

Methylrhenium Trioxide Revisited: Mechanisms for Non-redox Oxygen Insertion in a M-CH₃ Bond

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Supplementary Information

We include the final enthalpies (in Hartrees) and Cartesian coordinates (in Angstroms) for all species discussed in the manuscript. Entries in the left column correspond to gas-phase optimized structures corrected for the effects of diffuse functions (see Equation 1 in the main article), while the right column consists of species fully optimized in THF with corrections for effect of diffuse functions.

Reactants and Products

MTO (GP)

Enthalpy: -344.786670

Re	.0224237496	-.0388390503	.9841259194
O	-.0419935106	.0728596252	-.7227035751
O	-.8679444675	-1.3582076769	1.6137131725
O	1.6101354153	.0729264270	1.6139016154
C	-.9612104870	1.6644750135	1.6797266787
H	-.4341193098	2.5442320420	1.3067218281
H	-.9511390158	1.6477522949	2.7708424836
H	-1.9867859933	1.6475865064	1.3071985218

H₂O₂ (GP)

Enthalpy: -151.584473

H	-1.1006690384	-0.5206373830	-0.0954511095
O	-0.6943094409	0.2157955346	0.3796238949
O	0.6939263941	-0.2157303974	0.3790608434
H	1.1000177098	0.5213968575	-0.0951401514

H₂O (GP)

Enthalpy: -76.445475

H	0.0014695806	0.0000000000	0.0028929797
O	0.0000619653	0.0000000000	0.9648918569
H	0.9339733346	0.0000000000	1.1956587480

OH⁻ (GP)

Enthalpy: -75.961648

O	.7304213406	-.2277112506	.3810797385
H	1.0987377304	.5282618291	-.1186899415

OOH⁻ (GP)

Enthalpy: -151.109231

O	-.7315372201	.2277500128	.3799373805
O	.7316492713	-.2275499445	.3807685439
H	1.0868993184	.5167295626	-.1099588120

ReO₄⁻ (GP)

Enthalpy: -380.343554

Re	-.3320218271	.3615191069	.0079380508
O	-.9134910072	-.4608848362	-1.4167794454
O	1.4127937530	.3613440330	.0079263582
O	-.9136708098	2.0065236668	.0079010531
O	-.9134905534	-.4609283318	1.4326568354

HReO₄

Enthalpy: -380.751626

Re	-.2944155843	.2615839237	.0055241737
O	-.1050947641	-.2898313287	-1.6027710459
O	1.2177857997	.1356721598	.7952885091
O	-.9087595732	2.0374169861	.0271566205
O	-1.4577249066	-.6922991733	.8173538722
H	-.4085726839	2.7580609196	-.3761760194

MTO (SP)

Enthalpy: -344.788460

Re	.0320030207	-.0469834454	.9842080292
O	-.0899330794	.1499320024	-.7159232472
O	-.9162313524	-1.3077976037	1.6599246919
O	1.6001961096	.1475227599	1.6529302402
C	-.9488562180	1.6508734692	1.6766086888
H	-.4103870187	2.5247763427	1.3033580120
H	-.9426989135	1.6222438824	2.7683470514
H	-1.9696956262	1.6283800058	1.2889500843

H₂O₂ (SP)

Enthalpy: -151.584971

H	-1.0881883071	-0.4973767710	-0.5294262598
O	-0.6999609109	0.1897190677	0.0333586674
O	0.6999609109	-0.1897190677	0.0333586674
H	1.0881883071	0.4973767710	-0.5294262598

H₂O (SP)

Enthalpy: -76.445555

H	0.0000000000	0.7573867586	0.5297923251
O	0.0000000000	0.0000000000	-0.0667634657
H	0.0000000000	-0.7573867586	0.5297923251

OH⁻ (SP)

Enthalpy: -75.961315

O	0.0000000000	0.0000000000	-0.0571353615
H	0.0000000000	0.0000000000	0.9067796488

OOH⁻ (SP)

Enthalpy: -151.109214

O	-0.0413861541	0.7796284599	0.0000000000
O	-0.0170941569	-0.7233345243	0.0000000000
H	0.9281249736	-0.8934256111	0.0000000000

ReO₄⁻ (SP)

Enthalpy: -380.344069

Re	-.0003060375	-.0000430827	-.0000061341
O	.8210959002	.5798837918	1.4210698750
O	.0024701037	-1.7412723897	-.0000247045
O	-1.6411745197	.5820780178	.0000840435
O	.8211856195	.5798141496	-1.4210575162

HReO₄ (SP)

Enthalpy: -380.751171

Re	-.2965428275	.2700754516	.0028299553
O	-.1401014167	-.4375885294	-1.5505416510
O	1.2111264587	.1659342754	.8047114842
O	-.9591446878	2.0040371211	-1.561954946
O	-1.4546935205	-.6440592230	.8724770144
H	-.4055607996	2.7971386290	-.0632895069

CH₃OH (GP)

