

Supporting Information for

Theoretical Study on the Catalytic Oxidation Mechanism of 5-Hydroxymethylfurfural to 2, 5-Diformylfuran by PMo- Containing Keggin Heteropolyacid

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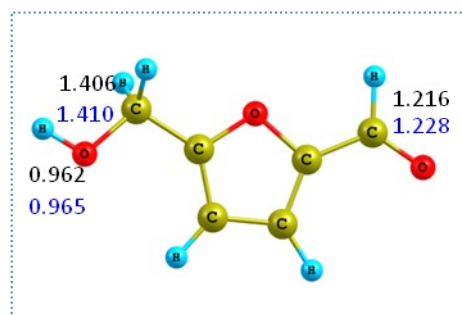
C.-W. Hu; e-mail: changweihu@scu.edu.cn

Catal. Sci. & Technol.

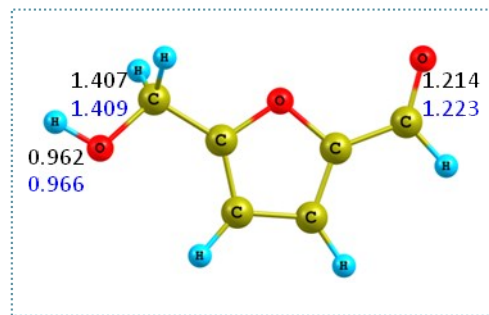
Catalog

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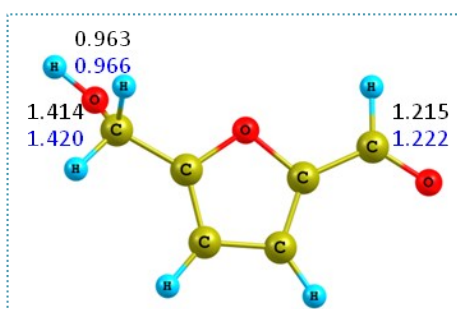
Figure S1: The four configurations and the relative Gibbs free energy (G_r) (kJ mol⁻¹) of HMF molecules are shown below. Black and blue numbers present the value in the gas phase and in the DMSO solvent, respectively. Distance lengths are reported in Å.



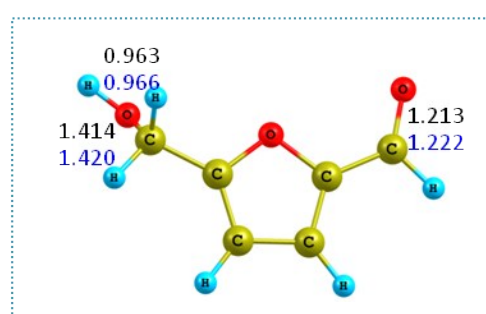
HMF 0.0 0.0



HMF-2 2.1 -2.1



HMF-3 4.6 1.9



HMF-4 7.2 -0.3

Table S1: The standard orientations of four configurations of HMF in the gas phase calculated at the M06/6-31++G(d, p) level.

HMF

C	0.337885	3.507784	-0.001906
C	0.552316	2.077128	0.023649
C	1.674432	1.295153	0.050624
C	1.231037	-0.051896	0.069673
C	-0.134326	0.004250	0.053560
C	-1.185710	-1.042326	0.054896
O	1.237734	4.325826	-0.006973
O	-0.565617	1.278669	0.026149
O	-0.542700	-2.288298	0.164079
H	-0.733157	3.809782	-0.016232
H	2.689588	1.669919	0.056010
H	1.821356	-0.957044	0.093019
H	-1.775703	-0.963327	-0.874182
H	-1.877138	-0.856768	0.894280
H	-1.196966	-2.991523	0.116587

HMF-3

C	0.398735	3.529613	0.223512
C	0.554914	2.093807	0.091203
C	1.626449	1.298802	-0.213822
C	1.144399	-0.033559	-0.198974
C	-0.185226	0.040225	0.116492
C	-1.230892	-0.992313	0.293122
O	1.310582	4.319247	0.075588
O	-0.554259	1.324614	0.298483
O	-2.186699	-0.860811	-0.740331
H	-0.633577	3.858234	0.474768
H	2.625805	1.656386	-0.423342
H	1.696027	-0.942254	-0.402551
H	-1.698142	-0.864236	1.282690
H	-0.740357	-1.977970	0.273938
H	-2.970153	-1.372395	-0.513873

HMF-2

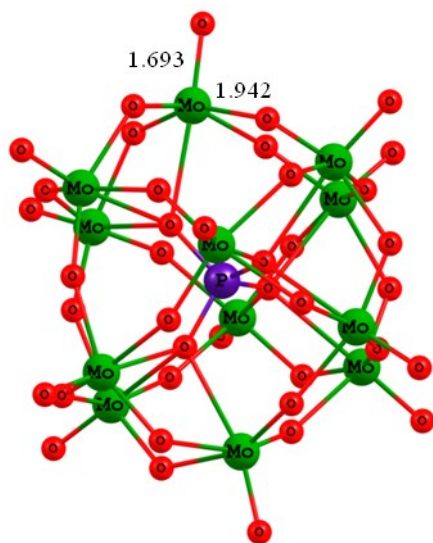
C	0.427975	3.534452	0.241308
C	0.525647	2.095229	0.095818
C	1.599726	1.309202	-0.233129
C	1.133288	-0.029114	-0.209158
C	-0.189817	0.037942	0.130903
C	-1.233310	-0.997939	0.306920
O	-0.568701	4.145516	0.564363
O	-0.566460	1.319539	0.321420
O	-2.108345	-0.963444	-0.803367
H	1.390777	4.052194	0.024525
H	2.596931	1.663843	-0.462370
H	1.688491	-0.932760	-0.423844
H	-1.771752	-0.798913	1.245914
H	-0.735792	-1.976036	0.398339
H	-2.945604	-1.372175	-0.561434

HMF-4

C	0.342571	3.512735	-0.005478
C	0.513052	2.077181	0.022275
C	1.647743	1.309329	0.053703
C	1.224644	-0.044579	0.073727
C	-0.140718	-0.000171	0.053214
C	-1.183032	-1.055095	0.054856
O	-0.720316	4.099525	-0.030559
O	-0.587552	1.268367	0.022383
O	-0.529610	-2.297380	0.146580
H	1.314443	4.058320	-0.001364
H	2.662993	1.686759	0.061531
H	1.825594	-0.942427	0.099607
H	-1.781915	-0.969676	-0.867530
H	-1.867301	-0.880542	0.901981
H	-1.181181	-3.004087	0.117035

Table S2: Snapshot and standard orientation of all the species in the solvent of DMSO under the temperature of 433 K calculated at the M06/6-31++G(d, p), Lanl2dz level. Distance lengths are reported in Å.

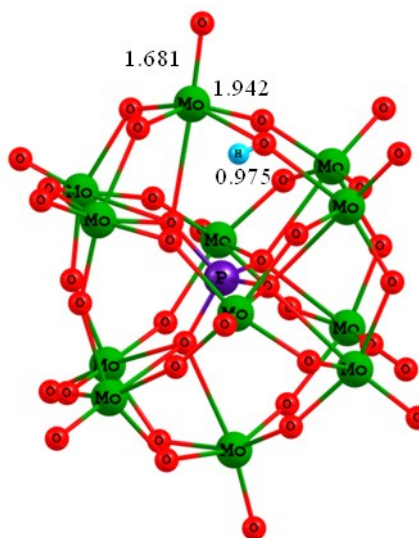
[PMo₁₂O₄₀]³⁻



P	0.000092	-0.000258	-0.000284
O	-1.237590	-0.327412	0.879773
O	1.230828	0.268913	0.908684
O	-0.294907	1.262342	-0.855974
O	0.302037	-1.204875	-0.933619
Mo	-1.198194	-2.226076	-2.639364
Mo	2.136698	-1.243015	-2.547686
Mo	0.872707	-3.507012	-0.217005
Mo	-1.334278	-2.207280	2.438424
Mo	-2.323856	1.123549	2.593331
Mo	-3.512229	-0.875014	0.064182
Mo	1.314950	2.043887	2.586491
Mo	2.304134	-1.290232	2.533068
Mo	3.511587	0.867605	0.147931
Mo	1.217269	2.395472	-2.484127
Mo	-2.117002	1.405377	-2.478366
Mo	-0.871698	3.513389	0.003756
O	0.421150	-1.992522	-3.447763
O	-0.660214	-3.615983	-1.573549
O	1.964836	-3.107289	-1.621047
O	-2.118328	-0.516387	3.359098
O	-3.163712	-2.007127	1.450080
O	-3.669919	0.616700	1.462725
O	2.092260	0.296730	3.401799
O	3.152046	1.907691	1.601482
O	3.658799	-0.711576	1.448130
O	-0.393816	2.213569	-3.314397
O	0.669764	3.709302	-1.334719

O	-1.952802	3.205694	-1.431652
O	3.252263	-1.678017	-3.752923
O	-2.142618	-2.969802	-3.831268
O	1.133240	-5.166153	0.029885
O	-3.117258	2.032870	3.787215
O	-1.812726	-3.356279	3.594797
O	-5.161327	-1.126665	-0.250029
O	3.088480	-2.275150	3.671685
O	1.784125	3.115477	3.818514
O	5.163009	1.138659	-0.136524
O	-3.223294	1.917787	-3.661524
O	2.169307	3.221617	-3.621148
O	-1.134555	5.153128	0.355531
O	-2.654436	-1.801953	-1.263798
O	-0.740445	-3.189096	1.030035
O	1.600211	0.435139	-2.998033
O	-0.349673	1.489664	3.064719
O	0.731813	3.114987	1.240068
O	2.660382	1.871976	-1.125563
O	0.326445	-1.685605	2.964433
O	-1.573907	-0.238380	-3.036155
O	3.158265	-0.699606	-1.147233
O	-1.839334	2.615518	1.273640
O	1.830238	-2.693496	1.115821
O	-3.149265	0.772683	-1.124005

[HPMo₁₂O₄₀]²⁻

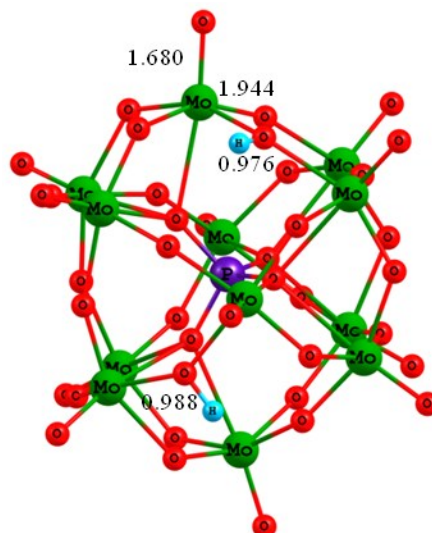


P	-0.015081	0.002283	0.003116
O	0.278719	-1.189910	0.954821

O	-0.587130	1.193691	0.819630
O	-1.053241	-0.435493	-1.066446
O	1.301326	0.440845	-0.695541
Mo	2.791343	-0.930235	-2.152089
Mo	1.434284	2.268239	-2.312822
Mo	3.518494	1.137387	0.345677
Mo	1.831506	-1.070560	2.838237
Mo	-1.335910	-2.436131	2.390597
Mo	1.222734	-3.386370	0.304100
Mo	-2.643284	1.072920	2.135033
Mo	0.508347	2.438446	2.682976
Mo	-1.285975	3.390843	-0.087661
Mo	-2.024107	0.937053	-2.909021
Mo	-0.682831	-2.261467	-2.647984
Mo	-3.345871	-1.267225	-0.629289
O	2.530501	0.649768	-3.020179
O	3.979904	-0.272035	-0.862439
O	3.140986	2.267708	-1.011344
O	0.097399	-2.043875	3.444064
O	2.028069	-2.910576	1.869000
O	-0.477356	-3.714742	1.403131
O	-1.179176	2.045473	3.244998
O	-2.532931	2.913802	1.153866
O	-0.005622	3.718030	1.480665
O	-1.509050	-0.642233	-3.656419
O	-3.459901	0.241949	-2.013266
O	-2.654363	-2.305408	-1.958895
O	1.958935	3.426744	-3.439285
O	3.854365	-1.780428	-3.166418
O	5.026345	1.635062	0.898674
O	-2.357600	-3.329067	3.410657
O	2.789699	-1.414251	4.198403
O	1.713327	-4.995566	0.077408
O	1.167263	3.330359	3.968290
O	-3.972946	1.415562	3.135486
O	-1.683457	5.000302	-0.452671
O	-0.836013	-3.418923	-3.882140
O	-2.724354	1.788270	-4.200064
O	-4.982160	-1.716748	-0.583799
O	2.272583	-2.424705	-0.848338
O	3.000290	-0.296831	1.623437
O	-0.058137	1.542730	-3.056560
O	-2.004362	-0.517192	2.743436
O	-3.370015	0.371051	0.625264
O	-1.931023	2.430321	-1.507663
O	1.036394	0.519111	3.222392

O	0.965779	-1.535516	-2.896804
O	0.526056	3.220221	-1.060219
O	-2.598802	-2.125740	0.805959
O	2.296360	2.289867	1.537880
O	-0.203061	-3.214658	-1.177812
H	2.430809	3.208178	1.238232

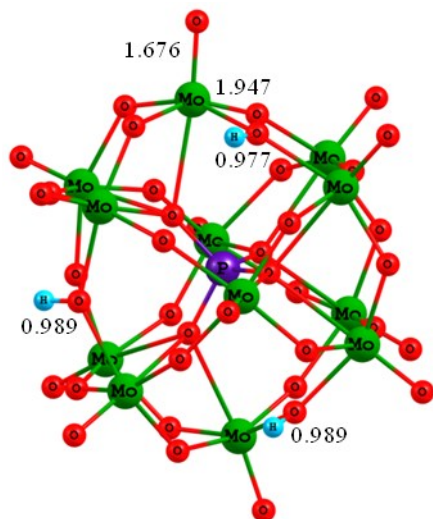
[H₂PMo₁₂O₄₀]⁻



P	-0.012580	-0.003029	0.002092
O	0.207756	1.237708	-0.906428
O	-0.614646	-1.164015	-0.836368
O	-0.992170	0.365889	1.149999
O	1.348740	-0.451699	0.601167
Mo	2.902174	0.874060	2.033210
Mo	1.602557	-2.351076	2.117937
Mo	3.512062	-1.062117	-0.597964
Mo	1.648641	1.234101	-2.880379
Mo	-1.506076	2.522831	-2.184233
Mo	1.157059	3.416654	-0.206386
Mo	-2.746105	-1.016131	-2.022816
Mo	0.386958	-2.300337	-2.818061
Mo	-1.227600	-3.413231	0.002888
Mo	-1.833377	-1.108672	2.977453
Mo	-0.555414	2.120988	2.793627
Mo	-3.318141	1.178233	0.887327
O	2.715336	-0.749477	2.837728
O	4.019378	0.297166	0.640754
O	3.228601	-2.261776	0.717581
O	-0.131762	2.205341	-3.336835
O	1.875663	3.029251	-1.836535
O	-0.609217	3.767694	-1.187733
O	-1.336114	-1.909984	-3.261544

