Electronic Supplementary Material (ESI) for RSC Advances.

Theoretical Study on the Reaction Mechanism of Reverse Water-Gas Shift Reaction using Rh-Mo_6S_8 cluster

[supporting information]

Zhaoru Cao, Ling Guo*, Naying Liu, Xiaoli Zheng, Wenli Li, Yayin Shi, Juan Guo, Yaru Xi

School of Chemistry and Material Science, School of Modern Arts and Sciences, Shanxi Normal University, Linfen 041004, China

Figure S1 Combined free energy profile of redox mechanism for RWGS reaction on Rh-Mo_6S_8 and Ti-Mo_6S_8 clusters including reaction intermediates and transition states.

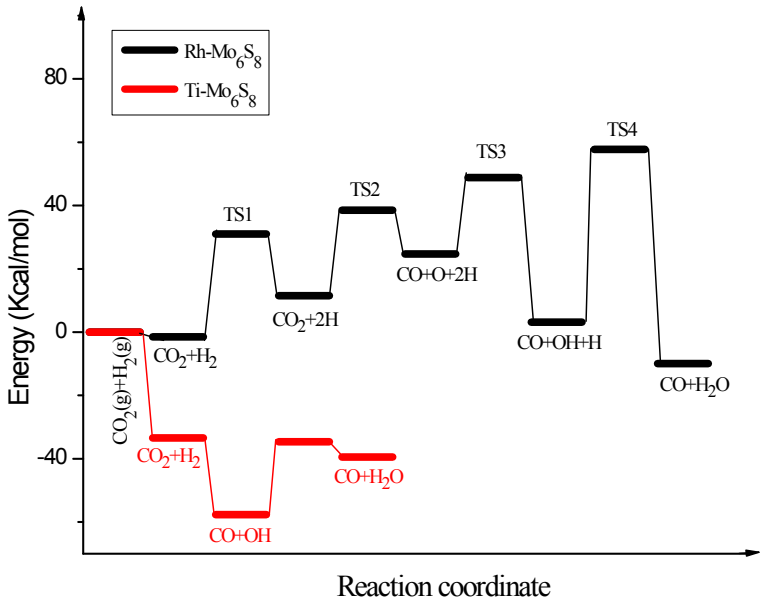

Figure S2 Combined free energy profile of carboxyl mechanism (HOCO intermediate) for RWGS reaction on Rh-Mo_6S_8, K-Mo_6S_8 and Mo_6S_8 clusters including reaction intermediates and transition states.

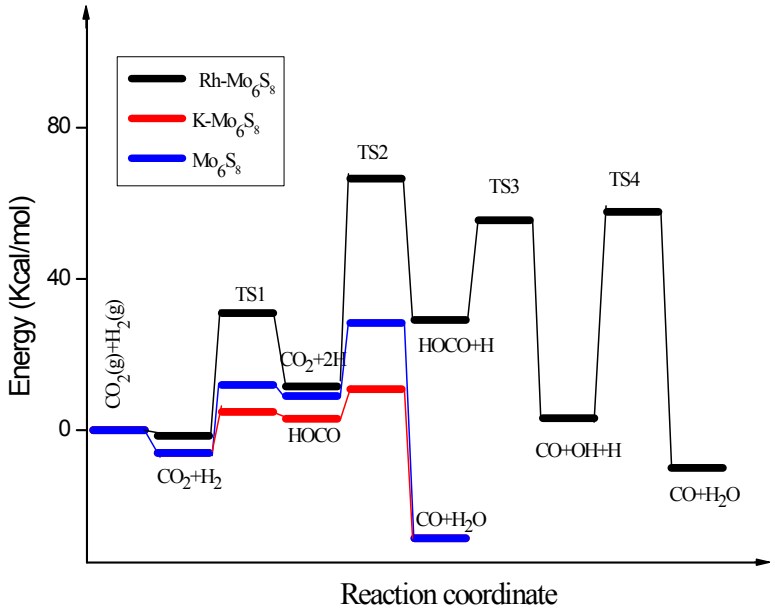

Table S1. Calculated binding Energies (BE) and Vibrational Frequencies of Gas Phase and Adsorbed Species at their Preferred Adsorption Site.

species	Preferred adsorption site	BE/eV	frequencies/cm^{-1}
H_2	gas		4646
CO	gas		2439
CO_2	gas		2585,1518,745,745
H_2O	gas		4187,4069,1827
HOCO	gas		4095,2125,1390,1207,683,545
HCOOH	gas		4041,3319,2035,1552,1440,1274,1192,715,691
H^*	S-Mo bridge	-1.31	2401,552,537
O^*	S-Mo bridge	-5.65	685,462
OH^*	Mo-top	-2.28	3747,762,667,198,194
H_2	Mo-top	-0.08	4057,821,461
H_2O^*	Mo-top	-0.67	3817,3706,1656,611,443,136,87,70
CO^*	Mo-top	-0.52	2122, 397,65,46
CO_2^*	Rh-top	-0.14	1905,1211,697,576,341,331,257,169,155,151,146,124,93
$HOCO^*$	Mo-top	-1.22	3717,1540,1319,1205,725,646,480,393,299,192,188,128,104,42,57
HCOO	Mo-top,Rh-top	-2.74	3105,1575,1394,1369,1045,775,414,315,315,160,150,137,126,109,91,65
CHO	Mo-top	-0.83	2977,1519,1308,813,544,221,145,115
$HCOOH^*$	Rh-top	-0.43	3480,3167,1737,1419,1376,1218,1048,726,672,146,133,112,84,59,46,23

Table S2. DFT Calculated free energy barrier (E_a) and Reaction Energies (△G) of Elementary Reaction Steps; the Imaginary Vibrational Frequency (w) of the Transition State for Each Elementary Reaction Step.