Enthalpy: -115.717910

C	.1608002116	.5020546667	.2679392343
H	.5338270391	-.5229418018	.2853226783
H	.5199524880	.9787516720	-.6544570251
H	-.9367540731	.4637532846	.2376248052
O	.6520232885	1.1399307878	1.4384592653
H	.3308996303	2.0459057202	1.4367395940

CH₃OH (SP)

Enthalpy: -115.718070

C	.1609589010	.4978910071	.2655736295
H	.5332281232	-.5282833377	.2808287967
H	.5207735395	.9785804659	-.6521237371
H	-.9348756865	.4637106329	.2392116165
O	.6517546770	1.1430021514	1.4400679204
H	.3311726811	2.0522923268	1.4399497027

Reaction I**1 (GP)**

Enthalpy: -496.333586

Re	.0512378444	.0033223610	.9783361944
O	.6086619890	.3990207227	-.5816343558
O	-.4894075318	-1.7348114311	.8930372081
O	1.3189493830	.1622767195	2.0998261735
C	-.9715103878	1.8394389945	1.2769681840
H	-.2523300261	2.6219857980	1.0307763361
H	-1.2967121317	1.9007837013	2.3128734928
H	-1.8241976237	1.8748504008	.5981370100
O	-1.9160160248	-.5239039576	2.0365036936
O	-2.0923643107	-.2141877694	3.4276131226
H	-3.0273809914	.0357995999	3.4340088218
H	-1.4160021369	-1.5474849319	1.6878593205

1 (SP)

Enthalpy: -496.333668

Re	.0512378444	.0033223610	.9783361944
O	.6086619890	.3990207227	-.5816343558
O	-.4894075318	-1.7348114311	.8930372081
O	1.3189493830	.1622767195	2.0998261735
C	-.9715103878	1.8394389945	1.2769681840
H	-.2523300261	2.6219857980	1.0307763361
H	-1.2967121317	1.9007837013	2.3128734928
H	-1.8241976237	1.8748504008	.5981370100
O	-1.9160160248	-.5239039576	2.0365036936
O	-2.0923643107	-.2141877694	3.4276131226
H	-3.0273809914	.0357995999	3.4340088218
H	-1.4160021369	-1.5474849319	1.6878593205

2 (GP)

Enthalpy: -496.355315

Re	.0584528757	-.0095141158	.9910293586
O	-.0452272157	.3174384369	-.6772500031
O	.1611553292	-1.9109257322	1.0813440898
O	1.5263790780	.5489645872	1.6489830520
C	-.9415701148	1.8288224215	1.4718767532
H	-.3365424241	2.5679252853	.9454357993
H	-.9295023339	1.9811755266	2.5456058318
H	-1.9586080531	1.7991017096	1.0935513281
O	-1.4512434458	-.6994046739	2.1630487432
O	-2.3894360802	.1175509320	2.8676954574
H	-3.2198310807	-.2305609288	2.5127458081
H	-.5028636071	-2.3259895078	1.6556418911

2 (SP)

Enthalpy: -496.355839

Re	.0584528757	-.0095141158	.9910293586
O	-.0452272157	.3174384369	-.6772500031
O	.1611553292	-1.9109257322	1.0813440898
O	1.5263790780	.5489645872	1.6489830520
C	-.9415701148	1.8288224215	1.4718767532
H	-.3365424241	2.5679252853	.9454357993
H	-.9295023339	1.9811755266	2.5456058318
H	-1.9586080531	1.7991017096	1.0935513281
O	-1.4512434458	-.6994046739	2.1630487432
O	-2.3894360802	.1175509320	2.8676954574
H	-3.2198310807	-.2305609288	2.5127458081
H	-.5028636071	-2.3259895078	1.6556418911

3 (GP)

Enthalpy: -496.338469

Re	-.0018336741	.0034269616	-.0024114178
O	.0041423374	-.0080967675	2.1579026409
H	1.2005889184	-.0096758381	1.9587712929
O	1.9440615461	-.1262693717	.9994845468
O	.5967037847	.9510660452	-1.2750342043
O	-1.6646398382	.4042955722	.1472684546
C	-.5799943972	-1.7116713540	-1.1340741389
H	-1.3662362791	-1.4124407407	-1.8216806439
H	-.9523497315	-2.4161335372	-.3893527515
H	.3062888369	-2.0931251358	-1.6320629332
O	1.3798864506	-1.3412105020	.4809102692
H	-.4185472597	.7333132405	2.6039804549

3 (SP)

Enthalpy: -496.339468

Re	-.0018336741	.0034269616	-.0024114178
O	.0041423374	-.0080967675	2.1579026409
H	1.2005889184	-.0096758381	1.9587712929
O	1.9440615461	-.1262693717	.9994845468
O	.5967037847	.9510660452	-1.2750342043
O	-1.6646398382	.4042955722	.1472684546
C	-.5799943972	-1.7116713540	-1.1340741389
H	-1.3662362791	-1.4124407407	-1.8216806439
H	-.9523497315	-2.4161335372	-.3893527515
H	.3062888369	-2.0931251358	-1.6320629332
O	1.3798864506	-1.3412105020	.4809102692
H	-.4185472597	.7333132405	2.6039804549