O	-2.552067	-2.899250	-1.139683
O	-0.037163	-3.643966	-1.651084
O	-1.297781	0.442002	3.769020
O	-3.329105	-0.396487	2.201153
O	-2.564481	2.163932	2.223087
O	2.208970	-3.552507	3.154825
O	4.010801	1.693256	3.023953
O	4.986614	-1.510400	-1.265677
O	-2.598583	3.445532	-3.098978
O	2.520204	1.658056	-4.275710
O	1.637190	5.021432	0.068825
O	0.981772	-3.119059	-4.180999
O	-4.127288	-1.333615	-2.959751
O	-1.579992	-5.044698	0.312273
O	-0.652207	3.215948	4.089005
O	-2.444311	-2.031847	4.264393
O	-4.960502	1.601484	0.958656
O	2.286435	2.419524	0.835409
O	2.893604	0.427993	-1.781330
O	0.146284	-1.687098	2.981207
O	-2.166753	0.611646	-2.589850
O	-3.392707	-0.398992	-0.441296
O	-1.801628	-2.532127	1.502636
O	0.855011	-0.348908	-3.293981
O	1.115137	1.412243	2.910993
O	0.635876	-3.258017	0.875702
O	-2.669054	2.116321	-0.545773
O	2.227463	-2.170760	-1.777527
O	-0.176537	3.150736	1.345790
H	2.404645	-3.100955	-1.541234
H	-2.105060	0.595875	-3.576099

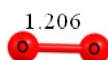
H₃PMo₁₂O₄₀



P	0.017539	0.004979	0.002912
O	-0.347277	-1.093412	-1.033348
O	0.734573	1.181929	-0.714051
O	0.962747	-0.595534	1.079646
O	-1.279887	0.526931	0.679403
Mo	-2.954317	-0.777546	1.989428
Mo	-1.307591	2.257870	2.404433
Mo	-3.373547	1.508870	-0.411949
Mo	-1.799791	-0.710048	-2.961010
Mo	1.201501	-2.402394	-2.485723
Mo	-1.522670	-3.222544	-0.559761
Mo	2.824272	0.940686	-1.958079
Mo	-0.157040	2.637489	-2.532818
Mo	1.599620	3.241841	0.357162
Mo	1.980012	0.562367	3.040763
Mo	0.353266	-2.468593	2.526306
Mo	3.182549	-1.618992	0.674614
O	-2.581856	0.714347	2.965931
O	-3.988644	0.028634	0.685016
O	-2.965672	2.483252	1.038514
O	-0.141718	-1.809545	-3.563834
O	-2.211541	-2.577139	-2.119494
O	0.183930	-3.648333	-1.614382
O	1.507975	2.116414	-3.056496
O	2.847514	2.721122	-0.865732
O	0.424341	3.786138	-1.232953
O	1.285756	-1.001301	3.666048
O	3.380220	-0.214210	2.155666
O	2.339339	-2.662974	1.908696
O	-1.767440	3.392068	3.582755
O	-4.135683	-1.579571	2.907490
O	-4.820983	2.155428	-0.954584
O	2.176373	-3.327641	-3.522667
O	-2.727305	-0.876153	-4.374671
O	-2.173187	-4.786957	-0.454778
O	-0.672696	3.665161	-3.781697
O	4.222007	1.211672	-2.885018
O	2.132273	4.779965	0.838863
O	0.342894	-3.707671	3.688583
O	2.702162	1.261966	4.408523
O	4.769163	-2.222349	0.660554
O	-2.524673	-2.234247	0.612567
O	-2.941191	0.079892	-1.751824
O	0.075989	1.346848	3.154486
O	2.063732	-0.540024	-2.690137
O	3.415840	0.081679	-0.470694

O	2.089209	2.139253	1.735457
O	-0.841539	0.814761	-3.213092
O	-1.228025	-1.601670	2.760393
O	-0.260322	3.190453	1.249583
O	2.419300	-2.312593	-0.839145
O	-2.032257	2.589875	-1.511538
O	-0.151644	-3.280206	0.981472
H	-2.195166	3.526990	-1.288283
H	2.006569	-0.408570	-3.668588
H	-3.431981	-2.621342	0.535727

O₂



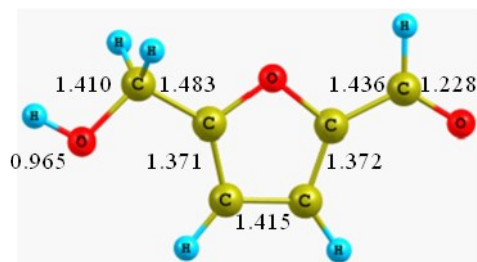
O	0.000000	0.000000	0.603047
O	0.000000	0.000000	-0.603047

H₂O



O	0.000000	0.118043	0.000000
H	0.763293	-0.472131	0.000000
H	-0.763293	-0.472212	0.000000

HMF



C	2.496622	-0.640840	-0.010917
C	1.202860	-0.016950	0.003195
C	0.774914	1.286503	0.009737
C	-0.639286	1.249876	0.018752
C	-0.982979	-0.077323	0.016424
C	-2.287739	-0.781796	0.028468
O	3.555994	-0.021084	-0.016727
O	0.111673	-0.855870	0.006442
O	-3.305000	0.190303	-0.056665
H	2.475407	-1.749145	-0.017144
H	1.415681	2.159579	0.008156
H	-1.325539	2.085698	0.027264
H	-2.369718	-1.376232	0.952280

H	-2.323322	-1.488459	-0.815590
H	-4.160201	-0.255050	-0.013318

HMF-2

C	0.342571	3.512735	-0.005478
C	0.513052	2.077181	0.022275
C	1.647743	1.309329	0.053703
C	1.224644	-0.044579	0.073727
C	-0.140718	-0.000171	0.053214
C	-1.183032	-1.055095	0.054856
O	-0.720316	4.099525	-0.030559
O	-0.587552	1.268367	0.022383
O	-0.529610	-2.297380	0.146580
H	1.314443	4.058320	-0.001364
H	2.662993	1.686759	0.061531
H	1.825594	-0.942427	0.099607
H	-1.781915	-0.969676	-0.867530
H	-1.867301	-0.880542	0.901981
H	-1.181181	-3.004087	0.117035

HMF-3

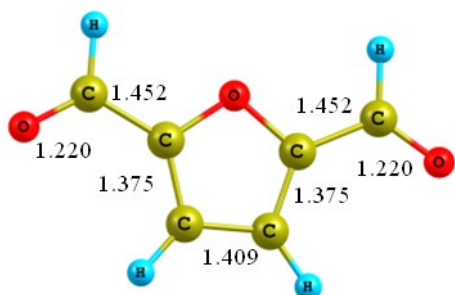
C	0.398735	3.529613	0.223512
C	0.554914	2.093807	0.091203
C	1.626449	1.298802	-0.213822
C	1.144399	-0.033559	-0.198974
C	-0.185226	0.040225	0.116492
C	-1.230892	-0.992313	0.293122
O	1.310582	4.319247	0.075588
O	-0.554259	1.324614	0.298483
O	-2.186699	-0.860811	-0.740331
H	-0.633577	3.858234	0.474768
H	2.625805	1.656386	-0.423342
H	1.696027	-0.942254	-0.402551
H	-1.698142	-0.864236	1.282690
H	-0.740357	-1.977970	0.273938
H	-2.970153	-1.372395	-0.513873

HMF-4

C	0.427975	3.534452	0.241308
C	0.525647	2.095229	0.095818
C	1.599726	1.309202	-0.233129
C	1.133288	-0.029114	-0.209158
C	-0.189817	0.037942	0.130903
C	-1.233310	-0.997939	0.306920
O	-0.568701	4.145516	0.564363
O	-0.566460	1.319539	0.321420

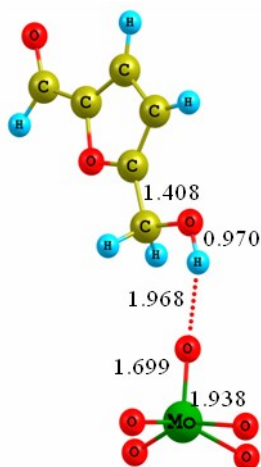
O	-2.108345	-0.963444	-0.803367
H	1.390777	4.052194	0.024525
H	2.596931	1.663843	-0.462370
H	1.688491	-0.932760	-0.423844
H	-1.771752	-0.798913	1.245914
H	-0.735792	-1.976036	0.398339
H	-2.945604	-1.372175	-0.561434

DFE



C	-2.385246	-0.680041	0.000977
C	-1.086780	-0.030186	-0.002011
C	-0.704690	1.290731	-0.000910
C	0.704581	1.290610	-0.002189
C	1.086608	-0.030431	-0.002764
C	2.385464	-0.680031	-0.000392
O	-3.436130	-0.059466	0.003828
O	-0.000178	-0.840537	-0.003572
O	3.436268	-0.059346	0.005341
H	-2.355001	-1.786763	0.000700
H	-1.372781	2.142307	0.001804
H	1.372975	2.142040	-0.000786
H	2.355506	-1.786713	-0.002753

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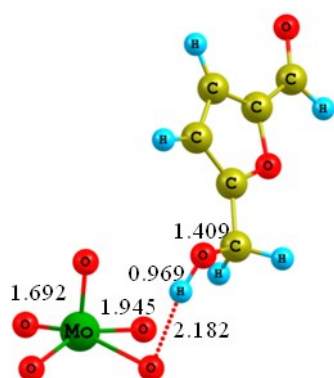


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O	-0.973376	1.427004	-0.561049

O	-1.980140	-0.901994	-0.452784
O	-0.745832	0.042193	1.550658
O	0.536862	-0.609563	-0.542054
Mo	2.840075	0.280109	-0.243187
Mo	1.343488	-2.846762	0.020921
Mo	1.109774	-0.992133	-2.922064
Mo	-1.122556	1.945140	-2.944728
Mo	-2.845190	3.015204	-0.118922
Mo	0.573550	3.334650	-0.234025
Mo	-4.313488	-0.432038	0.101537
Mo	-2.668698	-1.471119	-2.781631
Mo	-2.317930	-3.290898	0.111196
Mo	-0.497783	-1.863749	3.140438
Mo	0.930071	1.291300	2.817041
Mo	-2.527880	0.906022	3.039664
O	2.921781	-1.498768	0.141480
O	2.640242	0.056519	-2.047342
O	1.702290	-2.447727	-1.997927
O	-2.584790	3.011392	-1.921755
O	0.024874	3.394341	-1.971624
O	-1.318173	3.943754	0.272312
O	-4.182841	-0.968294	-1.902673
O	-3.947256	-2.483705	0.243839
O	-2.496280	-3.076075	-1.920563
O	0.681355	-0.584018	3.678911
O	-1.991450	-0.962819	3.692104
O	-0.942394	1.494731	3.720481
O	2.240085	-4.284689	0.142525
O	4.447198	0.803967	-0.075497
O	1.774345	-1.205720	-4.469419
O	-4.082905	4.154145	0.110392
O	-1.263339	2.723020	-4.448521
O	1.395973	4.804970	-0.025791
O	-3.220130	-1.897947	-4.329355
O	-6.004727	-0.480740	0.255326
O	-2.681146	-4.943991	0.241348
O	1.865495	2.000049	4.045441
O	-0.316609	-3.094834	4.295130
O	-3.651657	1.302381	4.248633
O	1.910672	2.092079	-0.414586
O	0.376931	0.929754	-3.088574
O	0.900994	-2.431286	1.735101
O	-3.940862	1.285402	-0.365777
O	-3.699894	-0.257698	1.802497
O	-1.653706	-2.840677	1.757769
O	-2.265484	0.534294	-3.045044

O	2.144512	0.565465	1.671557
O	-0.330571	-3.383628	-0.436749
O	-2.769309	2.190416	1.756254
O	-0.645208	-1.481920	-3.109796
O	0.491048	2.669211	1.717596
C	12.023004	-1.532467	0.147833
C	11.130328	-0.410708	0.059345
C	11.317161	0.944765	-0.052438
C	10.029896	1.528900	-0.100548
C	9.138861	0.489267	-0.014559
C	7.657674	0.431934	-0.009695
O	13.247101	-1.436315	0.135389
O	9.782471	-0.685735	0.082277
O	7.169196	1.748454	-0.105964
H	11.521014	-2.517835	0.228795
H	12.276414	1.445908	-0.094747
H	9.776024	2.576913	-0.186781
H	7.319046	-0.064203	0.915032
H	7.317540	-0.193437	-0.851760
H	6.200801	1.697723	-0.106004

1-IM1b

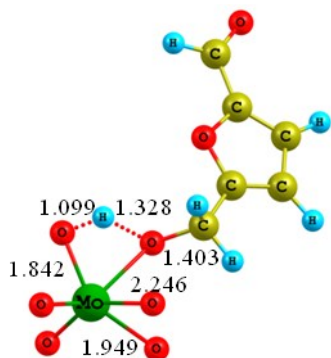


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O	0.389299	-1.032694	1.121595
O	2.113477	0.276369	-0.206219
O	-0.104215	1.346706	0.397936
O	-0.018691	-0.515399	-1.326819
Mo	-2.381927	-1.161119	-1.768247
Mo	0.003358	0.728184	-3.430545
Mo	0.653908	-2.575824	-2.527359
Mo	1.284496	-3.305042	1.033819
Mo	1.083943	-0.872603	3.511864
Mo	-1.782954	-1.909993	1.928257
Mo	3.593293	1.112652	1.549748
Mo	3.868318	-1.364816	-0.875989
Mo	3.128960	1.853114	-1.825388