Mechanism	Reaction no.	Elementary steps	E_a	△G	w
A	R1	$H_2 \rightarrow H^* + H^*$	32.51	13.05	-136.81
	R2	$CO_2 \rightarrow CO^* + O^*$	26.99	13.21	-581.60
	R3	$O^* + H^* \rightarrow OH^*$	24.07	-21.60	-1316.63
	R4	$OH^* + H^* \rightarrow H_2O^*$	54.61	-13.10	-594.30
B	R5	$H_2 \rightarrow 2H^*$	32.51	13.05	-136.81
	R6	$CO_2^* + H^* \rightarrow HOCO^*$	55.02	17.62	-1078.73
	R7	$HOCO^* \rightarrow CO^* + OH^*$	26.37	-26.01	-55.42
	R8	$OH^* + H^* \rightarrow H_2O^*$	54.61	-13.10	-594.30
C	R9	$H_2 \rightarrow H^* + H^*$	32.51	13.05	-136.81
	R10	$CO_2^* + H^* \rightarrow HCOO^*$	46.36	5.07	-529.12
	R11	$HCOO^* + H^* \rightarrow HCOOH^*$	21.92	-19.36	-1114.85
	R12	$HCOOH^* \rightarrow CO^* + H_2O^*$	27.69	-5.75	-1108.64
D	R13	$HCOOH^* \rightarrow HCO^* + OH^*$	76.01	33.87	-155.26
	R14	$HCO^* \rightarrow CO^* + H^*$	13.34	-27.97	-542.66
	R15	$OH^* + H^* \rightarrow H_2O^*$	54.61	-13.10	-594.30

cartesian coordinates and the absolute energy values of all the optimized intermediates:

Mechansim A:

CO_2+H_2: -3890.605895 a.u.

Mo	2.148030	-0.891623	-0.270225
Mo	1.537209	1.456402	0.654110
Mo	0.493225	-0.728676	1.746306
Mo	-0.446238	-1.490136	-0.652581
Mo	0.748807	0.705390	-1.712635
Mo	-1.019202	1.169521	0.198004
S	-1.735949	-0.008809	-2.117089
S	1.264842	-1.620800	-2.443698
S	3.088021	1.165847	-1.240134
S	0.143877	2.930300	-0.850930
S	-0.417431	1.364876	2.481259
S	2.826646	-0.207307	2.006264
S	1.170919	-2.904469	0.692735
S	-1.747094	-1.870907	1.341253
Rh	-3.070708	-0.636928	-0.176232
C	-3.749831	1.210984	0.334512
O	-4.913076	0.859403	0.323873
O	-2.998992	2.182651	0.487022
H	2.754089	2.861660	1.746078
H	2.325106	3.341206	1.330452

Ts1: -3890.554085a.u.

Mo	2.148784	-0.941687	-0.178181
Mo	1.599885	1.529322	0.427357
Mo	0.571972	-0.473401	1.818349
Mo	-0.479942	-1.552013	-0.444303
Mo	0.720455	0.443934	-1.792666
Mo	-1.012415	1.098094	0.153231
S	-1.749674	-0.304718	-2.110685
S	1.212288	-1.953926	-2.209794
S	3.073188	0.999424	-1.430583
S	0.025115	2.806376	-1.239385
S	-0.247588	1.747099	2.273760
S	2.917792	0.142867	1.948402
S	1.138732	-2.780003	1.058354
S	-1.750718	-1.538686	1.611121
Rh	-3.111668	-0.649226	-0.117589
C	-3.749265	1.235025	0.256235
O	-4.930736	0.954345	0.247945
O	-2.951161	2.177897	0.373238
H	1.644242	3.116049	1.295967
H	0.978349	3.357638	-0.249362

CO_2+2H: -3890.585098a.u.

Mo	2.132999	-0.968211	-0.034665
Mo	1.666176	1.539074	0.101197
Mo	0.593296	-0.108060	1.849187
Mo	-0.499534	-1.623796	-0.106142
Mo	0.649471	0.103482	-1.849883
Mo	-0.956369	1.067665	0.027462
S	-1.737576	-0.729892	-2.001514
S	1.162466	-2.339952	-1.809280
S	3.041633	0.676454	-1.680988
S	-0.063281	2.509741	-1.785255
S	-0.125256	2.282875	2.029265
S	2.987950	0.479099	1.816744
S	1.137038	-2.529362	1.549969
S	-1.754122	-1.018841	1.885328
Rh	-3.164622	-0.658348	-0.030426
C	-3.713766	1.263366	0.056461
O	-4.914736	1.070947	0.057199
O	-2.870865	2.181089	0.083473
H	0.968761	3.070039	1.683961
H	1.011339	3.250776	-1.307799

TS2: -3890.542098a.u.