A (GP)

Enthalpy: -419.925250

Re	-.0624554772	.3549456675	.9166435941
O	-.1498559675	.3381883569	-.7835105219
O	-1.2593436355	1.3222865713	1.6448057252
C	-1.0242591385	-1.5087574225	1.2321293826
H	-.4043921992	-2.2774627523	.7751876626
H	-2.0036626715	-1.4454223316	.7590177166
H	-1.1042039320	-1.6568249526	2.3071069159
O	1.3420401356	-.5767262649	1.9359728682
O	1.6918801508	.7655443003	1.5518211267

A (SP)

Enthalpy: -419.922168

Re	-.0624554772	.3549456675	.9166435941
O	-.1498559675	.3381883569	-.7835105219
O	-1.2593436355	1.3222865713	1.6448057252
C	-1.0242591385	-1.5087574225	1.2321293826
H	-.4043921992	-2.2774627523	.7751876626
H	-2.0036626715	-1.4454223316	.7590177166
H	-1.1042039320	-1.6568249526	2.3071069159
O	1.3420401356	-.5767262649	1.9359728682
O	1.6918801508	.7655443003	1.5518211267

Reaction II**4 (GP)**

Enthalpy: -571.463208

H	.1106434172	.0082002669	.3283425438
O	.0644145197	-.1706174539	1.5834779244
O	.8309596680	.6103479794	2.4935075454
H	1.0517130241	-.0541610538	3.1608420768
Re	-1.9888668005	.4746644898	.8469245786
O	-1.8946554552	1.9068249579	1.7366726062
O	-3.6640768306	-.4904387878	.9803105085
C	-3.1019473590	1.3698490672	-.7456104549
H	-2.4908560556	2.1828655406	-1.1345575734
H	-4.0465336891	1.7326689387	-.3431748766
H	-3.2610899458	.6051281672	-1.5029998730
O	-.7541478063	.1533288673	-.4545078138
O	-2.6643294665	-.9906121000	1.8792638217

4 (SP)

Enthalpy: -571.463695

H	0.1335334449	0.0373398699	0.3264851737
O	0.0629327030	-0.1550689347	1.5849241508
O	0.8090154996	0.5682455758	2.5538444895
H	1.0703052745	-0.1345769769	3.1713361272
Re	-1.9879750841	0.4760506913	0.8408480341
O	-1.8956831177	1.9160681431	1.7182786522
O	-3.6625415496	-0.4902081823	0.9962407233
C	-3.1168313833	1.3481330068	-0.7526428349
H	-2.5080256752	2.1539263629	-1.1615928385
H	-4.0509716012	1.7196069521	-0.3315430352
H	-3.2948595554	0.5697073613	-1.4930373493
O	-0.7416884784	0.1694671394	-0.4517016524
O	-2.6522511389	-0.9814714378	1.8932382102

5 (GP)

Enthalpy: -571.491295

Re	0.1140012207	0.4235650793	1.0273362210
O	0.0642679461	0.2166382926	-0.8653278707
O	-1.3056707106	1.1349234341	1.5831886496
C	-0.8440727424	-1.4980527558	0.6801859433
H	-0.0839576808	-2.1521099486	0.2597819588
H	-1.6452129137	-1.3178235958	-0.0303732978
H	-1.2044185661	-1.8653859626	1.6393717767
O	0.8892887270	-0.7660253495	2.3388906545
O	1.4788352972	0.5314578228	2.4226577957
O	1.2685258237	2.0008726171	0.4647296300
O	1.1157078035	2.5330690915	-0.8528946391
H	2.0435453496	2.6384784976	-1.1104560673
H	0.4152566044	1.0246650932	-1.2998784616

5 (SP)

Enthalpy: -571.490400

Re	0.1403450867	0.4021148106	1.0120648002
O	-0.1268190755	0.3777653919	-0.8676518290
O	-1.2489539923	1.1490354038	1.5954090185
C	-0.7373607534	-1.5418780943	0.6478849782
H	0.0583188130	-2.1601611596	0.2313994935
H	-1.5453784708	-1.4025105709	-0.0650446938
H	-1.0836538814	-1.9376130320	1.6029190160
O	0.7859358987	-0.7209724900	2.4710804657
O	1.4427511242	0.5453309085	2.4726234193
O	1.3733988716	1.9261546353	0.4620923839
O	1.2357183812	2.4982499044	-0.8322950022
H	2.1285912771	2.3980830582	-1.2062237199
H	0.2626737739	1.1875072895	-1.2774134791

6 (GP)