Mo	-0.186452	3.482517	-0.887791
Mo	-2.501277	1.539187	0.833470
Mo	0.379956	2.707684	2.410982
O	-1.882184	-0.095740	-3.157005
O	-1.381692	-2.607625	-2.273603
O	0.382642	-1.293523	-3.794631
O	1.618266	-2.512691	2.926508
O	-0.642530	-3.329667	1.839846
O	-0.699679	-1.277847	3.550881
O	4.533439	-0.449978	0.551848
O	4.072212	2.012883	-0.273418
O	4.026105	0.023497	-2.056980
O	-1.890679	3.140556	-0.343086
O	0.435002	3.938455	0.771416
O	-1.432454	2.685289	2.214696
O	-0.191187	1.228107	-5.042544
O	-3.968684	-1.606097	-2.153069
O	0.838991	-3.998709	-3.434401
O	1.533143	-0.859279	5.148858
O	1.703490	-4.917007	1.368966
O	-3.137884	-2.537783	2.735490
O	5.130777	-2.413104	-1.310725
O	4.926977	1.664851	2.445669
O	4.044572	2.746541	-2.941195
O	-4.059410	2.099030	1.214401
O	-0.309446	4.969225	-1.697903
O	0.634191	3.864933	3.626598
O	-2.336840	-1.877872	0.173252
O	0.536446	-3.356747	-0.620844
O	-0.513774	2.160441	-2.436540
O	2.783098	-0.105596	2.629696
O	2.319776	2.386708	1.784478
O	1.724269	2.951772	-1.407190
O	2.831631	-2.532388	0.471492
O	-2.726510	0.554225	-0.681399
O	1.774585	0.945237	-3.090245
O	0.583480	1.099886	3.264598
O	2.360331	-2.122886	-2.039442
O	-2.250937	0.099783	1.913103
C	-9.149985	1.776102	0.225000
C	-8.427489	0.577680	-0.097892
C	-8.586488	-0.405408	-1.042961
C	-7.534900	-1.331029	-0.846547
C	-6.802445	-0.853444	0.210995
C	-5.578229	-1.340190	0.894449
O	-10.156696	2.151890	-0.369420

O	-7.325487	0.293562	0.675264
O	-5.296098	-2.654899	0.474555
H	-8.726589	2.356524	1.069628
H	-9.373787	-0.442112	-1.786092
H	-7.332298	-2.236097	-1.403577
H	-5.721144	-1.288590	1.986194
H	-4.749006	-0.656527	0.652708
H	-4.345553	-2.721516	0.299269

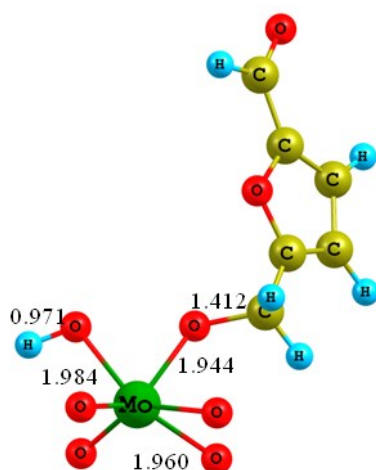
1-TS1



P	-0.606696	-0.002756	-0.001994
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O	-2.136179	0.183023	-0.201003
O	-0.114693	-1.193447	-0.870091
O	0.130453	1.295767	-0.430618
Mo	2.721273	1.796239	-0.352481
Mo	0.027281	2.232250	-2.685567
Mo	-0.200319	3.554574	0.532033
Mo	-0.875882	1.229467	3.315833
Mo	-1.117835	-2.211586	2.870320
Mo	1.929481	-0.670431	2.493543
Mo	-3.790531	-1.537902	0.322617
Mo	-3.618291	1.896998	0.841614
Mo	-3.288996	0.652093	-2.343398
Mo	-0.272410	-1.450467	-3.346112
Mo	2.212302	-1.934630	-0.960785
Mo	-0.866950	-3.547351	-0.690379
O	2.043090	2.233387	-1.960776
O	1.781395	3.065081	0.558269
O	-0.054321	3.768414	-1.272457
O	-1.395916	-0.708171	3.860509
O	1.000062	0.377535	3.660552
O	0.701271	-2.210264	3.064930
O	-4.463265	0.295066	1.036165
O	-4.310586	-0.567038	-1.452399
O	-3.915121	2.029264	-0.958739
O	1.437874	-1.879767	-2.889242

O	-1.020875	-2.968668	-2.651888
O	0.938008	-3.589922	-0.943815
O	0.219723	3.194357	-4.072551
O	4.147276	2.961552	-0.367829
O	-0.148983	5.143927	1.126508
O	-1.633999	-3.469051	3.887214
O	-1.082950	1.970459	4.830524
O	3.322210	-1.097687	3.364903
O	-4.704776	3.013869	1.515371
O	-5.224502	-2.422893	0.539019
O	-4.270422	1.115442	-3.648690
O	3.660883	-2.752951	-1.305041
O	-0.320734	-1.704580	-5.023829
O	-1.329637	-5.172706	-0.850769
O	2.519764	0.656531	1.349989
O	-0.057915	2.488799	2.293498
O	0.299521	0.529321	-3.262670
O	-2.867195	-1.767237	1.872355
O	-2.715644	-2.631224	-0.651768
O	-2.067993	-0.498204	-3.078998
O	-2.489210	1.398243	2.493952
O	2.563832	-0.172990	-1.111958
O	-1.769875	2.039577	-2.502976
O	-0.883498	-3.246418	1.116328
O	-1.972098	3.096875	0.612107
O	2.116588	-1.908279	0.853080
C	9.881065	0.785170	-0.190302
C	8.737103	-0.080894	-0.071249
C	8.560230	-1.436253	-0.201165
C	7.187053	-1.681884	0.031702
C	6.615496	-0.463638	0.296002
C	5.225046	-0.063550	0.626657
O	11.011476	0.390140	-0.455576
O	7.541345	0.514562	0.236049
O	4.748417	0.829741	-0.344415
H	9.666975	1.859643	-0.020762
H	9.335103	-2.153814	-0.440916
H	6.668311	-2.632258	0.014300
H	4.621606	-0.980945	0.658019
H	5.192923	0.391508	1.631513
H	4.885816	2.150285	-0.301168

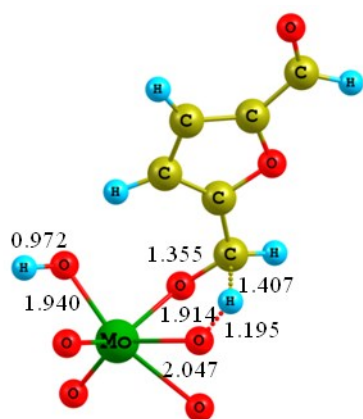
1-IM2



P	-0.595044	-0.004382	0.004313
O	-0.277697	-0.419148	1.467408
O	-2.105505	0.334379	-0.126593
O	-0.245051	-1.177793	-0.951720
O	0.248076	1.245036	-0.371842
Mo	2.860523	1.512616	-0.389672
Mo	0.164024	2.328634	-2.560767
Mo	0.162484	3.458925	0.737394
Mo	-0.643385	1.033689	3.398257
Mo	-1.223559	-2.334825	2.754680
Mo	1.942725	-1.061325	2.359807
Mo	-3.898234	-1.255959	0.352569
Mo	-3.385740	2.108245	1.071715
Mo	-3.274652	1.043526	-2.192809
Mo	-0.503082	-1.260964	-3.431245
Mo	1.997417	-2.123891	-1.172806
Mo	-1.210734	-3.458653	-0.887139
O	2.139629	2.062884	-1.963930
O	2.105673	2.775464	0.680794
O	0.272033	3.772699	-1.055203
O	-1.327297	-0.878241	3.843547
O	1.153309	-0.008314	3.621492
O	0.592675	-2.514202	2.881836
O	-4.372060	0.582219	1.199969
O	-4.378885	-0.130117	-1.340113
O	-3.724412	2.381748	-0.705234
O	1.172243	-1.874823	-3.064511
O	-1.369964	-2.744513	-2.803033
O	0.573365	-3.651793	-1.208923
O	0.403566	3.355209	-3.893087
O	4.175077	2.934917	-0.817835
O	0.382380	4.995555	1.424413
O	-1.824605	-3.601333	3.711974
O	-0.732351	1.692736	4.961604

O	3.315158	-1.670199	3.151816
O	-4.340254	3.275656	1.851305
O	-5.402106	-2.016475	0.567728
O	-4.247831	1.677835	-3.430611
O	3.350713	-3.048995	-1.618993
O	-0.627249	-1.402175	-5.118358
O	-1.829885	-5.020717	-1.128365
O	2.568026	0.276262	1.274593
O	0.257941	2.274532	2.424563
O	0.255892	0.648103	-3.249395
O	-2.953127	-1.667925	1.850531
O	-2.962356	-2.379764	-0.725093
O	-2.191366	-0.165616	-3.041079
O	-2.258224	1.402991	2.648095
O	2.559355	-0.398732	-1.226584
O	-1.636728	2.291908	-2.323903
O	-1.142696	-3.273123	0.933863
O	-1.641320	3.162820	0.854486
O	1.960965	-2.204202	0.641686
C	9.770154	0.743911	0.308229
C	8.634931	-0.095449	0.019797
C	8.487557	-1.287145	-0.645882
C	7.110418	-1.605222	-0.589140
C	6.510005	-0.592652	0.113780
C	5.100011	-0.351129	0.499739
O	10.915472	0.482348	-0.041592
O	7.420199	0.328919	0.487596
O	4.657492	0.796932	-0.192910
H	9.533657	1.662575	0.881539
H	9.284112	-1.850055	-1.116406
H	6.606222	-2.468258	-1.006156
H	4.521528	-1.245081	0.234843
H	5.019892	-0.192434	1.584639
H	3.688618	3.680689	-1.204760

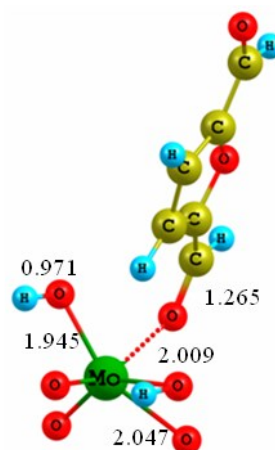
1-TS2



P	-0.553891	0.026088	-0.013975
O	0.234077	1.153183	-0.736534
O	-1.952001	-0.137678	-0.671192
O	-0.728797	0.398081	1.484156
O	0.231052	-1.309263	-0.132354
Mo	2.778851	-2.036140	0.652271
Mo	-0.532855	-3.421184	0.831334
Mo	0.830825	-2.475260	-2.234625
Mo	0.791466	1.107192	-3.115591
Mo	-0.385380	3.560026	-0.948502
Mo	2.533013	1.907583	-0.203301
Mo	-3.613111	1.651081	-0.788229
Mo	-2.470865	-0.747115	-3.033582
Mo	-3.713433	-1.740975	0.011286
Mo	-1.900839	-0.905876	3.258304
Mo	1.138873	0.767261	3.016377
Mo	-1.866141	2.412889	2.370747
O	1.554085	-3.151448	1.315653
O	2.512600	-2.216134	-1.169678
O	0.300690	-3.759286	-1.053963
O	0.099498	3.002009	-2.613289
O	2.403227	1.861032	-2.021204
O	1.311751	3.554026	-0.265165
O	-3.513147	0.691043	-2.629377
O	-4.551899	-0.165397	-0.360680
O	-3.412418	-1.934115	-2.008130
O	-0.296009	-0.404773	3.959341
O	-2.641687	0.765931	3.315258
O	-0.367694	2.167879	3.379961
O	-0.686529	-5.041677	1.317971
O	4.112005	-3.397772	0.287990
O	1.473234	-3.365936	-3.529139
O	-0.732953	5.208398	-1.157703
O	1.371467	1.465976	-4.671597
O	4.018398	2.682832	0.069707

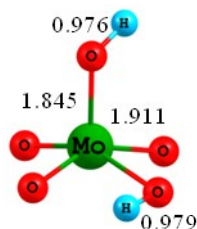
O	-2.918732	-1.139487	-4.623290
O	-5.007605	2.578387	-1.074237
O	-4.994590	-2.838541	0.200012
O	2.107015	1.101614	4.371958
O	-2.661127	-1.730485	4.532532
O	-2.712688	3.625933	3.203492
O	3.097471	0.094093	0.175732
O	1.406154	-0.566618	-2.768129
O	-0.906223	-2.452593	2.324456
O	-2.234173	2.718149	-1.304685
O	-3.288331	1.841481	0.988967
O	-3.177694	-1.369375	1.723015
O	-0.929935	0.580874	-3.373632
O	1.770017	-0.724999	2.320277
O	-2.105913	-3.034899	0.008812
O	-1.102259	3.284089	0.952102
O	-0.820616	-1.944946	-2.823368
O	1.772382	1.864343	1.714505
C	8.916149	1.439376	-0.228381
C	7.852735	0.477928	-0.165195
C	7.490167	-0.592026	-0.952900
C	6.347128	-1.163515	-0.365763
C	6.078308	-0.409765	0.765547
C	4.994126	-0.386220	1.719141
O	9.769305	1.460159	-1.112994
O	6.983091	0.583575	0.893008
O	4.166834	-1.453360	1.834164
H	8.916754	2.182929	0.593762
H	8.003245	-0.913332	-1.851162
H	5.782757	-2.026494	-0.696476
H	4.024979	0.241407	0.914366
H	5.208960	0.113087	2.668961
H	3.892347	-3.876307	-0.528899

1-IM3



P	-0.578017	0.024249	-0.000701
O	0.100221	1.403340	-0.228779
O	-1.974285	0.010176	-0.681578
O	-0.745073	-0.222257	1.523836
O	0.307399	-1.093457	-0.617068
Mo	2.918328	-1.891449	-0.097160
Mo	-0.262786	-3.469013	-0.544334
Mo	0.946224	-1.310530	-3.001076
Mo	0.601178	2.319247	-2.438459
Mo	-0.713271	3.647329	0.495214
Mo	2.344330	2.082410	0.572281
Mo	-3.774440	1.563208	-0.115734
Mo	-2.500741	0.312520	-3.100915
Mo	-3.585727	-1.871877	-0.681298
Mo	-1.766272	-2.198844	2.651675
Mo	1.124341	-0.315591	3.094910
Mo	-2.016680	1.197203	3.107256
O	1.850178	-3.284487	0.012453
O	2.647891	-1.448801	-1.932849
O	0.548642	-2.988291	-2.408204
O	-0.226463	3.812470	-1.252393
O	2.174327	2.726324	-1.125736
O	0.995289	3.520420	1.136612
O	-3.643671	1.394275	-2.183548
O	-4.555408	-0.349234	-0.426165
O	-3.319812	-1.250404	-2.617528
O	-0.189565	-1.874058	3.504112
O	-2.635798	-0.744060	3.340532
O	-0.479345	0.708541	3.956894
O	-0.275440	-5.158950	-0.718708
O	4.507419	-2.680754	-0.894041
O	1.625379	-1.580554	-4.533051
O	-1.195506	5.215178	0.932377
O	1.112655	3.293817	-3.732654
O	3.769835	2.814086	1.133128
O	-2.954827	0.524037	-4.722847
O	-5.244688	2.410621	-0.034660
O	-4.770767	-3.059748	-0.938794
O	2.095715	-0.447973	4.482716
O	-2.427334	-3.508767	3.505334
O	-2.936206	1.923761	4.335333
O	2.905694	0.326907	-0.201923
O	1.355037	0.697151	-2.755779
O	-0.675186	-3.181374	1.203263
O	-2.497555	2.856753	-0.171752
O	-3.422431	1.083795	1.600778