Mo	2.687318	-0.277993	0.120383
Mo	1.655613	1.987210	0.901613
Mo	0.794714	-0.354406	1.940436
Mo	0.278386	-1.231257	-0.431443
Mo	1.220969	1.095923	-1.480948
Mo	-0.852129	1.546734	0.284452
S	-1.045726	0.230092	-1.919521
S	2.113986	-1.106670	-2.140804
S	3.434838	1.857133	-0.842267
S	0.238079	3.257572	-0.758664
S	-0.253230	1.703963	2.642550
S	3.025519	0.541084	2.408855
S	1.938199	-2.398017	1.063117
S	-1.233130	-1.725149	1.418314
Rh	-2.494420	-0.466500	-0.110411
C	-3.687291	1.026843	0.417608
O	-4.801075	1.280613	0.665838
O	-2.631481	2.389317	0.507025
H	0.612847	2.792381	2.630825
H	1.043621	4.051489	0.065453

CO+O+2H: -3890.564055a.u.

Mo	2.048508	-0.985370	-0.246405
Mo	1.638202	1.398309	0.578477
Mo	0.469834	-0.696900	1.770837
Mo	-0.568793	-1.567919	-0.611210
Mo	0.642416	0.593915	-1.716369
Mo	-1.063040	0.929657	0.369103
S	-1.733808	-0.103081	-2.156477
S	1.142279	-1.755954	-2.385061
S	3.053279	1.021627	-1.344924
S	0.210233	3.058610	-1.271570
S	-0.220772	1.555249	2.613292
S	2.856256	-0.147228	1.971294
S	1.022400	-2.933520	0.776518
S	-1.847266	-1.588798	1.441465
Rh	-3.233839	-0.540717	-0.251909
C	-3.182433	1.352602	0.662685
O	-4.224762	1.816914	0.907134
O	-1.058845	2.986844	-0.286567
H	0.899082	2.379834	2.451071
H	1.246171	3.485201	-0.434542

TS3: -3890.525695a.u.

Mo	1.987645	-1.171587	0.256407
Mo	2.019485	1.632610	-0.142480
Mo	0.282970	0.044213	1.865820
Mo	-0.505352	-1.716260	0.104784
Mo	0.699077	-0.380686	-1.778529
Mo	-1.119236	0.886320	-0.121284
S	-1.734014	-0.932414	-1.928394
S	1.131822	-2.771729	-1.396615
S	3.104502	0.167950	-1.621173
S	0.066000	2.083927	-1.870031
S	-0.783793	2.315828	1.963236
S	2.573216	0.846155	1.961287
S	0.830761	-2.371388	2.058172
S	-2.121182	-0.782953	1.709094
Rh	-3.524312	-0.246067	-0.293180
C	-3.116838	1.738889	-0.282398
O	-3.974750	2.535260	-0.221594
O	2.182212	3.339418	-0.660716
H	0.201218	3.202800	1.682493
H	1.044336	3.179796	-1.503905

CO+OH+H: -3890.598473a.u.

Mo	1.729969	-1.306660	0.355979
Mo	2.162640	1.283642	-0.205963
Mo	0.145282	0.150341	1.855305
Mo	-0.922109	-1.610347	0.078890
Mo	0.609855	-0.359803	-1.759972
Mo	-0.915827	1.127948	-0.180602
S	-1.813354	-0.799993	-2.057388
S	0.713591	-2.832579	-1.278843
S	3.069029	-0.415503	-1.542573
S	0.541591	2.210127	-1.708282
S	-0.396013	2.604639	1.773593
S	2.518271	0.472345	2.016504
S	0.388449	-2.362581	2.072201
S	-2.274629	-0.559907	1.802349
Rh	-3.306247	-0.032419	-0.293462
C	-2.892788	2.018255	-0.426941
O	-3.825222	2.710801	-0.541165
O	3.689974	2.408972	-0.468147
H	0.755837	3.260866	1.467801
H	4.501013	2.090438	-0.899587

TS4: -3890.511442a.u.

Mo	1.742191	-1.352324	0.107021
Mo	2.092504	1.278146	0.128883
Mo	0.066163	-0.315595	1.877881
Mo	-0.909782	-1.535818	-0.303563
Mo	0.722263	0.017867	-1.764222
Mo	-0.957829	1.229034	-0.015694
S	-1.672209	-0.261345	-2.267620
S	0.791142	-2.475056	-1.844069
S	3.167166	-0.045106	-1.492938
S	0.541002	2.564550	-1.276861
S	-0.657253	1.920698	2.174832
S	2.387107	0.095756	2.199734
S	0.368630	-2.764578	1.525761
S	-2.336831	-1.161672	1.601159
Rh	-3.174076	0.016361	-0.268099
C	-2.915133	2.110645	-0.109521
O	-3.925436	2.689151	-0.195610
O	3.612841	2.660800	0.291575
H	2.141881	2.890199	1.047624
H	3.531610	3.443076	-0.286563

$CO+H_2O$: -3890.619343a.u.