Enthalpy: -571.462739

Re	0.0020895034	0.0018829791	-0.0056264330
O	-0.0038784389	0.0143807269	2.1490521292
H	1.3002527549	-0.0132206747	1.8809294427
O	1.9304463231	0.1162705336	0.9412589606
O	0.6207284673	-0.3291198897	-1.5414088971
C	-0.0995912516	-2.1228622935	0.3945634859
H	-0.8368668429	-2.3163788590	1.1689437114
H	0.8981766489	-2.4439475674	0.6928381772
H	-0.3917142088	-2.6035927276	-0.5366122747
O	-1.9022292428	-0.2111543964	-0.0863822356
O	-1.5102887627	1.1819331078	-0.2076754049
O	1.3133848979	1.3690170532	0.5628990066
H	-0.3823137967	-0.7477166965	2.5955526024

B (GP)

Enthalpy: -495.051528

Re	.0512605175	-.1471250990	-.4323659897
O	1.7097987247	-.3565135757	-.2912355051
O	-.4968664440	1.5364976041	.3759256591
C	-.1158039989	-.5313503343	-2.5266053424
H	.2375151888	-1.5456874674	-2.7046428298
H	.4876718436	.2107331321	-3.0467153584
H	-1.1691416439	-.4313124030	-2.7830867540
O	-.8945279420	-1.8154644224	-.4044282927
O	-.8878085148	-1.1993302889	.9089026501
O	-.4062793097	1.6027964485	-1.0703922024

B:H₂O (GP)

Enthalpy: -571.505466

Re	-.1676995720	-.1430831657	-.4434699749
O	1.4976552974	-.3633417683	-.4556345474
O	-.4897213762	1.5391137556	.5182207136
C	-.5001870650	-.4062472347	-2.5373069589
H	-.1641570902	-1.4077436039	-2.8019457784
H	.0680783752	.3610730942	-3.0609459618
H	-1.5684859027	-.2894730343	-2.6977919006
O	-.9362668639	-1.9169416531	-.3893925298
O	-.8686762655	-1.3468856901	.9412650734
O	-.4604841863	1.7080476882	-.9207377520
O	-2.6131827567	.1736693349	-.4724338219
H	-2.9499993774	-.4784246499	.1564849014
H	-2.7500794703	1.0397902809	-.0665256459

Reaction III**7 (GP)**

Enthalpy: -495.926334

Re	.0289071413	-.0219181511	.9682971995
O	.7707002427	.7075307574	-.4259498098
O	-.3579215731	-1.6545867244	.3910213404
O	1.1933086948	-.0665841522	2.2416343509
C	-.9245685236	1.9492065453	1.2112139743
H	-.1099550545	2.6768823282	1.2089895910
H	-1.4972677275	1.9814041011	2.1341103671
H	-1.5729258390	2.1235509274	.3516928888
O	-1.7966071930	-.2381152991	1.8757016346
O	-2.2365827534	-1.6002871929	2.0972266887
H	-1.7068451808	-2.0536891043	1.4015213289

6 (SP)

Enthalpy: -571.463560

Re	0.0025284415	0.0019608892	-0.0045206376
O	-0.0291302403	0.0273393686	2.1320629136
H	1.2844916832	-0.0071585481	1.9029277096
O	1.9296016442	0.1183694806	0.9636615618
O	0.6515405714	-0.3360676019	-1.5276058450
C	-0.1023807929	-2.1204012038	0.3938939240
H	-0.7736810131	-2.3094651088	1.2271304594
H	0.9180758260	-2.4429581695	0.6041550873
H	-0.4750655679	-2.5792114599	-0.5206487969
O	-1.9024087157	-0.2178335044	-0.1141064847
O	-1.5126880691	1.1804574628	-0.2324053005
O	1.3147005116	1.3675759022	0.5700828520
H	-0.3636201699	-0.7523240773	2.5920137395

B (SP)

Enthalpy: -495.049056

Re	.0444686286	-.1461377116	-.4313940214
O	1.6999556423	-.3567522112	-.2836414556
O	-.4886963002	1.5499821141	.3660840238
C	-.1163734817	-.5299123506	-2.5225029887
H	.2476664844	-1.5426194352	-2.6929847350
H	.4851069784	.2200117162	-3.0351937899
H	-1.1732634254	-.4357736091	-2.7696700429
O	-.8554348158	-1.8435416644	-.4046935062
O	-.8926968765	-1.2120358494	.9034850678
O	-.3592155429	1.6172166648	-1.0792062699

B:H₂O (SP)

Enthalpy: -571.507409

Re	-.1861792197	-.1425083193	-.4478968718
O	1.4811451452	-.3673516482	-.4903235432
O	-.4432632430	1.5556644216	.5050603525
C	-.5013897373	-.4113059181	-2.5481057201
H	-.1491424184	-1.4115719802	-2.7991559972
H	.0757394163	.3584457655	-3.0601409729
H	-1.5672450401	-.3023590147	-2.7290525346
O	-.9338908912	-1.9251921938	-.4015276519
O	-.8298711821	-1.3771867134	.9375611000
O	-.4568364240	1.7087017985	-.9371875364
O	-2.5856472945	.1722689573	-.4447662131
H	-3.0179448398	-.4650901482	.1422257179
H	-2.8237246563	1.0447773969	-.0978721831

7 (SP)