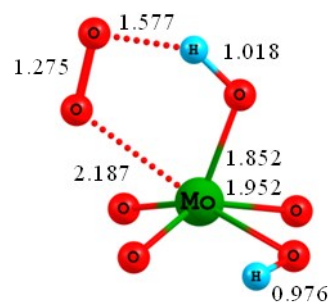
O	-3.039470	-2.142082	1.046048
O	-1.078836	1.791781	-2.892523
O	1.853883	-1.379972	1.877455
O	-1.881166	-2.928342	-1.167837
O	-1.359267	2.605614	2.138190
O	-0.756123	-0.733779	-3.353684
O	1.636838	1.244878	2.319562
C	9.579950	0.795680	0.216490
C	8.214936	0.435909	0.006271
C	7.319360	0.651506	-1.030073
C	6.118491	0.037722	-0.677220
C	6.321706	-0.536326	0.579790
C	5.526874	-1.282479	1.479316
O	10.288344	1.419957	-0.574227
O	7.597904	-0.288202	0.993580
O	4.316321	-1.612990	1.318235
H	9.980653	0.449818	1.197843
H	7.543817	1.201923	-1.934845
H	5.197929	-0.005960	-1.243728
H	2.664433	0.340347	-1.157060
H	6.006619	-1.580160	2.419213
H	4.342535	-2.698288	-1.850306



P	-0.017718	0.002889	-0.001830
O	0.212809	1.255373	-0.891509
O	-1.196130	-0.833303	-0.572370
O	-0.358611	0.453932	1.445146
O	1.271058	-0.864445	0.011412
Mo	3.578771	-0.243927	0.860315
Mo	1.486464	-2.953863	1.260643
Mo	2.348314	-1.918666	-1.955101
Mo	0.769382	1.146114	-3.268678
Mo	-1.387568	3.107351	-1.371628
Mo	1.947763	2.992139	-0.555923
Mo	-3.467483	0.029053	-0.836828
Mo	-1.364303	-1.908570	-2.816711
Mo	-2.095885	-2.936871	0.378671
Mo	-0.873472	-0.985724	3.415895
Mo	1.140764	1.790253	2.837542

Mo	-2.271066	1.874955	2.125032
O	3.226656	-1.880828	1.535707
O	3.755230	-0.885480	-0.883954
O	2.411491	-3.140073	-0.603054
O	-0.684262	2.602752	-2.974366
O	1.877497	2.658058	-2.346820
O	0.133512	3.924773	-0.767319
O	-2.933619	-1.023637	-2.548064
O	-3.530052	-1.942073	-0.148017
O	-1.711515	-3.241530	-1.612672
O	0.343918	0.246579	3.979297
O	-2.267780	0.192892	3.298342
O	-0.829809	2.435646	3.090570
O	2.045012	-4.402871	1.949635
O	5.340642	0.051466	1.322378
O	3.332597	-2.603816	-3.156491
O	-2.413632	4.400549	-1.767278
O	1.158484	1.514788	-4.880816
O	2.944692	4.361637	-0.445515
O	-1.574073	-2.659014	-4.324868
O	-5.122036	0.216140	-1.174121
O	-2.775622	-4.445673	0.756898
O	1.847666	2.683501	4.097982
O	-1.218497	-1.884621	4.813983
O	-3.572541	2.699410	2.837786
O	3.245701	1.455686	-0.393040
O	2.045038	-0.036289	-2.744482
O	0.707753	-2.057036	2.637648
O	-2.681667	1.510339	-1.540474
O	-3.283550	0.570434	0.887479
O	-1.799725	-2.151083	2.006529
O	-0.548512	-0.101494	-3.384700
O	2.629476	0.708930	2.106173
O	-0.085994	-3.396411	0.465857
O	-1.940952	2.798204	0.577863
O	0.639200	-2.236285	-2.532287
O	1.253633	2.873824	1.383825
H	3.463250	1.108834	-1.282143
H	5.564022	0.541972	2.135564

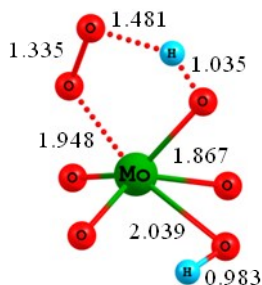
2a-IM1



P	-0.134093	0.002128	-0.003691
O	-0.275833	1.234730	-0.938565
O	-1.221497	-1.049455	-0.357405
O	-0.312317	0.451541	1.472673
O	1.273274	-0.628304	-0.191467
Mo	3.605005	0.379946	0.254046
Mo	2.054420	-2.591468	1.036720
Mo	2.189916	-1.567284	-2.293162
Mo	-0.098574	1.117434	-3.373204
Mo	-2.235685	2.759474	-1.174534
Mo	1.154183	3.258056	-0.922945
Mo	-3.622353	-0.604685	-0.253904
Mo	-1.554967	-2.236457	-2.525670
Mo	-1.568491	-3.232280	0.762375
Mo	-0.239443	-0.966173	3.523604
Mo	1.130134	2.087231	2.575623
Mo	-2.311981	1.550020	2.438968
O	3.580721	-1.203883	1.110036
O	3.573326	-0.260086	-1.473562
O	2.685682	-2.698031	-0.951713
O	-1.721159	2.312974	-2.863892
O	0.857121	2.837458	-2.671862
O	-0.806829	3.853230	-0.844199
O	-3.192468	-1.624573	-2.013598
O	-3.222263	-2.524378	0.466109
O	-1.461640	-3.554388	-1.260206
O	0.814320	0.481587	3.857678
O	-1.821325	-0.052301	3.621265
O	-0.856914	2.393463	3.142701
O	2.964850	-3.890200	1.645590
O	3.073872	-2.125082	-3.630721
O	-3.525144	3.837265	-1.414054
O	-0.045672	1.475578	-5.033097
O	1.896658	4.782596	-1.000979
O	-1.868043	-3.078238	-3.966188
O	-5.316193	-0.721164	-0.314310
O	-1.899656	-4.817395	1.271611
O	1.860643	3.144298	3.687053

O	-0.189844	-1.847974	4.973320
O	-3.607248	2.168393	3.345325
O	2.675373	1.969437	-0.906306
O	1.434217	0.197463	-3.050146
O	1.360718	-1.782086	2.509986
O	-3.235675	0.957173	-1.101201
O	-3.262460	0.036546	1.407258
O	-1.158558	-2.335482	2.306008
O	-1.175209	-0.342812	-3.249233
O	2.541882	1.170028	1.736529
O	0.478469	-3.333702	0.521327
O	-2.404369	2.446571	0.844365
O	0.494122	-2.200485	-2.573223
O	0.813400	3.108205	1.106796
H	2.817600	1.649485	-1.816984
H	5.905488	1.300951	0.512018
O	4.941394	1.611756	0.609839
O	5.570241	-0.535490	-0.032662
O	6.714712	0.004901	0.121591

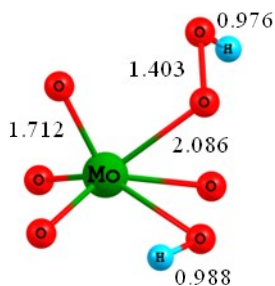
2a-TS1



P	-0.138793	0.002457	-0.004029
O	-0.217560	1.230270	-0.952534
O	-1.303683	-0.976064	-0.318534
O	-0.251210	0.481245	1.469576
O	1.217283	-0.725620	-0.214626
Mo	3.786635	0.082744	0.140895
Mo	1.890573	-2.722600	1.022869
Mo	2.017999	-1.751314	-2.323142
Mo	-0.105763	1.071036	-3.388676
Mo	-2.073294	2.883273	-1.165547
Mo	1.347728	3.150403	-0.997228
Mo	-3.665334	-0.365850	-0.167253
Mo	-1.768351	-2.163945	-2.462028
Mo	-1.773160	-3.115853	0.839022
Mo	-0.227703	-0.912724	3.537871
Mo	1.325354	2.027244	2.516943
Mo	-2.147738	1.726593	2.465231

O	3.487502	-1.432997	1.091649
O	3.536706	-0.528350	-1.599805
O	2.466356	-2.896875	-0.977585
O	-1.630241	2.381617	-2.859676
O	0.981705	2.729715	-2.733001
O	-0.565505	3.880073	-0.882680
O	-3.347640	-1.434531	-1.921814
O	-3.381008	-2.299504	0.570211
O	-1.735983	-3.469468	-1.180774
O	0.930326	0.463079	3.827987
O	-1.740518	0.109001	3.658366
O	-0.622224	2.476493	3.124257
O	2.723854	-4.073312	1.629113
O	2.830115	-2.385086	-3.672358
O	-3.291109	4.044229	-1.390972
O	-0.067290	1.404192	-5.054160
O	2.190907	4.619143	-1.113142
O	-2.171995	-2.999881	-3.883292
O	-5.364123	-0.366196	-0.187919
O	-2.200171	-4.668012	1.377578
O	2.152389	3.045146	3.596849
O	-0.204749	-1.777901	4.998230
O	-3.376021	2.443785	3.391803
O	2.656007	1.719177	-0.942913
O	1.367514	0.051795	-3.087411
O	1.288628	-1.849282	2.499964
O	-3.192458	1.155120	-1.044677
O	-3.223578	0.269525	1.476313
O	-1.266731	-2.230430	2.360421
O	-1.276744	-0.309999	-3.220220
O	2.618372	1.024274	1.770726
O	0.255836	-3.360896	0.553428
O	-2.215747	2.607644	0.860793
O	0.276711	-2.269692	-2.556155
O	1.045056	3.049406	1.041552
H	2.651525	1.241397	-1.801677
H	5.864889	1.304142	0.319737
O	4.870222	1.589908	0.336245
O	5.585980	-0.660959	0.208213
O	6.674032	0.095131	0.044256

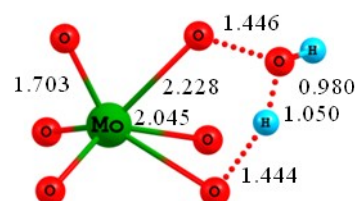
2a-IM2



P	-0.129973	-0.001673	0.004280
O	-0.106965	-0.625289	1.426940
O	-1.502502	0.682364	-0.244002
O	0.087621	-1.119567	-1.052296
O	1.001955	1.055801	-0.113521
Mo	3.694238	0.849283	0.108343
Mo	1.444113	2.348687	-2.139746
Mo	1.240802	3.105788	1.257443
Mo	-0.411010	0.666906	3.478875
Mo	-1.601972	-2.398134	2.345372
Mo	1.786268	-1.842225	2.463170
Mo	-3.639825	-0.500525	-0.171414
Mo	-2.525416	2.567942	1.028706
Mo	-2.206646	1.846063	-2.314998
Mo	0.152442	-0.887517	-3.534934
Mo	2.086831	-2.521759	-1.150594
Mo	-1.340316	-3.116316	-1.388493
O	3.222073	1.683392	-1.455586
O	3.023032	2.109507	1.306922
O	1.653703	3.568549	-0.456973
O	-1.538845	-1.075428	3.596169
O	1.076804	-0.772622	3.757954
O	0.100891	-2.996754	2.643637
O	-3.821499	1.300438	0.850849
O	-3.639073	0.872356	-1.745870
O	-2.557021	3.091737	-0.723918
O	1.594507	-1.899550	-3.072043
O	-1.086001	-2.192198	-3.201593
O	0.388675	-3.674974	-1.537989
O	2.072594	3.425182	-3.294078
O	1.688040	4.473813	2.157480
O	-2.581087	-3.586607	3.059916
O	-0.566597	1.165188	5.095605
O	2.879224	-2.824328	3.313172
O	-3.305783	3.835191	1.845295
O	-5.285885	-0.918144	-0.220320
O	-2.848009	2.807946	-3.557985
O	3.259997	-3.678917	-1.564087

O	0.228325	-0.823239	-5.229578
O	-2.239147	-4.464122	-1.895546
O	2.993675	-0.493102	1.730501
O	0.855504	1.764109	2.777273
O	1.268290	0.770755	-3.026341
O	-3.013260	-1.267354	1.353781
O	-2.828293	-1.690767	-1.278166
O	-1.301298	0.516234	-3.190782
O	-1.795105	1.467651	2.612895
O	3.207051	-1.120627	-0.910228
O	-0.338452	2.697187	-2.105537
O	-1.479053	-3.138661	0.437801
O	-0.583772	3.216035	1.139657
O	1.791348	-2.777221	0.623551
H	2.841497	0.279713	2.327516
H	5.487079	-1.384075	-1.137143
O	5.013576	-0.708201	0.537283
O	5.941580	-0.788825	-0.511721
O	5.204389	1.653736	0.060585

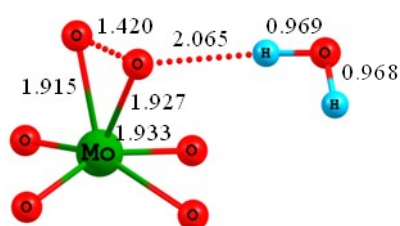
2a-TS2



P	0.129931	-0.001309	-0.005709
O	-0.173363	-0.954411	-1.194404
O	1.585370	0.529695	-0.120247
O	-0.032523	-0.776200	1.330906
O	-0.859760	1.195681	-0.039091
Mo	-3.632311	1.311884	0.123956
Mo	-0.854514	3.005547	1.603164
Mo	-1.101827	2.846441	-1.870875
Mo	-0.061661	-0.275332	-3.539402
Mo	0.979134	-3.088126	-1.777977
Mo	-2.314780	-2.123748	-1.625705
Mo	3.557971	-0.912987	-0.132877
Mo	2.582532	1.875864	-1.968230
Mo	2.711610	2.070951	1.459358
Mo	0.308531	0.081049	3.648308
Mo	-2.122072	-1.822464	2.046281
Mo	1.224721	-2.798879	2.014387
O	-2.781449	2.376241	1.322112
O	-2.980761	2.077211	-1.390562