Mo	-1.906497	-1.193555	0.190565
Mo	-1.535804	1.311228	-0.364416
Mo	-0.346873	-0.573956	-1.788301
Mo	0.756299	-1.597795	0.415810
Mo	-0.607979	0.275703	1.832828
Mo	1.114228	1.225513	-0.019388
S	1.952565	-0.149519	2.046378
S	-0.860993	-2.164012	2.210601
S	-3.000389	0.596356	1.484957
S	-0.222024	2.663620	1.346320
S	0.320583	1.725900	-2.218958
S	-2.737900	-0.212883	-1.921032
S	-0.798661	-2.945079	-1.075196
S	1.966566	-1.585343	-1.678081
Rh	3.173152	-0.418992	-0.073676
C	2.691253	2.603788	-0.094373
O	3.566850	3.341665	-0.139090
O	-2.762604	3.174923	-0.942690
H	-2.312580	3.695333	-1.630417
H	-2.858349	3.759422	-0.171592

Mechanism B:

CO_2+H_2: -3890.605895a.u.

Mo	2.148030	-0.891623	-0.270225
Mo	1.537209	1.456402	0.654110
Mo	0.493225	-0.728676	1.746306
Mo	-0.446238	-1.490136	-0.652581
Mo	0.748807	0.705390	-1.712635
Mo	-1.019202	1.169521	0.198004
S	-1.735949	-0.008809	-2.117089
S	1.264842	-1.620800	-2.443698
S	3.088021	1.165847	-1.240134
S	0.143877	2.930300	-0.850930
S	-0.417431	1.364876	2.481259
S	2.826646	-0.207307	2.006264
S	1.170919	-2.904469	0.692735
S	-1.747094	-1.870907	1.341253
Rh	-3.070708	-0.636928	-0.176232
C	-3.749831	1.210984	0.334512
O	-4.913076	0.859403	0.323873
O	-2.998992	2.182651	0.487022
H	2.754089	2.861660	1.746078
H	2.325106	3.341206	1.330452

TS1: -3890.554085a.u.

Mo	2.148784	-0.941687	-0.178181
Mo	1.599885	1.529322	0.427357
Mo	0.571972	-0.473401	1.818349
Mo	-0.479942	-1.552013	-0.444303
Mo	0.720455	0.443934	-1.792666
Mo	-1.012415	1.098094	0.153231
S	-1.749674	-0.304718	-2.110685
S	1.212288	-1.953926	-2.209794
S	3.073188	0.999424	-1.430583
S	0.025115	2.806376	-1.239385
S	-0.247588	1.747099	2.273760
S	2.917792	0.142867	1.948402
S	1.138732	-2.780003	1.058354
S	-1.750718	-1.538686	1.611121
Rh	-3.111668	-0.649226	-0.117589
C	-3.749265	1.235025	0.256235
O	-4.930736	0.954345	0.247945
O	-2.951161	2.177897	0.373238
H	1.644242	3.116049	1.295967
H	0.978349	3.357638	-0.249362

CO_2+2H: -3890.585098a.u.

Mo	2.132999	-0.968211	-0.034665
Mo	1.666176	1.539074	0.101197
Mo	0.593296	-0.108060	1.849187
Mo	-0.499534	-1.623796	-0.106142
Mo	0.649471	0.103482	-1.849883
Mo	-0.956369	1.067665	0.027462
S	-1.737576	-0.729892	-2.001514
S	1.162466	-2.339952	-1.809280
S	3.041633	0.676454	-1.680988
S	-0.063281	2.509741	-1.785255
S	-0.125256	2.282875	2.029265
S	2.987950	0.479099	1.816744
S	1.137038	-2.529362	1.549969
S	-1.754122	-1.018841	1.885328
Rh	-3.164622	-0.658348	-0.030426
C	-3.713766	1.263366	0.056461
O	-4.914736	1.070947	0.057199
O	-2.870865	2.181089	0.083473
H	0.968761	3.070039	1.683961
H	1.011339	3.250776	-1.307799

TS2: -3890.497413a.u.

Mo	2.203121	-0.620216	-0.303541
Mo	1.322083	1.480784	0.904322
Mo	0.457278	-1.017705	1.583991
Mo	-0.253095	-1.562325	-0.891981
Mo	0.693495	1.011414	-1.610756
Mo	-1.117271	0.892086	0.146805
S	-1.889403	-0.176565	-2.025501
S	1.456672	-1.091346	-2.622840
S	2.911368	1.693210	-0.912411
S	-0.152919	3.177569	-0.318531
S	-0.778868	0.955147	2.645414
S	2.690621	-0.168374	2.100088
S	1.580780	-2.861220	0.298799
S	-1.477669	-2.543736	0.902568
Rh	-2.918730	-0.888199	0.017325
C	-3.065736	1.820314	0.104155
O	-4.002333	0.959571	-0.039751
O	-3.117905	3.056345	0.294228
H	-1.614131	3.340334	0.050875
H	0.028313	2.094926	2.616088

HOCO+H: -3890.557025a.u.