Enthalpy: -495.928600

Re	.0289071413	-.0219181511	.9682971995
O	.7707002427	.7075307574	-.4259498098
O	-.3579215731	-1.6545867244	.3910213404
O	1.1933086948	-.0665841522	2.2416343509
C	-.9245685236	1.9492065453	1.2112139743
H	-.1099550545	2.6768823282	1.2089895910
H	-1.4972677275	1.9814041011	2.1341103671
H	-1.5729258390	2.1235509274	.3516928888
O	-1.7966071930	-.2381152991	1.8757016346
O	-2.2365827534	-1.6002871929	2.0972266887
H	-1.7068451808	-2.0536891043	1.4015213289

8 (GP)

Enthalpy: -495.890622

Re	.0010751338	-.0024075712	.0032718570
O	.0024982225	.0142221748	1.7504583266
O	1.7021893599	-.0250475828	-.3482405055
O	-.7827964038	-1.4944723746	-.3857451829
C	-1.5978762224	1.9284796336	.6334372578
H	-2.2800868857	1.2122793262	1.0847532245
H	-2.0907376962	2.6326732838	-.0253906793
H	-.9205998930	2.3765871059	1.3525753348
O	-.6865750978	1.3180320995	-1.1293435539
O	.0162522000	.4713801861	-2.6176852816
H	.8858289258	.8889754955	-2.5542324362

9 (GP)

Enthalpy: -496.027265

Re	-.0122251623	.4019125677	.8031775231
O	.7803073469	2.2341722472	.5568141222
O	.1024739979	.4291810103	2.5399520420
O	1.3907758412	-.2856898521	.0060457767
O	-1.4537760654	.9830467589	.0299648591
O	-.8531858329	-1.4205077356	.8089197293
C	-.1021694035	-2.5010284698	1.2629529397
H	-.6666793504	-3.4329748369	1.1168092424
H	.8562203296	-2.5745900262	.7201656132
H	.1411330772	-2.4024717885	2.3361701330
H	1.7362337456	2.1627609414	.6379101875

10a (GP)

Enthalpy: -495.990335

Re	.0972692421	-.0257119079	.0084528591
O	.3565930744	.3321951083	1.6646788528
O	1.5647063172	.1035403082	-.8654056135
O	-.5285704793	-1.6171094905	-1.098709467
C	-2.4795543723	1.4833088769	-.3699319803
H	-3.0980913672	.5899213041	-.4837183235
H	-2.8125286192	2.2587151232	-1.0589731417
H	-2.5319357096	1.8480955876	.6585880145
O	-1.1184217304	1.1829544925	-.7133645063

11a (GP)

Enthalpy: -496.448082

Re	.0044883619	.0004034545	-.0080186382
O	.2238260609	-.0021092652	1.6928255784
O	1.5331838065	.0767912567	-.7671724492
O	-.6112048600	-1.5615912400	-.3848273027
C	-2.4173552869	.2071386788	-2.1662280380
H	-2.3842936323	-.8810654546	-2.1157576914
H	-1.9952057622	.5525565294	-3.1121397061
H	-3.4455220317	.5559185065	-2.0591001850
O	-1.6494932533	.7176487907	-1.0706921863
H	-.4808573535	2.5006583207	.8969099655
O	-.3597700165	2.1171840570	.0220312735
H	-1.3461646990	1.7554401354	-.7168897025

8 (SP)

Enthalpy: -495.891415

Re	0.0003678728	-0.0014949469	0.0044113705
O	-0.0047534536	0.0078790807	1.7546002093
O	1.7050608691	-0.0183253703	-0.3296805530
O	-0.7923763289	-1.4955833961	-0.3719089318
C	-1.4910568939	1.9337436910	0.5810595527
H	-2.1713997452	1.2615251945	1.0983289599
H	-1.9939851287	2.6009889017	-0.1067171407
H	-0.7733220012	2.4200124639	1.2326920379
O	-0.6708360339	1.2477138406	-1.2023606782
O	0.0315603568	0.2984146088	-2.6279030771
H	0.8527790768	0.8043770321	-2.6960504119

9 (SP)

Enthalpy: -496.028120

Re	-.0130445516	.4004413470	.8034899651
O	.7482043394	2.2343437612	.5624457214
O	.1294963623	.4325838676	2.5374642571
O	1.3820319530	-.2904587412	.0060436558
O	-1.4577811579	.9883429394	.0336975106
O	-.8577370407	-1.3957715474	.8277778150
C	-.1222360249	-2.5010719524	1.2943284950
H	-.7182806043	-3.4109472829	1.1772656895
H	.8158237867	-2.6054881279	.7292346947
H	.1428512804	-2.3767760685	2.3547159956
H	1.6973493333	2.2623957569	.7356964133

10a (SP)

Enthalpy: -495.991339

Re	0.1041885936	-0.0172394490	0.0173681497
O	0.2556230286	0.2498565751	1.7043270427
O	1.6037359651	0.2772754031	-0.7656815942
O	-0.3511002261	-1.6569364352	-0.2097960582
C	-2.5005249543	1.5682757576	-0.3291083156
H	-3.1772689592	0.7179724238	-0.2273579739
H	-2.8242800549	2.2175700853	-1.1428605367
H	-2.4402148468	2.1294893663	0.6054776309
O	-1.1838870850	1.0930213200	-0.6872584900