O	-1.198188	3.778390	-0.306892
O	0.856082	-2.127761	-3.320892
O	-1.710188	-1.522192	-3.237058
O	-0.800262	-3.504909	-1.693768
O	3.758212	0.529860	-1.615980
O	3.935643	0.799462	1.002286
O	2.935102	2.815377	-0.438505
O	-1.280835	-0.808842	3.654505
O	1.345250	-1.421643	3.529212
O	-0.507545	-3.060896	2.518829
O	-1.187994	4.413593	2.493393
O	-1.544067	3.991000	-3.043901
O	1.713830	-4.540299	-2.260805
O	-0.107821	-0.226876	-5.236998
O	-3.617488	-3.130142	-2.040081
O	3.349983	2.777713	-3.184534
O	5.142275	-1.524954	-0.175132
O	3.628773	3.218592	2.309837
O	-3.326737	-2.666998	2.895902
O	0.500888	0.580343	5.259336
O	2.052505	-4.084686	2.751309
O	-3.226365	-0.627015	-1.042126
O	-1.089953	1.125284	-3.009258
O	-0.702013	1.693466	2.852972
O	2.631330	-1.946944	-1.307229
O	2.812143	-1.663638	1.343749
O	1.824177	1.141100	2.764325
O	1.511716	0.521689	-3.096597
O	-2.950563	-0.296485	1.541480
O	0.927280	3.088001	1.258821
O	1.078077	-3.299763	0.258623
O	0.720980	2.733248	-2.011080
O	-2.129747	-2.554882	0.383853
H	-4.413363	-1.306530	-0.580461
H	-5.236001	-1.877412	0.756305
O	-5.441830	0.019309	0.256348
O	-5.335525	-1.382686	-0.083418
O	-5.068085	2.223866	0.212458

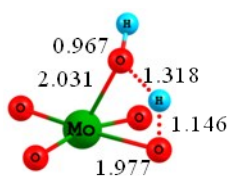
2a-IM3



P	0.117479	-0.005825	-0.005762
O	-0.346442	-0.968659	-1.133199
O	1.646721	0.240127	-0.125397
O	-0.195914	-0.641601	1.376613
O	-0.634450	1.346833	-0.141064
Mo	-3.097014	1.734056	-0.025118
Mo	-0.309351	3.236354	1.374412
Mo	-0.553219	2.880618	-2.085271
Mo	-0.092304	-0.488657	-3.515982
Mo	0.397997	-3.313157	-1.546341
Mo	-2.663014	-1.753349	-1.529169
Mo	3.319818	-1.536760	0.001354
Mo	2.889948	1.247074	-2.039029
Mo	3.024618	1.656475	1.369392
Mo	0.278196	0.299937	3.637204
Mo	-2.448247	-1.234237	2.117170
Mo	0.661530	-2.807045	2.222001
O	-2.298481	3.011366	1.064823
O	-2.532427	2.482599	-1.552319
O	-0.489076	3.922399	-0.590468
O	0.466643	-2.457762	-3.153082
O	-1.944743	-1.387915	-3.164528
O	-1.428356	-3.389900	-1.471521
O	3.794606	-0.263282	-1.571644
O	3.997171	0.153242	1.025462
O	3.396997	2.211610	-0.569464
O	-1.447904	-0.281024	3.670293
O	1.021280	-1.371844	3.642135
O	-1.093437	-2.711027	2.706489
O	-0.385021	4.740886	2.159884
O	-0.767389	4.001189	-3.342265
O	0.856529	-4.905727	-1.914005
O	-0.114812	-0.552424	-5.213551
O	-4.125382	-2.530727	-1.901657
O	3.820364	1.904986	-3.297277
O	4.764558	-2.430050	0.034047
O	4.130495	2.673744	2.159191
O	-3.794809	-1.781713	2.996574
O	0.546013	0.867906	5.214351
O	1.232191	-4.167508	3.061684
O	-3.153616	-0.072462	-1.081888
O	-0.849284	1.110484	-3.103803
O	-0.411441	2.010017	2.713258
O	2.228227	-2.463665	-1.119410
O	2.436372	-2.032017	1.509467
O	1.970392	0.999341	2.715453

O	1.597286	0.035839	-3.095241
O	-2.926354	0.430188	1.462659
O	1.459902	2.966485	1.062840
O	0.439538	-3.395156	0.501553
O	1.218625	2.425795	-2.179090
O	-2.577074	-2.068253	0.508450
H	-5.602458	-1.675730	-0.558537
H	-5.687019	-0.322437	0.160564
O	-4.989001	1.554093	-0.343918
O	-6.037119	-1.225886	0.179914
O	-4.687497	2.683298	0.461933

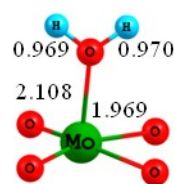
2b-TS1



P	0.009411	-0.000811	-0.006087
O	-1.191607	-0.452264	0.869851
O	1.336789	-0.238475	0.765243
O	-0.132074	1.510728	-0.335487
O	0.024433	-0.823239	-1.323822
Mo	-1.643342	-0.962047	-2.834178
Mo	1.690129	-0.528203	-3.087607
Mo	0.246953	-3.283817	-1.513128
Mo	-1.484442	-2.732925	1.697782
Mo	-1.872036	0.424815	3.103518
Mo	-3.584298	-0.366947	0.232257
Mo	1.858327	0.795742	2.917228
Mo	2.253096	-2.401077	1.604895
Mo	3.618152	0.283300	-0.048551
Mo	1.416922	2.937426	-1.672183
Mo	-2.026476	2.461939	-1.551672
Mo	-0.243251	3.364043	1.305213
O	-0.069298	-0.726901	-3.958494
O	-1.402562	-2.720888	-2.562844
O	1.275562	-2.559592	-2.832793
O	-1.890407	-1.392011	3.233532
O	-3.325548	-1.953472	1.092289
O	-3.371223	0.536585	2.060980
O	2.386962	-1.213766	2.979816
O	3.559967	0.776264	1.705718
O	3.595731	-1.659641	0.607555
O	-0.262692	3.278256	-2.289266
O	1.196806	3.816760	-0.083039

O	-1.472521	3.733368	0.010478
O	2.614421	-0.649968	-4.507868
O	-3.397523	-0.859840	-3.852963
O	0.237823	-4.941148	-1.880275
O	-2.399466	0.946721	4.630332
O	-2.058881	-4.143702	2.450114
O	-5.271949	-0.269078	0.077202
O	2.945345	-3.821323	2.225687
O	2.601538	1.286657	4.363931
O	5.263446	0.416063	-0.444739
O	-3.119524	3.503593	-2.330421
O	2.402511	3.979775	-2.579822
O	-0.191776	4.790800	2.223524
O	-3.359860	-0.843848	-1.595474
O	-1.182594	-3.219129	-0.026391
O	1.415327	1.255794	-2.866238
O	0.166981	0.333840	3.399752
O	1.361810	2.342932	2.104926
O	2.852802	1.778395	-0.779325
O	0.277867	-2.657796	2.139857
O	-1.760027	1.073322	-2.668676
O	2.898578	-0.659038	-1.737519
O	-1.245848	2.210147	2.314399
O	1.433530	-3.132313	-0.125984
O	-3.040281	1.531877	-0.365293
H	-3.846857	-0.705936	-2.623987
H	-3.563627	-0.271936	-4.602396

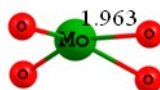
2b-IM1



P	-0.004541	0.001458	-0.000591
O	0.555372	1.137450	-0.900261
O	-0.627286	-1.109934	-0.889626
O	-1.095945	0.580253	0.941333
O	1.149696	-0.601938	0.846191
Mo	2.483372	0.434009	2.298911
Mo	0.846554	-2.419032	2.452092
Mo	3.188540	-1.704161	-0.029740
Mo	2.292270	0.800405	-2.586152
Mo	-0.697862	2.575400	-2.507510
Mo	1.696531	3.194755	-0.122900
Mo	-2.477853	-0.728386	-2.439616

Mo	0.508716	-2.501986	-2.619723
Mo	-1.713082	-3.188915	-0.090924
Mo	-2.452168	-0.638621	2.643258
Mo	-0.679136	2.352844	2.571313
Mo	-3.190152	1.704151	0.241201
O	1.992099	-0.952667	3.341759
O	3.838517	-0.222870	1.190003
O	2.629372	-2.690693	1.397826
O	0.786478	1.989678	-3.385972
O	2.612880	2.605395	-1.584686
O	0.197939	3.736655	-1.413856
O	-1.033030	-1.893789	-3.375467
O	-2.729156	-2.560511	-1.468081
O	-0.309273	-3.693706	-1.498229
O	-1.826087	0.864262	3.460201
O	-3.666534	0.233385	1.588758
O	-2.531259	2.651639	1.652578
O	1.075648	-3.628403	3.623096
O	3.830826	1.325617	3.652127
O	4.712982	-2.357186	-0.391976
O	-1.463800	3.587927	-3.634380
O	3.442746	1.004651	-3.819440
O	2.364584	4.726713	0.174407
O	1.192733	-3.482440	-3.824936
O	-3.712211	-0.899791	-3.594297
O	-2.360109	-4.729105	0.210327
O	-0.824346	3.529373	3.788279
O	-3.407529	-1.380495	3.834316
O	-4.735620	2.365409	0.004879
O	2.473169	2.133929	1.116511
O	3.191617	-0.040146	-1.250183
O	-0.615049	-1.497440	3.018852
O	-1.566761	0.758977	-2.953907
O	-3.280447	0.074284	-1.021263
O	-2.390465	-2.141301	1.250253
O	1.345909	-0.673150	-3.075918
O	0.804894	1.489845	3.084913
O	-0.023414	-3.251904	1.092077
O	-2.170556	2.446025	-1.087385
O	2.077533	-2.410246	-1.303398
O	0.094081	3.223596	1.177007
H	4.599857	0.888840	4.049113
H	3.626028	2.131052	4.151425

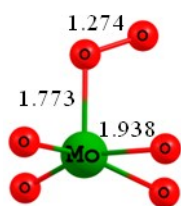
[PMo₁₂O₃₉]³⁻



P	-0.000323	0.003901	-0.052777
O	0.571056	1.445032	0.047492
O	-0.788369	-0.336751	1.241954
O	1.169494	-1.003774	-0.224552
O	-0.953474	-0.088903	-1.276001
Mo	-0.452003	0.356374	-3.608614
Mo	-2.130148	-2.129793	-1.926271
Mo	-3.024288	1.226425	-1.623388
Mo	-0.815684	3.436188	0.338855
Mo	2.176889	2.341048	1.732722
Mo	1.905171	2.616120	-1.681013
Mo	0.206408	-0.337073	3.474231
Mo	-2.798455	0.820493	2.159497
Mo	-1.931575	-2.477493	1.741298
Mo	1.033841	-3.485879	-0.430215
Mo	2.738130	-0.953719	-2.097923
Mo	3.049399	-1.349449	1.351996
O	-1.260323	-1.241315	-3.660481
O	-1.908439	1.490531	-3.309618
O	-3.388116	-0.478241	-2.157804
O	0.819794	3.550565	1.616989
O	0.733276	3.837665	-1.003998
O	2.905963	2.745948	0.104362
O	-1.639312	0.616401	3.549736
O	-1.103562	-1.952413	3.278355
O	-3.259207	-0.947249	2.060278
O	2.146593	-2.916946	-1.755405
O	2.216351	-3.175550	0.930820
O	3.757108	-1.391407	-0.327661
O	-3.107199	-3.283857	-2.700750
O	-4.381368	2.104250	-2.142368
O	3.251769	3.041578	2.844297
O	-1.383568	5.025973	0.529652
O	2.944614	3.552437	-2.642496
O	-4.155821	1.554748	2.866698
O	0.485037	-0.457688	5.145796
O	-2.898515	-3.782065	2.235969
O	4.004437	-1.268824	-3.185804
O	1.037638	-5.175517	-0.593971
O	4.333975	-1.859018	2.337787
O	0.784415	1.820483	-2.904141
O	-1.775882	2.766356	-1.050210
O	-0.541618	-2.973461	-1.658630

O	0.967646	1.242194	2.991253
O	1.500238	-1.361801	2.715221
O	-0.499195	-3.262372	0.912232
O	-1.698543	2.474656	1.604892
O	1.351612	-0.740033	-3.216568
O	-2.628935	-2.198970	-0.180824
O	2.993771	0.467006	1.581110
O	-3.283871	1.010969	0.176971
O	2.903286	0.810020	-1.695294

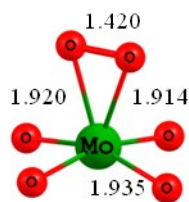
t-[PMo₁₂O₄₁]³⁻



P	-0.054001	0.001115	-0.004224
O	0.144949	0.773282	-1.337478
O	-1.401392	-0.771119	-0.043961
O	-0.072115	1.009161	1.177682
O	1.112555	-1.006864	0.186859
Mo	3.425221	-0.530985	0.311963
Mo	1.323666	-2.485555	2.121168
Mo	1.688689	-2.884968	-1.323053
Mo	0.240438	-0.305891	-3.528120
Mo	-1.303974	2.559527	-2.302618
Mo	2.091436	2.183984	-1.937598
Mo	-3.574485	0.307934	-0.337144
Mo	-2.095219	-2.557488	-1.640530
Mo	-2.335965	-2.181762	1.765927
Mo	-0.370903	0.517066	3.604638
Mo	1.794377	2.487972	1.727199
Mo	-1.660163	2.887206	1.477826
O	3.162369	-1.661862	1.721384
O	3.376548	-1.798878	-1.011237
O	1.864919	-3.507408	0.381462
O	-0.966262	1.382379	-3.651062
O	1.657563	1.225498	-3.426530
O	0.382317	3.268249	-2.268175
O	-3.482177	-1.380401	-1.546483
O	-3.724841	-1.223381	1.075718
O	-2.359270	-3.266128	0.025350
O	1.056593	1.641293	3.476571
O	-1.625642	1.788384	3.209127
O	-0.013644	3.509751	1.952452

O	1.837238	-3.647337	3.249360
O	5.175298	-0.273657	0.433797
O	2.354796	-4.125943	-2.270610
O	-2.237476	3.768643	-3.043105
O	0.365017	-0.635847	-5.190022
O	3.235435	3.302876	-2.504104
O	-2.659036	-3.766691	-2.690124
O	-5.232265	0.637801	-0.508220
O	-3.095659	-3.300632	2.791880
O	2.814006	3.649843	2.431985
O	-0.549715	0.276166	5.275476
O	-2.710576	4.128158	1.965936
O	3.093728	0.918030	-1.086451
O	1.453482	-1.409077	-2.746029
O	0.913772	-1.021549	3.118919
O	-2.773896	1.262474	-1.661811
O	-3.019112	1.411222	0.994950
O	-1.661919	-0.910674	2.899548
O	-1.204809	-1.260468	-2.974156
O	2.844268	1.024197	1.521058
O	-0.406763	-2.914277	1.771919
O	-1.520615	3.097461	-0.336400
O	-0.121636	-3.095320	-1.506280
O	1.756389	2.916591	-0.037738
O	6.417459	-0.000498	0.503263