Mo	2.271428	-0.460936	-0.004988
Mo	1.023593	1.460233	1.124210
Mo	0.098232	-1.161129	1.416423
Mo	0.121252	-1.412411	-1.199470
Mo	0.897169	1.222766	-1.430557
Mo	-1.239931	0.954589	-0.037985
S	-1.485185	0.026706	-2.279955
S	2.066584	-0.733977	-2.464121
S	2.948991	1.890075	-0.275849
S	-0.230452	3.132911	-0.191046
S	-1.271586	0.667569	2.545922
S	2.143388	-0.289102	2.474709
S	1.749399	-2.769662	0.248676
S	-1.202253	-2.860525	0.297410
Rh	-2.693711	-1.139865	-0.033015
C	-3.323826	1.574063	-0.078566
O	-4.056860	0.560751	-0.047739
O	-3.931050	2.757835	-0.108516
H	-3.237087	3.441230	-0.135147
H	-0.415052	1.504987	3.209702

TS3: -3890.515007a.u.

Mo	2.276125	-0.485120	-0.206573
Mo	1.142929	1.683642	0.732132
Mo	0.541308	-0.857755	1.623411
Mo	-0.113114	-1.655114	-0.728835
Mo	0.614035	0.795985	-1.665231
Mo	-1.402298	1.025316	0.139480
S	-1.675534	-0.203070	-2.103594
S	1.633694	-1.310921	-2.449437
S	2.796599	1.766678	-1.041417
S	-0.277562	2.904727	-0.930412
S	-0.970055	0.710789	2.683401
S	2.600096	0.343460	2.161153
S	1.772249	-2.736705	0.569004
S	-1.345653	-2.459608	1.199159
Rh	-2.761895	-1.290025	-0.210876
C	-3.447915	1.623718	-0.039017
O	-4.546947	1.943319	-0.119137
O	-2.159950	2.720926	1.270831
H	-2.059155	3.537405	0.752200
H	-0.331635	1.919739	2.787890

CO+OH+H: -3890.598473a.u.

Mo	1.729969	-1.306660	0.355979
Mo	2.162640	1.283642	-0.205963
Mo	0.145282	0.150341	1.855305
Mo	-0.922109	-1.610347	0.078890
Mo	0.609855	-0.359803	-1.759972
Mo	-0.915827	1.127948	-0.180602
S	-1.813354	-0.799993	-2.057388
S	0.713591	-2.832579	-1.278843
S	3.069029	-0.415503	-1.542573
S	0.541591	2.210127	-1.708282
S	-0.396013	2.604639	1.773593
S	2.518271	0.472345	2.016504
S	0.388449	-2.362581	2.072201
S	-2.274629	-0.559907	1.802349
Rh	-3.306247	-0.032419	-0.293462
C	-2.892788	2.018255	-0.426941
O	-3.825222	2.710801	-0.541165
O	3.689974	2.408972	-0.468147
H	0.755837	3.260866	1.467801
H	4.501013	2.090438	-0.899587

TS4：-3890.511442a.u.

Mo	1.742191	-1.352324	0.107021
Mo	2.092504	1.278146	0.128883
Mo	0.066163	-0.315595	1.877881
Mo	-0.909782	-1.535818	-0.303563
Mo	0.722263	0.017867	-1.764222
Mo	-0.957829	1.229034	-0.015694
S	-1.672209	-0.261345	-2.267620
S	0.791142	-2.475056	-1.844069
S	3.167166	-0.045106	-1.492938
S	0.541002	2.564550	-1.276861
S	-0.657253	1.920698	2.174832
S	2.387107	0.095756	2.199734
S	0.368630	-2.764578	1.525761
S	-2.336831	-1.161672	1.601159
Rh	-3.174076	0.016361	-0.268099
C	-2.915133	2.110645	-0.109521
O	-3.925436	2.689151	-0.195610
O	3.612841	2.660800	0.291575
H	2.141881	2.890199	1.047624
H	3.531610	3.443076	-0.286563

$CO+H_2O$: -3890.619343a.u.

Mo	-1.906497	-1.193555	0.190565
Mo	-1.535804	1.311228	-0.364416
Mo	-0.346873	-0.573956	-1.788301
Mo	0.756299	-1.597795	0.415810
Mo	-0.607979	0.275703	1.832828
Mo	1.114228	1.225513	-0.019388
S	1.952565	-0.149519	2.046378
S	-0.860993	-2.164012	2.210601
S	-3.000389	0.596356	1.484957
S	-0.222024	2.663620	1.346320
S	0.320583	1.725900	-2.218958
S	-2.737900	-0.212883	-1.921032
S	-0.798661	-2.945079	-1.075196
S	1.966566	-1.585343	-1.678081
Rh	3.173152	-0.418992	-0.073676
C	2.691253	2.603788	-0.094373
O	3.566850	3.341665	-0.139090
O	-2.762604	3.174923	-0.942690
H	-2.312580	3.695333	-1.630417
H	-2.858349	3.759422	-0.171592

Mechansim C and D:

CO_2+H_2: -3890.605895a.u.