11a (SP)

Enthalpy: -496.451637

Re	.0044883619	.0004034545	-.0080186382
O	.2238260609	-.0021092652	1.6928255784
O	1.5331838065	.0767912567	-.7671724492
O	-.6112048600	-1.5615912400	-.3848273027
C	-2.4173552869	.2071386788	-2.1662280380
H	-2.3842936323	-.8810654546	-2.1157576914
H	-1.9952057622	.5525565294	-3.1121397061
H	-3.4455220317	.5559185065	-2.0591001850
O	-1.6494932533	.7176487907	-1.0706921863
H	-.4808573535	2.5006583207	.8969099655
O	-.3597700165	2.1171840570	.0220312735
H	-1.3461646990	1.7554401354	-.7168897025

11b (GP)

Enthalpy: -496.019343

Re	-.0010455317	-.0015968304	.0065882980
O	-.0113326700	-.0220289011	1.7386993839
O	1.6799359049	-.0305416364	-.4216511404
O	-.7342130180	1.5022138870	-.4295516824
O	-1.0059355073	-1.5532395005	-.2947012824
H	-.8465269931	-1.4749767496	-1.3862764697
O	-.3254186128	-.6404709192	-2.2980957441
C	.7446837459	-.9720005841	-3.1254954128
H	1.6381008509	-1.2949162991	-2.5638829408
H	.4735589250	-1.7851594892	-3.8233000887
H	1.0560523781	-.1130745272	-3.7442668516

11b (SP)

Enthalpy: -496.019623

Re	-0.0006720948	0.0072842634	-0.0010992355
O	0.0182839585	0.0205792933	1.7324290613
O	1.6696337451	0.0556398861	-0.4579917266
O	-0.8048326750	1.4675933876	-0.4586208131
O	-0.9787582888	-1.5778816177	-0.2107794021
H	-0.8482787495	-1.5231188053	-1.3171741585
O	-0.3173178466	-0.6920131019	-2.2115206235
C	0.7775319637	-1.1179729253	-2.9903603608
H	1.4389873218	-1.8080197568	-2.4465004041
H	0.4179913329	-1.6329910106	-3.8910102285
H	1.3869405903	-0.2658210042	-3.3133412229

Reaction IV**12a (GP)**

Enthalpy: -495.906344

Re	-.1675698801	.3869475516	.8498739988
O	-.2740207931	-.1503269755	-.7905743582
O	-1.4146441405	1.0901889220	1.8476940643
C	-1.2319484644	-1.4870829852	1.2911901209
H	-.6831182279	-2.3244464513	.8565431523
H	-2.2210206874	-1.4075462401	.8364568820
H	-1.3216995091	-1.5932968898	2.3731464877
O	1.1566694694	-.6092039233	1.8886509062
O	1.6433667887	.7047274384	1.4897830709
O	-.0670583568	2.2696631464	.0111215781
H	-.4693167105	2.8576084920	.6585151230

12a (SP)

Enthalpy: -495.907117

Re	-0.1683711620	0.3865399823	0.8530043367
O	-0.2595105741	-0.1455546972	-0.7933817750
O	-1.3872440418	1.0869004157	1.8801603737
C	-1.2227033553	-1.4770845670	1.2778576269
H	-0.6581494916	-2.3098906566	0.8582306507
H	-2.1987607746	-1.4005157696	0.7968738096
H	-1.3367494670	-1.5770252955	2.3567962112
O	1.1621600917	-0.6107142695	1.8748098928
O	1.6408988077	0.7098049374	1.4772085837
O	-0.1144832251	2.2567766198	-0.0138052858
H	-0.4233857926	2.9006636894	0.6349503861

12b (GP)

Enthalpy: -495.916585

Re	.0225063375	.3829868016	.9428070001
O	.4257088908	.5889332611	-.7287398877
O	-.3689365032	1.4674910902	2.2537275038
C	-.8540888649	-1.5554957653	1.2694427460
H	-.0805858424	-2.3097260734	1.4061308797
H	-1.4931292608	-1.7607505443	.4135731571
H	-1.4704178250	-1.4705251373	2.1668363496
O	1.5090740295	-.6697783398	1.6562023281
O	2.0415237684	.6279378814	1.4273857009
O	-1.8863606742	.7047073504	.3360739590
H	-2.3544284330	1.0235376992	1.1137496314

12b (SP)

Enthalpy: -495.917893

Re	0.0008297386	0.4013114530	0.9915030552
O	-0.5627098472	1.0857724422	-0.5045930626
O	0.6633892212	0.9430654599	2.5127895853
C	-0.8486810543	-1.5502269557	1.2308851165
H	-0.8507574451	-1.9937032883	0.2357664881
H	-1.8526578874	-1.4648188082	1.6298385426
H	-0.1918291414	-2.1158450863	1.8901728422
O	1.4048418259	-0.8246412091	0.3705696211
O	1.9357384899	0.4839229458	0.2136513440
O	-1.7710339409	0.9816422077	1.7028635478
H	-1.7807113868	0.9040931906	2.6652348960