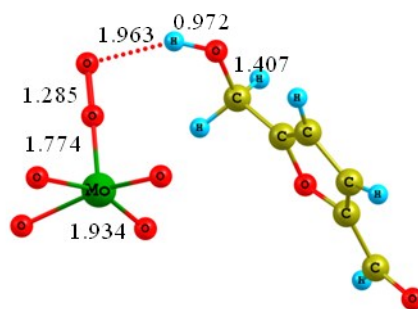
b-[PMo₁₂O₄₁]³⁻



P	-0.050813	0.001439	0.003686
O	0.212827	-0.475483	1.458481
O	-1.356510	0.841954	-0.041876
O	-0.200768	-1.234845	-0.925024
O	1.141200	0.874130	-0.476837
Mo	3.544089	0.216923	-0.612578
Mo	1.272246	1.886020	-2.697546
Mo	1.909480	2.996365	0.545368
Mo	0.517990	1.043041	3.348879
Mo	-1.236921	-1.923284	2.881029
Mo	2.135093	-1.835616	2.229174
Mo	-3.546822	-0.018807	0.617115
Mo	-1.851022	2.968143	1.164905

Mo	-2.360599	1.881718	-2.054271
Mo	-0.657437	-1.260821	-3.377028
Mo	1.553334	-2.904498	-1.253704
Mo	-1.887225	-3.036711	-0.705527
O	3.116409	1.013118	-2.154818
O	3.503087	1.793967	0.392454
O	1.985475	3.225245	-1.261756
O	-0.748790	-0.505068	3.914673
O	1.855413	-0.554868	3.496187
O	0.409580	-2.720684	2.896453
O	-3.291204	1.882114	1.418771
O	-3.734821	1.178047	-1.084622
O	-2.207030	3.315266	-0.595724
O	0.725176	-2.412965	-3.095997
O	-1.933601	-2.340936	-2.634192
O	-0.309318	-3.842668	-1.135065
O	1.750736	2.745007	-4.083006
O	5.434387	0.461686	-0.440433
O	2.697758	4.371059	1.153987
O	-2.164675	-2.887293	3.925859
O	0.780100	1.715597	4.886824
O	3.268102	-2.871369	2.953803
O	-2.281886	4.406199	1.957408
O	-5.200107	-0.205957	0.960532
O	-3.144902	2.795801	-3.250474
O	2.466020	-4.248892	-1.749607
O	-0.949316	-1.375694	-5.045356
O	-3.024208	-4.289735	-0.842571
O	3.113934	-0.798369	1.036175
O	1.716525	1.878389	2.269125
O	0.725756	0.268046	-3.322319
O	-2.692385	-0.710725	2.065570
O	-3.140754	-1.414031	-0.473123
O	-1.828868	0.358746	-2.921978
O	-0.921387	1.939055	2.691471
O	2.662359	-1.499605	-1.438825
O	-0.407044	2.480960	-2.342313
O	-1.622462	-2.858749	1.098171
O	0.128710	3.347365	0.791850
O	1.628022	-2.939563	0.561056
O	5.124647	-0.772430	-1.070377

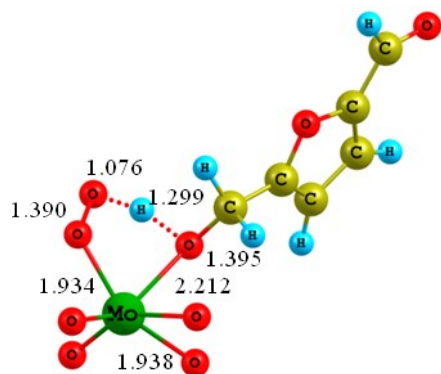
3-IM1



P	0.530863	0.017416	-0.001866
O	1.063063	-0.520308	-1.358702
O	0.899015	1.519485	0.145247
O	1.175089	-0.787561	1.160189
O	-1.013713	-0.141951	0.045802
Mo	-2.266455	-2.149103	-0.139305
Mo	-2.387681	0.527709	1.952740
Mo	-2.642822	0.897881	-1.504615
Mo	0.397526	0.382582	-3.529990
Mo	3.428050	-0.615969	-2.145613
Mo	0.798935	-2.826014	-2.226454
Mo	3.193343	2.361153	0.128071
Mo	0.213891	3.414407	-1.324929
Mo	0.369826	2.975488	2.078909
Mo	0.823753	-0.484673	3.610978
Mo	0.920266	-3.201780	1.441715
Mo	3.597514	-0.977691	1.644696
O	-3.017769	-1.326376	1.300446
O	-3.045032	-1.099235	-1.422451
O	-3.354476	1.025215	0.169061
O	2.456156	0.094069	-3.512836
O	0.525688	-1.699842	-3.633909
O	2.782096	-2.316346	-2.341849
O	2.008368	3.585419	-1.062939
O	2.072065	3.379874	1.566353
O	-0.255156	3.920533	0.369438
O	0.669183	-2.269740	3.282844
O	2.636144	-0.422809	3.369189
O	2.880177	-2.635583	1.891030
O	-3.673225	0.845304	3.017081
O	-3.298730	-3.586825	-0.262678
O	-3.919041	1.375382	-2.516958
O	5.003701	-0.705572	-2.770916
O	0.210471	0.692843	-5.189827
O	0.870978	-4.359077	-2.951788
O	-0.187898	4.761306	-2.276842
O	4.582390	3.338318	0.172896
O	-0.003503	4.185851	3.209055

O	1.003818	-4.806800	1.992387
O	0.634259	-0.362971	5.293532
O	5.175020	-1.132492	2.252226
O	-0.875307	-2.752102	-1.496936
O	-1.296528	0.194577	-2.901503
O	-1.129865	-0.292413	2.978475
O	3.444388	1.265801	-1.301619
O	3.501000	1.064222	1.362363
O	0.733902	1.498252	3.098869
O	0.651876	2.019252	-2.779357
O	-0.842479	-2.921373	1.114449
O	-1.482947	2.098945	1.839449
O	3.803575	-1.035306	-0.174457
O	-1.539034	2.358444	-1.445392
O	1.401929	-3.288080	-0.307774
O	-4.035919	-4.630443	-0.398448
C	-6.404573	2.670663	-0.860463
C	-6.377667	1.463109	-0.085804
C	-6.358377	1.191064	1.259253
C	-6.296636	-0.215456	1.387432
C	-6.283144	-0.711877	0.109580
C	-6.257309	-2.089100	-0.440723
O	-6.421695	3.799828	-0.375525
O	-6.337889	0.283025	-0.790462
O	-6.147073	-3.001223	0.625509
H	-6.409509	2.511899	-1.958112
H	-6.377923	1.928581	2.052307
H	-6.257050	-0.800045	2.297197
H	-5.416299	-2.171958	-1.148477
H	-7.175746	-2.260428	-1.026929
H	-5.654955	-3.779538	0.314088

3-TS1

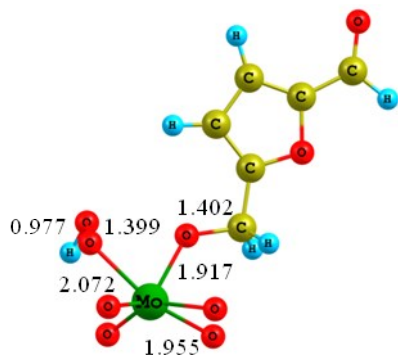


P	-0.633457	-0.033003	0.008192
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O	-0.068923	1.401887	-0.180665
Mo	2.452940	2.162828	-0.162779
Mo	-0.443321	2.753760	-2.181897
Mo	-0.553264	3.367143	1.248412
Mo	-0.767594	0.467623	3.519610
Mo	-0.689714	-2.818037	2.381133
Mo	2.144836	-0.888835	2.165593
Mo	-3.608084	-1.961803	0.181603
Mo	-3.748737	1.295011	1.394483
Mo	-3.543297	0.762344	-1.993320
Mo	-0.414665	-0.730440	-3.577398
Mo	2.285163	-1.391613	-1.486570
Mo	-0.582041	-3.372730	-1.388022
O	1.628817	2.862864	-1.594362
O	1.498733	3.086592	1.046678
O	-0.571268	3.954607	-0.477371
O	-1.042227	-1.586990	3.676629
O	1.206925	-0.212047	3.574921
O	1.129281	-2.644232	2.470755
O	-4.407330	-0.400535	1.297462
O	-4.361875	-0.721338	-1.320648
O	-4.197212	1.750848	-0.319619
O	1.361017	-1.040760	-3.315371
O	-0.947127	-2.433672	-3.174349
O	1.192463	-3.153256	-1.744317
O	-0.459306	3.990703	-3.346408
O	-0.618816	4.799570	2.156982
O	-0.993328	-4.305498	3.140736
O	-0.930619	0.859971	5.164534
O	3.637805	-1.317441	2.850364
O	-4.888016	2.119611	2.345156
O	-4.922523	-3.032902	0.287931
O	-4.665928	1.361109	-3.117038
O	3.778686	-1.949792	-2.073365
O	-0.567542	-0.646121	-5.265951
O	-0.886842	-4.975276	-1.857626
O	2.539073	0.690371	1.285899
O	-0.165337	1.993130	2.738411
O	-0.043901	1.245066	-3.115185
O	-2.547945	-2.388825	1.596025
O	-2.506193	-2.704446	-1.057138
O	-2.272019	-0.066703	-3.018807
O	-2.448952	0.609250	2.841525
O	2.382484	0.398844	-1.287158
O	-2.191461	2.320747	-1.944031

O	-0.488231	-3.444937	0.439822
O	-2.257144	2.699712	1.328977
O	2.329238	-1.741457	0.295462
C	9.750510	-0.852111	0.726213
C	8.490209	-0.671097	0.071615
C	7.964917	-1.093643	-1.128076
C	6.662507	-0.565888	-1.216724
C	6.459015	0.147828	-0.057746
C	5.300399	0.913037	0.483805
O	10.702488	-1.480605	0.275355
O	7.556198	0.098298	0.723493
O	4.506629	1.432497	-0.539024
H	9.808284	-0.353687	1.721340
H	8.482349	-1.719997	-1.843733
H	5.924937	-0.712874	-1.996550
H	5.698982	1.709124	1.141931
H	4.708889	0.247619	1.133640
H	4.912207	2.646122	-0.762062
O	3.633171	3.679633	0.052009
O	4.812889	3.714172	-0.682486

3-IM2

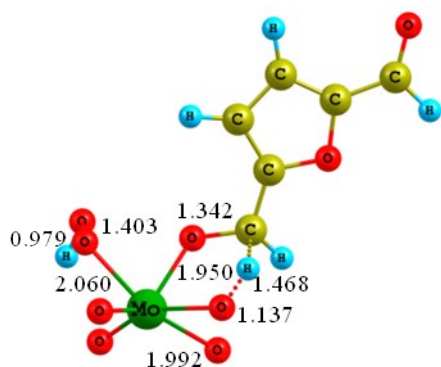


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O	0.242122	-0.831035	1.271945
O	-0.144841	1.307622	-0.041803
Mo	-2.673805	1.697834	-0.119557
Mo	0.028187	3.019659	1.693603
Mo	0.027158	3.052267	-1.792707
Mo	0.670904	-0.124996	-3.553951
Mo	1.100830	-3.144299	-1.881629
Mo	-1.993953	-1.652700	-1.904683
Mo	3.864581	-1.500740	0.054443
Mo	3.500750	1.487254	-1.688314
Mo	3.394920	1.511746	1.745529
Mo	0.538280	-0.142132	3.650863

Mo	-2.038770	-1.544602	1.782822
Mo	1.096776	-3.061993	1.928779
O	-1.978512	2.664355	1.244282
O	-1.948918	2.516007	-1.567569
O	-0.036630	3.919680	-0.190402
O	1.255214	-2.111913	-3.374404
O	-1.176958	-1.091938	-3.435017
O	-0.723798	-3.262419	-1.943532
O	4.410893	-0.049385	-1.329973
O	4.427222	0.074994	1.305126
O	3.882422	2.288885	-0.088700
O	-1.170422	-0.754619	3.498454
O	1.322610	-1.789902	3.521507
O	-0.688733	-3.053416	2.297210
O	-0.139336	4.424287	2.634489
O	-0.130987	4.303438	-2.928992
O	1.624376	-4.676533	-2.391399
O	0.764414	0.002838	-5.245467
O	-3.407190	-2.409711	-2.462605
O	4.496331	2.299896	-2.797430
O	5.326603	-2.365411	0.088278
O	4.418254	2.453450	2.718958
O	-3.426779	-2.212394	2.499617
O	0.684423	0.249011	5.296268
O	1.644825	-4.497857	2.649556
O	-2.548263	-0.020168	-1.288536
O	-0.153479	1.403277	-3.020161
O	-0.131862	1.648388	2.877172
O	2.875427	-2.315056	-1.236021
O	2.894789	-2.179135	1.432647
O	2.269918	0.687698	2.933138
O	2.314104	0.379506	-2.960484
O	-2.525157	0.132851	1.290489
O	1.820827	2.819117	1.478229
O	1.006510	-3.456134	0.142273
O	1.812536	2.643454	-1.812628
O	-2.037235	-2.193939	0.086202
C	-9.566381	-1.750542	0.137367
C	-8.606393	-0.691088	-0.006303
C	-8.698081	0.637425	-0.338479
C	-7.381691	1.155211	-0.309254
C	-6.572464	0.105682	0.040386
C	-5.106880	-0.015159	0.255949
O	-10.773388	-1.607888	-0.035104
O	-7.289160	-1.014260	0.226633
O	-4.529806	1.224373	-0.054801

H	-9.134777	-2.731630	0.420568
H	-9.614133	1.165049	-0.574209
H	-7.058633	2.166727	-0.517095
H	-4.697479	-0.816477	-0.381446
H	-4.906672	-0.291996	1.302773
H	-3.842015	4.063911	1.402364
O	-3.735346	3.459935	-0.369986
O	-4.510805	3.776538	0.750432

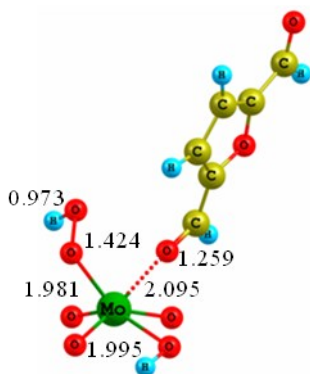
3a-TS2



P	0.606967	-0.048286	-0.009620
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O	2.129768	0.149301	-0.245086
O	0.374701	-0.606812	1.421293
O	-0.119582	1.316350	-0.161898
Mo	-2.569558	1.887071	0.052904
Mo	0.355027	3.267955	1.230367
Mo	-0.136154	2.750366	-2.182415
Mo	0.143296	-0.696246	-3.468501
Mo	0.700359	-3.433474	-1.396096
Mo	-2.313491	-1.790815	-1.250281
Mo	3.764256	-1.664681	-0.142311
Mo	3.261585	1.026820	-2.287263
Mo	3.641550	1.598579	1.079042
Mo	1.026630	0.430731	3.593857
Mo	-1.834670	-1.100301	2.342009
Mo	1.236059	-2.751127	2.315174
O	-1.669450	3.040656	1.170270
O	-2.043475	2.387789	-1.632839
O	0.056393	3.861864	-0.750128
O	0.678325	-2.659898	-3.045049
O	-1.701578	-1.525870	-2.946994
O	-1.117816	-3.456154	-1.193554
O	4.159693	-0.483222	-1.806426
O	4.551412	0.054081	0.746483
O	3.892199	2.047735	-0.906289