Mo	2.148030	-0.891623	-0.270225
Mo	1.537209	1.456402	0.654110
Mo	0.493225	-0.728676	1.746306
Mo	-0.446238	-1.490136	-0.652581
Mo	0.748807	0.705390	-1.712635
Mo	-1.019202	1.169521	0.198004
S	-1.735949	-0.008809	-2.117089
S	1.264842	-1.620800	-2.443698
S	3.088021	1.165847	-1.240134
S	0.143877	2.930300	-0.850930
S	-0.417431	1.364876	2.481259
S	2.826646	-0.207307	2.006264
S	1.170919	-2.904469	0.692735
S	-1.747094	-1.870907	1.341253
Rh	-3.070708	-0.636928	-0.176232
C	-3.749831	1.210984	0.334512
O	-4.913076	0.859403	0.323873
O	-2.998992	2.182651	0.487022
H	2.754089	2.861660	1.746078
H	2.325106	3.341206	1.330452

TS1: -3890.554085a.u.

Mo	2.148784	-0.941687	-0.178181
Mo	1.599885	1.529322	0.427357
Mo	0.571972	-0.473401	1.818349
Mo	-0.479942	-1.552013	-0.444303
Mo	0.720455	0.443934	-1.792666
Mo	-1.012415	1.098094	0.153231
S	-1.749674	-0.304718	-2.110685
S	1.212288	-1.953926	-2.209794
S	3.073188	0.999424	-1.430583
S	0.025115	2.806376	-1.239385
S	-0.247588	1.747099	2.273760
S	2.917792	0.142867	1.948402
S	1.138732	-2.780003	1.058354
S	-1.750718	-1.538686	1.611121
Rh	-3.111668	-0.649226	-0.117589
C	-3.749265	1.235025	0.256235
O	-4.930736	0.954345	0.247945
O	-2.951161	2.177897	0.373238
H	1.644242	3.116049	1.295967
H	0.978349	3.357638	-0.249362

CO_2+2H: -3890.585098a.u.

Mo	2.132999	-0.968211	-0.034665
Mo	1.666176	1.539074	0.101197
Mo	0.593296	-0.108060	1.849187
Mo	-0.499534	-1.623796	-0.106142
Mo	0.649471	0.103482	-1.849883
Mo	-0.956369	1.067665	0.027462
S	-1.737576	-0.729892	-2.001514
S	1.162466	-2.339952	-1.809280
S	3.041633	0.676454	-1.680988
S	-0.063281	2.509741	-1.785255
S	-0.125256	2.282875	2.029265
S	2.987950	0.479099	1.816744
S	1.137038	-2.529362	1.549969
S	-1.754122	-1.018841	1.885328
Rh	-3.164622	-0.658348	-0.030426
C	-3.713766	1.263366	0.056461
O	-4.914736	1.070947	0.057199
O	-2.870865	2.181089	0.083473
H	0.968761	3.070039	1.683961
H	1.011339	3.250776	-1.307799

TS2: -3890.511225a.u.

Mo	2.174652	-0.769270	0.413631
Mo	1.502097	1.293288	-1.007070
Mo	0.791126	1.125572	1.478772
Mo	-0.397059	-1.264831	0.996430
Mo	0.492909	-1.101582	-1.541960
Mo	-1.033268	1.128808	-0.396783
S	-1.901958	-1.471667	-0.535261
S	1.197613	-2.967010	-0.024742
S	2.791954	-0.599657	-1.990332
S	-0.556708	0.704615	-2.685991
S	0.175337	3.096926	0.130594
S	3.115899	1.465935	0.830176
S	1.343447	-0.957194	2.717271
S	-1.706452	0.474781	2.075634
Rh	-2.988650	-0.628238	0.241996
C	-3.739317	1.147828	-0.438897
O	-4.867847	0.824291	-0.140575
O	-3.022741	2.068278	-0.846659
H	-3.037889	-1.091874	-1.6136971

HCOO+H: -3890.542089a.u.

Mo	1.330919	1.540222	-0.803557
Mo	2.237884	-0.555102	0.394145
Mo	0.630634	-0.910970	-1.643849
Mo	-1.196496	1.038603	-0.432848
Mo	0.520858	0.963706	1.600561
Mo	-0.176820	-1.546830	0.790470
S	-1.781210	-0.246601	2.057857
S	-0.261911	3.006874	0.493282
S	2.800244	1.716584	1.155037
S	1.406011	-1.108643	2.650027
S	1.683012	-2.797157	-0.334560
S	2.868474	-0.034263	-1.952411
S	-0.500351	0.962891	-2.671783
S	-1.397611	-2.396531	-1.053292
Rh	-2.835166	-0.891274	0.037953
C	-4.191426	1.606725	-0.168975
O	-4.387320	0.444328	0.306870
O	-3.091542	2.095916	-0.552054
H	-5.077747	2.250193	-0.245884
H	-1.634539	-0.058658	-2.769003

TS3: -3890.577017a.u.