13a (GP)

Enthalpy: -495.877096

Re	-0.0109173575	-0.0306695954	-0.0054707563
O	1.4246542631	-0.9339812244	-0.3844467015
O	0.5068679233	0.0933406702	1.9105387773
C	-0.6416006015	-0.6962774360	-2.3290262936
H	-1.6547213810	-0.4001103142	-2.5806147914
H	-0.5670590006	-1.7398703561	-2.0298650845
H	0.1111463090	-0.4102713182	-3.0563206163
O	-0.3591982267	1.1936930095	-1.3215769976
O	0.0838075745	1.8963785105	0.3048715892
O	-1.4517497629	-0.9175779450	0.3917678319
H	0.5604485831	1.0404388579	2.0893808395

13a (SP)

Enthalpy: -495.876356

Re	0.0036338164	-0.0243303146	-0.0204562572
O	1.5550037280	-0.6169199985	-0.5368423281
O	0.7090679984	0.0607326564	1.8405723827
C	-0.6754236734	-0.7373408906	-2.2573462290
H	-1.7492003988	-0.6537625695	-2.3830927285
H	-0.3532943625	-1.7540734604	-2.0385054556
H	-0.0845082751	-0.2676325053	-3.0360562386
O	-0.6844847809	1.1760910687	-1.2071528229
O	-0.2527845249	1.8500099712	0.4380092904
O	-1.2321482313	-1.1519524935	0.4536059800
H	0.3288676807	0.8178176613	2.3047016691

13b (GP)

Enthalpy: -495.862243

Re	-0.0000705418	0.0000249549	0.0000814831
O	-0.0023632559	-0.0004359326	1.7431002674
O	1.6931669516	-0.0018596270	-0.3467197293
C	-0.0312083545	-0.9341614260	-2.4015161037
H	-0.9961897650	-1.0858141645	-2.8803757856
H	0.4270975218	-1.8644141547	-2.0625035273
H	0.6518790037	-0.3291828636	-2.9857389734
O	-0.8540223312	0.8131456769	-1.4464733166
O	-0.7036948614	1.7784049714	0.1151427707
O	-1.0907041360	-1.6517158153	0.1246552793
H	-1.3588105686	-1.9159698933	-0.7600154028

14a (GP)

Enthalpy: -495.982962

Re	-0.0225069868	0.4294115762	0.7999555624
O	0.7070256229	1.9002416545	1.7200949436
O	0.8339201065	-0.2292877724	2.3779788635
O	0.7639020123	0.6319056668	-0.7325763912
O	-1.6793826124	0.9356598997	0.7185948297
O	-0.3931206615	-1.4741315640	0.5752429372
C	-0.0647900715	-2.5904210894	1.3482426242
H	-0.9836293022	-3.1106692078	1.6579832435
H	0.5432875943	-3.2887263649	0.7535813090
H	0.4968673315	-2.2743535785	2.2336604626
H	1.0354566266	1.0240715308	2.4552765189

15 (GP)

Enthalpy: -496.030773

Re	.0540795407	.4252651299	.8699414737
O	.3613718951	2.1376436086	.8165137885
O	.7030505026	-.0467645812	2.4089287202
O	1.0724106617	-.1998902280	-.3889576985
O	-1.8372249350	.9044106373	.5953029311
H	-2.2781799433	.0410845035	.5840643526
O	-1.0669628910	-1.3479367834	.8182530259
C	-.3965728482	-2.5586099470	.9710362397
H	-1.1136176899	-3.3940904304	.9212511878
H	.3615050295	-2.7089562452	.1828323906
H	.1303634274	-2.6152897317	1.9393905083

16 (GP)

Enthalpy: -496.019343

Re	-.0010455317	-.0015968304	.0065882980
O	-.0113326700	-.0220289011	1.7386993839
O	1.6799359049	-.0305416364	-.4216511404
O	-.7342130180	1.5022138870	-.4295516824
O	-1.0059355073	-1.5532395005	-.2947012824
H	-.8465269931	-1.4749767496	-1.3862764697
O	-.3254186128	-.6404709192	-2.2980957441
C	.7446837459	-.9720005841	-3.1254954128
H	1.6381008509	-1.2949162991	-2.5638829408
H	.4735589250	-1.7851594892	-3.8233000887
H	1.0560523781	-.1130745272	-3.7442668516

13b (SP)

Enthalpy: -495.859973

Re	-0.0004236287	-0.0086631298	-0.0157740568
O	0.0011718845	-0.0514568110	1.7402709487
O	1.6954582860	0.0388171923	-0.3407263737
C	-0.0119982021	-0.9275602125	-2.3117255430
H	-0.9998117608	-1.1205970362	-2.7192811315
H	0.4911022457	-1.8315075856	-1.9662570786
H	0.6205189289	-0.3211528533	-2.9490332232
O	-0.8238238016	0.8821622769	-1.4202526643
O	-0.6989698243	1.7712042779	0.1869127326
O	-1.1402525981	-1.6043397776	0.1212891069
H	-1.4114287888	-1.9578348112	-0.7338883531