O	-0.706571	-0.100116	3.773437
O	1.727714	-1.258638	3.633055
O	-0.478348	-2.583174	2.912256
O	0.370153	4.810701	1.941805
O	-0.409607	3.813613	-3.477135
O	1.093799	-5.054145	-1.712826
O	0.001886	-0.842316	-5.155205
O	-3.816556	-2.545035	-1.482701
O	4.118341	1.596521	-3.637495
O	5.185819	-2.594767	-0.162535
O	4.823624	2.622384	1.739344
O	-3.129979	-1.566739	3.337518
O	1.416526	1.067568	5.118367
O	1.830443	-4.084093	3.182062
O	-3.014300	-0.040951	-0.804894
O	-0.544550	0.941385	-3.087458
O	0.316198	2.111945	2.633383
O	2.575706	-2.614864	-1.137968
O	2.975552	-2.061059	1.445452
O	2.667397	1.037338	2.525100
O	1.870106	-0.198549	-3.190546
O	-2.314344	0.506042	1.661026
O	2.091410	2.934659	0.813248
O	0.881469	-3.416329	0.645797
O	1.613508	2.242874	-2.373112
O	-2.094535	-2.008067	0.790191
C	-9.221909	-1.849835	0.216981
C	-8.319785	-0.758735	-0.016997
C	-8.432412	0.437899	-0.692463
C	-7.194304	1.089690	-0.575053
C	-6.387114	0.251698	0.178549
C	-5.016249	0.333382	0.588187
O	-10.380314	-1.879835	-0.193575
O	-7.061172	-0.866678	0.520560
O	-4.443117	1.540328	0.467172
H	-8.794708	-2.685509	0.806466
H	-9.318814	0.785035	-1.209038
H	-6.903109	2.050468	-0.979255
H	-4.061697	-0.200085	-0.390887
H	-4.702561	-0.307221	1.421670
H	-3.302517	4.466434	1.284426
O	-3.563241	3.638975	-0.377684
O	-4.103652	4.220373	0.779186

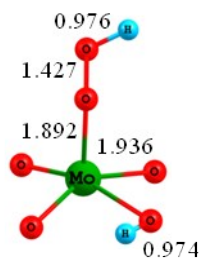
3a-IM3



P	-0.650939	-0.034318	0.005391
O	-0.392671	-0.547970	1.448598
O	-2.171171	0.213735	-0.196476
O	-0.162027	-1.098111	-1.015734
O	0.122114	1.295074	-0.214823
Mo	2.741385	1.805572	-0.099621
Mo	0.091835	2.549777	-2.311832
Mo	-0.186661	3.398093	1.058365
Mo	-0.975184	0.711212	3.460508
Mo	-1.274948	-2.622712	2.515639
Mo	1.810648	-1.114444	2.430194
Mo	-3.871631	-1.525932	0.037274
Mo	-3.643452	1.792926	1.052559
Mo	-3.262549	1.014233	-2.271840
Mo	-0.265240	-0.990763	-3.505587
Mo	2.151225	-1.872330	-1.164386
Mo	-0.965193	-3.435154	-1.195154
O	2.110574	2.409833	-1.646881
O	1.824000	2.999911	1.017908
O	0.006948	3.867027	-0.692771
O	-1.546722	-1.272192	3.707388
O	0.874553	-0.224903	3.717168
O	0.538627	-2.691788	2.746340
O	-4.524640	0.199748	0.994929
O	-4.329380	-0.296853	-1.588624
O	-3.894200	2.190922	-0.715427
O	1.424652	-1.521163	-3.080181
O	-1.060326	-2.575575	-3.054745
O	0.844124	-3.482543	-1.414210
O	0.336751	3.697602	-3.540174
O	-0.117937	4.883130	1.877830
O	-1.840394	-4.001651	3.328355
O	-1.203814	1.230075	5.062014
O	3.173253	-1.695401	3.259276
O	-4.723334	2.825581	1.858280
O	-5.327756	-2.399376	0.092990

O	-4.202860	1.684068	-3.516315
O	3.591064	-2.665573	-1.593266
O	-0.278271	-0.998467	-5.203079
O	-1.456211	-5.009069	-1.599228
O	2.272154	0.669568	1.679245
O	-0.107951	2.085825	2.649024
O	0.343860	0.942373	-3.123970
O	-2.990590	-1.998269	1.556319
O	-2.795640	-2.491565	-1.062706
O	-2.047390	-0.045679	-3.140789
O	-2.564606	1.034460	2.638267
O	2.588532	-0.109154	-1.102929
O	-1.712654	2.374598	-2.196544
O	-1.019180	-3.398271	0.635371
O	-1.968605	2.974811	1.033765
O	2.012490	-2.106130	0.631790
C	9.821916	-1.507286	-0.483544
C	8.755396	-0.686425	0.000317
C	8.710924	0.347524	0.924195
C	7.387335	0.782954	0.986199
C	6.671321	-0.010051	0.091602
C	5.303199	0.028554	-0.275718
O	10.996204	-1.416810	-0.123278
O	7.502785	-0.901295	-0.508009
O	4.548871	0.836388	0.326947
H	9.503578	-2.259759	-1.238751
H	9.570205	0.717961	1.468708
H	6.951959	1.580271	1.574498
H	1.722735	1.345741	2.133600
H	4.928085	-0.612219	-1.084213
H	4.525193	3.377681	-1.812688
O	4.047921	3.291685	-0.008839
O	5.022855	3.090566	-1.027460

3a-IM4

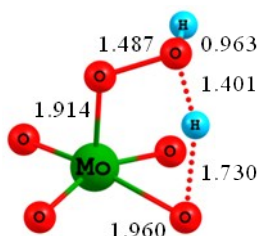


P	-0.072437	0.003133	-0.001134
O	-0.194123	1.444793	-0.566993
O	-1.373677	-0.789002	-0.305575
O	0.143412	0.069030	1.535894

O	1.134639	-0.712289	-0.667861
Mo	3.523633	-0.103896	-0.560355
Mo	1.808201	-3.003541	-0.149093
Mo	1.414157	-1.168328	-3.087145
Mo	-0.555423	1.947410	-2.931201
Mo	-1.868765	3.190931	0.039737
Mo	1.532369	3.217728	-0.444670
Mo	-3.586537	-0.116589	0.484206
Mo	-2.353912	-1.323265	-2.536101
Mo	-1.846402	-3.134246	0.338940
Mo	0.401703	-1.833444	3.128194
Mo	2.044010	1.185252	2.591554
Mo	-1.389873	1.097378	3.188340
O	3.552724	-1.902391	-0.288473
O	3.063164	-0.246306	-2.352948
O	1.979525	-2.658688	-2.202247
O	-1.805196	3.145151	-1.780124
O	0.806695	3.304619	-2.114911
O	-0.236560	3.990762	0.247652
O	-3.717501	-0.684064	-1.511368
O	-3.379122	-2.190245	0.627885
O	-2.223954	-2.927473	-1.666228
O	1.734339	-0.652567	3.512434
O	-0.943708	-0.802946	3.817392
O	0.303153	1.556845	3.684738
O	2.589893	-4.510960	-0.094707
O	1.888185	-1.454604	-4.691803
O	-2.975501	4.433285	0.376483
O	-0.792062	2.717807	-4.426795
O	2.491915	4.615135	-0.354617
O	-3.102361	-1.718781	-4.007529
O	-5.249541	-0.019853	0.817926
O	-2.329791	-4.749004	0.540118
O	3.161961	1.825538	3.699042
O	0.603060	-3.062660	4.281534
O	-2.340057	1.601006	4.501767
O	2.964440	1.962204	-1.120245
O	0.830134	0.806878	-3.213297
O	1.588945	-2.533130	1.593741
O	-3.124769	1.557764	-0.054445
O	-2.781017	0.023779	2.106425
O	-0.973621	-2.723908	1.896173
O	-1.815925	0.637656	-2.881078
O	3.097799	0.469759	1.150633
O	0.055765	-3.401377	-0.415275
O	-1.660345	2.383403	1.912376

O	-0.385472	-1.509411	-3.077312
O	1.605369	2.583252	1.517612
H	3.034932	2.013701	-2.090336
H	6.331275	0.452785	0.966270
O	5.359073	0.346400	-0.647737
O	6.018561	-0.305387	0.436749

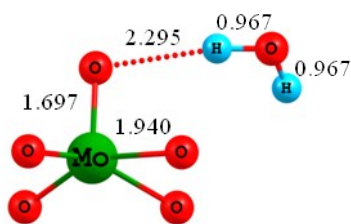
3a-TS3



P	-0.068733	0.002422	-0.005311
O	0.169875	0.782457	-1.327431
O	-1.506326	-0.586362	0.001558
O	0.098862	0.967721	1.200299
O	0.962655	-1.154126	0.104328
Mo	3.373007	-1.030604	0.150831
Mo	1.064290	-2.706039	1.989502
Mo	1.218619	-3.044275	-1.477082
Mo	0.024259	-0.232621	-3.545776
Mo	-1.073643	2.770647	-2.177317
Mo	2.255919	1.945557	-1.986718
Mo	-3.529747	0.774698	-0.159465
Mo	-2.499858	-2.217720	-1.602533
Mo	-2.535922	-1.917976	1.819737
Mo	-0.152700	0.444867	3.626177
Mo	2.166264	2.173651	1.694494
Mo	-1.213549	3.026384	1.622818
O	2.974972	-2.151294	1.552693
O	3.076718	-2.178054	-1.223716
O	1.387901	-3.736068	0.201198
O	-0.954435	1.601260	-3.568847
O	1.633439	1.097548	-3.475765
O	0.690983	3.252557	-2.207463
O	-3.714487	-0.873603	-1.412648
O	-3.816408	-0.766426	1.221286
O	-2.779652	-2.936476	0.056429
O	1.402937	1.377185	3.456444
O	-1.245995	1.880104	3.323109
O	0.520135	3.414634	2.032035
O	1.470896	-3.958643	3.062798
O	1.672656	-4.331875	-2.485804

O	-1.872479	4.112968	-2.841954
O	0.029640	-0.525119	-5.219313
O	3.510414	2.922851	-2.580619
O	-3.264236	-3.310694	-2.652696
O	-5.135803	1.322520	-0.241822
O	-3.389199	-2.959269	2.853763
O	3.360334	3.170932	2.377091
O	-0.286398	0.178414	5.297355
O	-2.068805	4.377982	2.191414
O	3.290504	0.539369	-1.238514
O	1.115716	-1.507603	-2.850578
O	0.895544	-1.232276	3.041348
O	-2.670977	1.656928	-1.497755
O	-2.774960	1.755187	1.170610
O	-1.650477	-0.780579	2.949964
O	-1.507539	-1.007496	-2.945779
O	3.017478	0.598672	1.405441
O	-0.721392	-2.895113	1.714272
O	-1.129200	3.271951	-0.190378
O	-0.610036	-3.011608	-1.577338
O	2.105702	2.657219	-0.055550
H	6.019272	0.358641	1.141139
H	4.776138	0.600435	-0.353399
O	5.271383	-1.200705	0.321279
O	5.960789	0.111889	0.212003

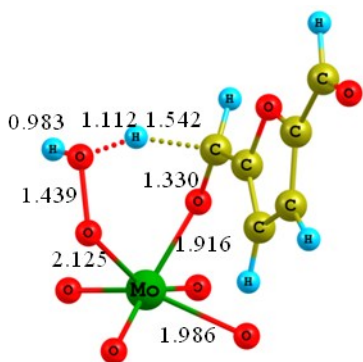
3a-IM5



P	0.072266	-0.000435	0.004076
O	-0.374585	-0.130671	1.486219
O	1.623231	0.045983	-0.071681
O	-0.512715	1.306798	-0.597860
O	-0.446868	-1.223850	-0.800376
Mo	-2.804211	-1.953065	-1.108753
Mo	-0.050833	-1.541718	-3.190933
Mo	0.117975	-3.599714	-0.381737
Mo	0.262431	-1.992223	2.935867
Mo	0.063694	1.454034	3.361897
Mo	-2.708129	-0.279312	2.305680
Mo	2.983628	1.755903	1.022915
Mo	3.244997	-1.695108	0.676663

Mo	2.983918	0.268478	-2.130337
Mo	-0.209802	2.197613	-2.907890
Mo	-2.906163	1.776299	-0.751546
Mo	-0.104702	3.608809	0.222696
O	-2.037978	-1.978402	-2.763003
O	-1.927090	-3.432690	-0.486798
O	0.135805	-3.365560	-2.189695
O	0.471104	-0.208938	3.983648
O	-1.732617	-1.475043	3.276486
O	-1.747497	1.195921	3.357762
O	3.846334	-0.108715	1.339823
O	3.760801	1.331177	-0.868995
O	3.688843	-1.333194	-1.060884
O	-1.991659	2.299315	-2.543649
O	0.270877	3.566216	-1.793025
O	-1.874927	3.507687	-0.201493
O	-0.007294	-2.137535	-4.781347
O	0.240841	-5.282710	-0.197321
O	0.326779	2.464053	4.700686
O	0.456835	-3.063399	4.240130
O	-4.206561	-0.248070	3.102741
O	4.421438	-2.814409	1.171498
O	4.263247	2.715179	1.596217
O	4.112879	0.265285	-3.398020
O	-4.423724	2.484015	-1.038697
O	-0.073301	2.871354	-4.460033
O	0.141904	5.263757	0.508902
O	-3.001002	-1.317456	0.823589
O	-0.298097	-3.037169	1.559620
O	-0.510160	0.209115	-3.365393
O	1.926054	1.479097	2.476100
O	1.843996	2.929915	0.233550
O	1.674569	1.420181	-2.690944
O	1.939781	-1.762466	2.272132
O	-3.070361	0.076555	-1.370604
O	1.684707	-1.197746	-2.778930
O	-0.180201	2.864881	1.894811
O	1.799763	-2.977727	-0.007811
O	-2.941542	1.303260	1.002062
H	-5.782668	-0.746005	-0.815298
H	-5.894927	0.781598	-0.751138
O	-4.393089	-2.482295	-1.380776
O	-6.136539	-0.025308	-0.276727