Mo	-1.419292	1.189666	-1.211249
Mo	-2.229279	-0.486532	0.588318
Mo	-0.636243	1.407993	1.245293
Mo	1.116302	0.869360	-0.635065
Mo	-0.659737	-1.343274	-1.321668
Mo	0.325646	-1.175002	1.162101
S	1.668748	-1.993779	-0.348464
S	0.517456	0.174325	-2.791787
S	-2.935162	-0.723341	-1.776023
S	-1.527001	-2.797270	0.548260
S	-1.278181	-0.380937	2.863364
S	-2.938268	1.865686	0.596662
S	0.125379	3.027625	-0.451271
S	1.759382	0.812344	2.021483
Rh	2.845493	-0.918877	0.048354
C	4.425151	1.516236	-0.314427
O	4.597846	0.281945	-0.218505
O	3.315622	2.134408	-0.090648
H	5.279523	2.142103	-0.603216
H	2.657755	1.550679	0.956992

HCOOH: -3890.607888a.u.

Mo	1.500283	0.213939	1.670170
Mo	2.154652	0.590211	-0.804667
Mo	0.063278	1.837877	0.149442
Mo	-0.860827	-0.743201	1.082127
Mo	1.280017	-1.711995	-0.062873
Mo	-0.298608	-0.126759	-1.636417
S	-1.077249	-2.373123	-0.963812
S	0.632967	-2.092344	2.306576
S	3.454118	-0.886076	0.673607
S	1.794732	-1.206820	-2.437190
S	0.849120	2.048965	-2.231613
S	2.293219	2.431046	0.841647
S	-0.901825	1.281594	2.301759
S	-2.063810	1.453284	-1.225925
Rh	-2.808405	-0.685350	-0.555317
C	-5.154332	0.659791	0.953168
O	-4.750636	-0.333316	0.349652
O	-4.484563	1.765275	1.171750
H	-3.582354	1.704017	0.774150
H	-6.161594	0.694903	1.377187

TS4: -3890.563755a.u.

Mo	1.554592	1.609089	-0.093098
Mo	2.176680	-0.865656	0.247630
Mo	0.770807	-0.233034	-1.839679
Mo	-1.031379	1.246623	-0.237464
Mo	0.470515	0.211589	1.869395
Mo	-0.352338	-1.640020	0.145945
S	-1.861134	-0.788100	1.871041
S	-0.193610	2.551440	1.527866
S	2.821528	0.895523	1.874978
S	1.155607	-2.162346	2.058309
S	1.431639	-2.579012	-1.339848
S	3.091673	0.469480	-1.642565
S	0.051997	2.072320	-2.164406
S	-1.505692	-1.317598	-1.980713
Rh	-2.966505	-0.678738	-0.223378
C	-4.358978	0.684316	0.324466
O	-5.342550	0.275353	0.817732
O	-2.713172	2.393208	-0.570846
H	-2.685411	3.298322	-0.918379
H	-3.827183	1.722411	-0.120725

$CO+H_2O$ (Mechanism C): -3890.617047a.u.

Mo	-1.420849	-0.659463	-1.498297
Mo	-2.098623	0.244297	0.821841
Mo	-0.499259	1.686665	-0.665942
Mo	1.163786	-0.693012	-0.922910
Mo	-0.626102	-1.843630	0.657980
Mo	0.478610	0.497868	1.557395
S	1.823548	-1.564914	1.484204
S	0.056024	-2.703905	-1.555741
S	-2.954543	-1.910130	-0.038765
S	-1.193022	-0.820271	2.849696
S	-1.220172	2.352597	1.658742
S	-2.824917	1.382693	-1.246087
S	0.540297	0.769608	-2.672996
S	2.024608	1.868923	0.537586
Rh	3.084951	0.365191	0.545645
C	3.170700	-1.190098	-1.404566
O	4.249734	-1.457575	-1.663527
O	-0.203558	3.810855	-1.604279
H	-0.455675	3.830517	-2.538602
H	0.764760	3.967971	-1.580739

TS5: -3890.486746 a.u.

Mo	1.251715	1.565396	0.695870
Mo	2.201422	-0.699162	-0.154975
Mo	0.722892	0.712432	-1.695276
Mo	-1.243126	1.114452	0.069209
Mo	0.373387	-0.795455	1.705477
Mo	-0.224760	-1.651291	-0.707318
S	-1.529286	-2.392939	1.143255
S	-0.751937	1.176047	2.413020
S	2.588727	0.082219	2.172278
S	1.519837	-2.836064	0.718262
S	1.545094	-1.500586	-2.415808
S	2.957805	1.449062	-1.080568
S	-0.093489	2.905820	-1.025212
S	-1.803536	-0.382958	-2.068583
Rh	-2.906711	-0.899310	-0.027735
C	-3.353413	1.693920	0.055221
O	-4.121862	0.772310	-0.304398
O	-1.415041	3.818895	1.063111
H	-3.840654	2.642886	0.346837
H	-1.297345	4.575693	0.448463

CHO+OH: -3890.553906a.u.

Mo	-1.498882	1.630411	-0.398929
Mo	-1.973115	-1.219156	0.117937
Mo	-0.674800	0.215252	1.764019
Mo	1.118130	1.234263	0.066218
Mo	-0.360030	-0.504067	-1.747175
Mo	0.655361	-1.649726	0.387325
S	1.906506	-1.549543	-1.682390
S	0.488704	1.706318	-2.171049
S	-2.750124	-0.015552	-1.865411
S	-0.906716	-2.946474	-1.160231
S	-1.040929	-2.222580	2.138480
S	-3.042178	0.653210	1.330093
S	-0.204564	2.605473	1.516291
S	1.852270	-0.331666	2.061725
Rh	3.109643	-0.358198	-0.076161
C	2.955654	2.374031	0.109839
O	3.967455	1.657838	-0.004120
O	-2.042997	3.378793	-0.964598
H	3.145110	3.464568	0.162391
H	-2.256029	4.037064	-0.279185

TS6: -3890.532641a.u.

Mo	2.011601	-1.105402	0.242010
Mo	1.622748	1.491366	-0.032841
Mo	0.117388	-0.082581	1.901271
Mo	-0.475038	-1.696946	-0.111491
Mo	0.721949	-0.123669	-1.758817
Mo	-1.193717	1.129271	-0.077688
S	-1.676343	-0.743470	-2.090771
S	1.263660	-2.556854	-1.595129
S	3.149752	0.174611	-1.537944
S	0.214001	2.348345	-1.560905
S	-0.995631	1.956791	2.096368
S	2.516559	0.602789	2.173934
S	0.777743	-2.479055	1.900576
S	-2.209710	-1.190127	1.491463
Rh	-3.381152	-0.278985	-0.397194
C	-3.353204	1.699565	-0.133130
O	-4.292250	2.399265	-0.029803
O	2.974558	2.836086	-0.136556
H	-2.038505	2.626123	-0.230441
H	3.781824	2.760911	-0.672274

CO+OH+H: -3890.598473a.u.

Mo	1.729969	-1.306660	0.355979
Mo	2.162640	1.283642	-0.205963
Mo	0.145282	0.150341	1.855305
Mo	-0.922109	-1.610347	0.078890
Mo	0.609855	-0.359803	-1.759972
Mo	-0.915827	1.127948	-0.180602
S	-1.813354	-0.799993	-2.057388
S	0.713591	-2.832579	-1.278843
S	3.069029	-0.415503	-1.542573
S	0.541591	2.210127	-1.708282
S	-0.396013	2.604639	1.773593
S	2.518271	0.472345	2.016504
S	0.388449	-2.362581	2.072201
S	-2.274629	-0.559907	1.802349
Rh	-3.306247	-0.032419	-0.293462
C	-2.892788	2.018255	-0.426941
O	-3.825222	2.710801	-0.541165
O	3.689974	2.408972	-0.468147
H	0.755837	3.260866	1.467801
H	4.501013	2.090438	-0.899587

TS7: -3890.511442a.u.

Mo	1.742191	-1.352324	0.107021
Mo	2.092504	1.278146	0.128883
Mo	0.066163	-0.315595	1.877881
Mo	-0.909782	-1.535818	-0.303563
Mo	0.722263	0.017867	-1.764222
Mo	-0.957829	1.229034	-0.015694
S	-1.672209	-0.261345	-2.267620
S	0.791142	-2.475056	-1.844069
S	3.167166	-0.045106	-1.492938
S	0.541002	2.564550	-1.276861
S	-0.657253	1.920698	2.174832
S	2.387107	0.095756	2.199734
S	0.368630	-2.764578	1.525761
S	-2.336831	-1.161672	1.601159
Rh	-3.174076	0.016361	-0.268099
C	-2.915133	2.110645	-0.109521
O	-3.925436	2.689151	-0.195610
O	3.612841	2.660800	0.291575
H	2.141881	2.890199	1.047624
H	3.531610	3.443076	-0.286563

$CO+H_2O$: -3890.619343a.u.

Mo	-1.906497	-1.193555	0.190565
Mo	-1.535804	1.311228	-0.364416
Mo	-0.346873	-0.573956	-1.788301
Mo	0.756299	-1.597795	0.415810
Mo	-0.607979	0.275703	1.832828
Mo	1.114228	1.225513	-0.019388
S	1.952565	-0.149519	2.046378
S	-0.860993	-2.164012	2.210601
S	-3.000389	0.596356	1.484957
S	-0.222024	2.663620	1.346320
S	0.320583	1.725900	-2.218958
S	-2.737900	-0.212883	-1.921032
S	-0.798661	-2.945079	-1.075196
S	1.966566	-1.585343	-1.678081
Rh	3.173152	-0.418992	-0.073676
C	2.691253	2.603788	-0.094373
O	3.566850	3.341665	-0.139090
O	-2.762604	3.174923	-0.942690
H	-2.312580	3.695333	-1.630417
H	-2.858349	3.759422	-0.171592