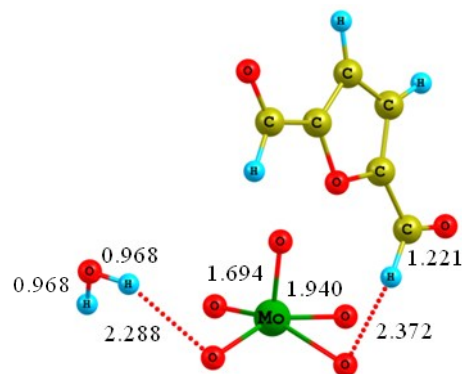
3b-TS2



P	-0.621463	0.027937	-0.002922
O	-0.010784	1.448110	-0.156442
O	-1.981187	-0.039591	-0.751239
O	-0.846449	-0.276466	1.503765
O	0.352567	-1.020303	-0.607774
Mo	2.863314	-1.517256	0.023658
Mo	-0.087869	-3.424048	-0.633685
Mo	1.114210	-1.125369	-2.963172
Mo	0.542330	2.460559	-2.310892
Mo	-0.980658	3.620476	0.593034
Mo	2.152068	2.221578	0.772460
Mo	-3.889369	1.394977	-0.228267
Mo	-2.408871	0.311790	-3.183350
Mo	-3.484041	-2.004900	-0.885516
Mo	-1.808524	-2.340617	2.521232
Mo	0.949054	-0.319739	3.161154
Mo	-2.268089	1.020440	3.064538
O	1.937292	-3.047091	0.028050
O	2.745320	-1.118489	-1.777829
O	0.782729	-2.840277	-2.440612
O	-0.421868	3.867893	-1.122941
O	2.026773	2.909320	-0.911336
O	0.700003	3.564924	1.313689
O	-3.652006	1.300181	-2.291315
O	-4.547592	-0.545794	-0.633068
O	-3.161909	-1.307785	-2.787164
O	-0.294285	-1.958912	3.459002
O	-2.788929	-0.957864	3.209600
O	-0.747764	0.588500	3.973326
O	0.001467	-5.105644	-0.858549
O	1.878850	-1.308652	-4.467603
O	-1.569199	5.145023	1.052473
O	1.059488	3.502573	-3.549061
O	3.506601	3.010057	1.424475
O	-2.796920	0.550796	-4.818588
O	-5.406521	2.158777	-0.194073
O	-4.587920	-3.246017	-1.235747

O	1.859713	-0.443958	4.589993
O	-2.435521	-3.711175	3.302355
O	-3.283384	1.656361	4.267186
O	2.760456	0.557556	0.314918
O	1.399084	0.892585	-2.638907
O	-0.597575	-3.215634	1.099404
O	-2.684942	2.756659	-0.183423
O	-3.592714	0.880095	1.488431
O	-3.005752	-2.300833	0.857688
O	-1.082559	1.858159	-2.861965
O	1.800825	-1.305869	1.948421
O	-1.702430	-2.951537	-1.319312
O	-1.644753	2.492863	2.170939
O	-0.598851	-0.629939	-3.381582
O	1.410208	1.290606	2.458097
C	9.552611	0.990093	0.072902
C	8.145395	0.729934	-0.009811
C	7.121200	1.277365	-0.752089
C	5.944719	0.606290	-0.386669
C	6.312204	-0.326075	0.579012
C	5.618431	-1.326018	1.332127
O	10.133420	1.841890	-0.598366
O	7.644268	-0.255358	0.804561
O	4.291687	-1.418235	1.297224
H	10.098005	0.357161	0.801290
H	7.226524	2.078808	-1.473077
H	4.943729	0.791440	-0.757467
H	6.072406	-1.668209	2.266968
H	5.748529	-2.586642	0.453252
H	4.852622	-4.006474	0.065889
O	4.427305	-2.451506	-1.070070
O	5.359180	-3.266762	-0.336129

3b-IM3



P	-0.624212	-0.005224	0.013656
O	-0.204431	-0.658308	1.359261

O	-2.008452	0.681098	0.175612	O	-1.407065	2.736602	-1.896363
O	-0.717011	-1.100417	-1.084218	O	-1.809257	-3.153253	0.744569
O	0.433045	1.056733	-0.396030	O	-0.727625	3.187209	1.296752
Mo	2.857738	0.702719	-0.817931	O	1.382753	-2.789235	0.010246
Mo	0.292518	2.392449	-2.437784	C	8.959341	1.193964	1.024567
Mo	1.055964	3.078173	0.894237	C	8.374404	0.102915	0.266552
Mo	0.086070	0.590229	3.439984	C	8.827992	-0.647359	-0.793428
Mo	-1.387729	-2.452891	2.624496	C	7.801833	-1.567828	-1.089790
Mo	1.899015	-1.892796	1.795830	C	6.793944	-1.317901	-0.188432
Mo	-4.043718	-0.507310	0.822158	C	5.475970	-1.897014	0.009019
Mo	-2.624628	2.537695	1.723164	O	10.068019	1.648197	0.788442
Mo	-3.262095	1.886300	-1.589298	O	7.135456	-0.302626	0.639697
Mo	-1.352206	-0.816545	-3.479523	O	5.026619	-2.783141	-0.700269
Mo	1.168281	-2.496262	-1.769734	H	8.323009	1.588975	1.840377
Mo	-2.189733	-3.092572	-1.046144	H	9.785822	-0.533396	-1.285024
O	2.236787	1.695833	-2.213720	H	7.786001	-2.325284	-1.863092
O	2.775455	2.073033	0.407462	H	2.947387	4.452482	-1.447581
O	0.971788	3.577389	-0.857207	H	4.900470	-1.470602	0.856352
O	-0.970106	-1.156418	3.833950	H	3.984649	3.732470	-0.601278
O	1.586619	-0.851829	3.259611	O	4.515903	0.551667	-1.131132
O	0.327901	-3.054198	2.419327	O	3.893456	4.452854	-1.240947
O	-3.923404	1.271589	1.891053				
O	-4.480438	0.898086	-0.660356				
O	-3.145865	3.097840	0.061358				
O	0.157831	-1.835126	-3.461888				
O	-2.452027	-2.130359	-2.838169				
O	-0.574818	-3.644541	-1.687423				
O	0.575179	3.494021	-3.699906				
O	1.743704	4.428032	1.660053				
O	-2.131011	-3.657950	3.561017				
O	0.393486	1.054396	5.045087				
O	3.183046	-2.890217	2.283679				
O	-3.138790	3.786089	2.752173				
O	-5.638711	-0.927104	1.229688				
O	-4.223388	2.872599	-2.581625				
O	2.173197	-3.642207	-2.520244				
O	-1.755802	-0.716810	-5.125388				
O	-3.200212	-4.431308	-1.307483				
O	2.688581	-0.623059	0.732400				
O	1.108426	1.704343	2.433157				
O	-0.131816	0.832991	-3.271369				
O	-3.016476	-1.304509	2.093410				
O	-3.580962	-1.672605	-0.492416				
O	-2.644897	0.576824	-2.711543				
O	-1.482553	1.406085	3.014973				
O	2.144978	-0.957408	-1.786856				

Table S3: Thermal correction to Gibbs free energy (G_0) (hartree), sum of electronic and thermal free energies (G_c) (hartree) with ZPE and thermal corrections, and the relative Gibbs free energies (G_r) (kJ mol⁻¹) of various species with respect to the reactants [PMo₁₂O₄₀]³⁻ + 2HMF + O₂ for the oxidation of HMF to DFF catalyzed by [PMo₁₂O₄₀]³⁻ at M06/6-31++G(d, p) level in the solvent of DMSO under the temperature of 433 K.

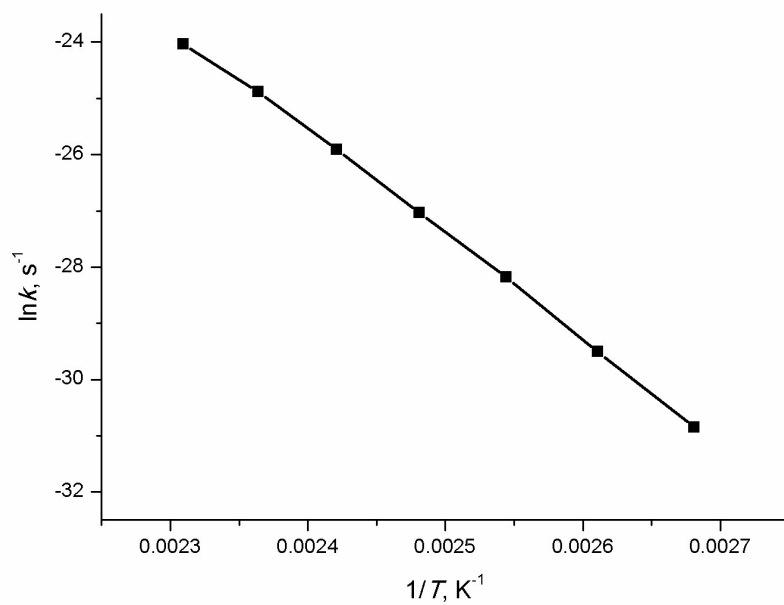
Species	Aqueous phase		
	G_0	G_c	G_r
HMF	0.05716	-457.59724	
O ₂	-0.02690	-150.28146	
DFF	0.03601	-456.40937	
H ₂ O	-0.00729	-76.41833	
[PMo ₁₂ O ₄₀] ³⁻	-0.05083	-4161.35913	
HMF×2 + O ₂	0.08743	-1065.47594	
DFF×2 + H ₂ O×2	0.05744	-1065.65540	
[PMo ₁₂ O ₄₀] ³⁻ + HMF×2 + O ₂	0.03659	-5226.83506	0.0
1-IM1a	0.02951	-4618.96762	
1-IM1a + HMF + O ₂	0.05978	-5226.84632	-29.6
1-IM1b	0.03761	-4618.96495	
1-IM1b + HMF + O ₂	0.06787	-5226.84365	-22.5
1-TS1	0.03473	-4618.90304	
1-TS1 + HMF + O ₂	0.06499	-5226.78174	140.0
1-IM2	0.03660	-4618.94247	
1-IM2 + HMF + O ₂	0.06687	-5226.82117	36.5
1-TS2	0.03293	-4618.89297	
1-TS2 + HMF + O ₂	0.06320	-5226.77167	166.4
1-IM3	0.03522	-4618.93235	
1-IM3 + HMF + O ₂	0.06548	-5226.81105	63.0
[H ₂ PMo ₁₂ O ₄₀] ³⁻	-0.03187	-4162.54187	
[H ₂ Mo ₁₂ O ₄₀] ³⁻ + DFF + HMF + O ₂	0.03440	-5226.82994	13.5
2b-TS1	-0.03607	-4162.51556	
2b-TS1 + DFF + HMF + O ₂	0.03020	-5226.80362	82.5
2a-IM1	-0.03176	-4312.83800	
2a-IM1 + DFF + HMF + O ₂	0.06141	-5226.84460	-25.0
2b-IM1	-0.03461	-4162.54738	
2b-IM1 + DFF + HMF + O ₂	0.03166	-5226.83544	-1.0
2a-TS1	-0.03281	-4312.79553	
2a-TS1 + DFF + HMF + O ₂	0.06036	-5226.80213	86.5
[PMo ₁₂ O ₃₉] ³⁻	-0.05399	-4086.11577	
[PMo ₁₂ O ₃₉] ³⁻ + DFF + H ₂ O + HMF + O ₂	0.00500	-5226.82216	33.9
2a-IM2	-0.02969	-4312.84780	

2a-IM2 + DFF + HMF + O ₂	0.06348	-5226.85440	-50.8
2a-TS2	-0.02912	-4312.79958	
2a-TS2 + DFF + HMF + O ₂	0.06405	-5226.80618	75.8
2a-IM3	-0.03287	-4312.86280	
2a-IM3 + DFF + HMF + O ₂	0.06030	-5226.86940	-90.1
t-[PMo ₁₂ O ₄₁] ³⁻	-0.05291	-4236.41811	
t-[PMo ₁₂ O ₄₀] ³⁻ + DFF + H ₂ O + HMF	0.03297	-5226.84304	-21.0
b-[PMo ₁₂ O ₄₁] ³⁻	-0.05000	-4236.43578	
b-[PMo ₁₂ O ₄₁] ³⁻ + DFF + H ₂ O + HMF	0.03589	-5226.86071	-67.3
3-IM1	0.03553	-4694.02364	
3-IM1 + DFF + H ₂ O	0.06425	-5226.85134	-42.7
3-TS1	0.03698	-4693.97335	
3-TS1 + DFF + H ₂ O	0.06570	-5226.80105	89.3
3-IM2	0.03710	-4694.04423	
3-IM2 + DFF + H ₂ O	0.06582	-5226.87193	-96.8
3a-TS2	0.03345	-4693.99347	
3a-TS2 + DFF + H ₂ O	0.06217	-5226.82117	36.5
3b-TS2	0.03519	-4693.98975	
3b-TS2 + DFF + H ₂ O	0.06391	-5226.81745	46.2
3a-IM3	0.04145	-4694.03142	
3a-IM3 + DFF + H ₂ O	0.07017	-5226.85912	-63.2
3a-IM4	-0.03308	-4237.63261	
3a-IM4 + DFF×2 + H ₂ O	0.03165	-5226.86967	-90.9
3a-TS3	-0.03643	-4237.58294	
3a-TS3 + DFF×2 + H ₂ O	0.02830	-5226.82000	39.5
3a-IM5	-0.03460	-4237.78751	
3a-IM5 + DFF×2 + H ₂ O	0.03013	-5227.02457	-497.6
3b-IM3	0.03048	-4694.20708	
3b-IM3 + DFF + H ₂ O	0.05920	-5227.03477	-524.3
[PMo ₁₂ O ₄₀] ³⁻ + H ₂ O	-0.05812	-4237.77746	
[PMo ₁₂ O ₄₀] ³⁻ + DFF×2 + H ₂ O×2	0.00661	-5227.01453	-471.2
[PMo ₁₂ O ₄₀] ³⁻ + DFF + H ₂ O	-0.02211	-4694.18683	
[PMo ₁₂ O ₄₀] ³⁻ + DFF×2 + H ₂ O×2	0.00661	-5227.01453	-471.2

Figure S2: Arrhenius plots of calculated rate constants for the crucial reaction step in the catalytic oxidation of HMF to DFF over PMo-containing Keggin heteropolyacid catalyst.

Reaction step of 1-IM1 $\rightarrow$ 1-TS2 (k_H):

$$k_H = 1.345 \times 10^8 \exp(-153,476 / RT)$$



Reaction step of 1-IM1 $\rightarrow$ 1-TS2 (k_D):

$$k_D = 2.741 \times 10^8 \exp(-161,175 / RT)$$