14a (SP)

Enthalpy: -495.984431

Re	-0.0263779818	0.4209479820	0.8006230430
O	0.6828463317	1.9180774010	1.7059588025
O	0.8405137409	-0.1935784006	2.3870593482
O	0.7753429215	0.6445242405	-0.7218652860
O	-1.6728087547	0.9586590370	0.6994470193
O	-0.3854028454	-1.4523443948	0.6155884399
C	-0.0653097854	-2.6110059889	1.3576871075
H	-0.9908237002	-3.1135268683	1.6536732857
H	0.5260429029	-3.2876465728	0.7302748464
H	0.5067943105	-2.3268031982	2.2428079675
H	1.0300288015	1.0602067330	2.4553360742

15 (SP)

Enthalpy: -496.031095

Re	0.0505267768	0.4154709039	0.8698060733
O	0.3385805933	2.1380485311	0.8320861827
O	0.7292392481	-0.0524746989	2.3967076999
O	1.0777260232	-0.1780564284	-0.3955289706
O	-1.8279589313	0.9351439672	0.5897534291
H	-2.3292720584	0.1052405404	0.5682878356
O	-1.0540501134	-1.3086370254	0.8214599587
C	-0.3803937687	-2.5353123888	0.9797676003
H	-1.1062822780	-3.3543425098	0.9217452228
H	0.3780677106	-2.6773344568	0.1962352728
H	0.1336965660	-2.5851425745	1.9507050202

16 (SP)

Enthalpy: -496.019623

Re	-0.0006720948	0.0072842634	-0.0010992355
O	0.0182839585	0.0205792933	1.7324290613
O	1.6696337451	0.0556398861	-0.4579917266
O	-0.8048326750	1.4675933876	-0.4586208131
O	-0.9787582888	-1.5778816177	-0.2107794021
H	-0.8482787495	-1.5231188053	-1.3171741585
O	-0.3173178466	-0.6920131019	-2.2115206235
C	0.7775319637	-1.1179729253	-2.9903603608
H	1.4389873218	-1.8080197568	-2.4465004041
H	0.4179913329	-1.6329910106	-3.8910102285
H	1.3869405903	-0.2658210042	-3.3133412229

Transition States Connecting Intermediates from Reaction III and IV

17 (GP)

Enthalpy: -495.871336

Re	.0003059008	.0002163594	.0022989562
O	.0005186552	.0110029035	1.7121443268
O	1.7881404187	.0011964190	-.6801551433
C	.6420377084	-2.0922766352	-.0728578328
H	-.1432686625	-2.6866771360	.4011113250
H	1.5905059537	-2.1765074793	.4491218944
H	.7551284453	-2.3607458567	-1.1206814027
O	-1.5451852425	-.9622264149	-.6997597720
O	-1.8379632825	.4588781585	-.6183648548
H	1.4933904668	1.2078972551	-.8055113579
O	.4505322171	1.7461630483	-.5799279545

18 (GP)

Enthalpy: -495.904362

Re	0.0212645860	-0.0125153306	0.9804313517
O	0.6171488182	0.7432254540	-0.4727290927
O	-0.2985445866	-1.7404168392	0.3004306333
O	1.2569848960	0.1396158339	2.1733724150
C	-1.1267002842	1.8431679558	1.0959593019
H	-0.3954365982	2.6488399015	1.1850671064
H	-1.7998782435	1.8098021657	1.9478987188
H	-1.6719230732	1.9588653807	0.1585466643
O	-1.6317546053	-0.4240731925	1.9760092454
O	-1.4398364354	-1.7466580975	2.4116793555
H	-0.8825928264	-2.1223302913	1.0882766257

17 (SP)

Enthalpy: -495.871810

Re	.0003059008	.0002163594	.0022989562
O	.0005186552	.0110029035	1.7121443268
O	1.7881404187	.0011964190	-.6801551433
C	.6420377084	-2.0922766352	-.0728578328
H	-.1432686625	-2.6866771360	.4011113250
H	1.5905059537	-2.1765074793	.4491218944
H	.7551284453	-2.3607458567	-1.1206814027
O	-1.5451852425	-.9622264149	-.6997597720
O	-1.8379632825	.4588781585	-.6183648548
H	1.4933904668	1.2078972551	-.8055113579
O	.4505322171	1.7461630483	-.5799279545

18 (SP)

Enthalpy: -495.905770

Re	0.0203363757	-0.0100708800	0.9771689240
O	0.6253451006	0.7336498159	-0.4723874846
O	-0.2940663604	-1.7453597521	0.3091992975
O	1.2268947228	0.1513185261	2.1951079131
C	-1.1210009580	1.8372630634	1.1004469565
H	-0.3740080668	2.6291416058	1.1799918301
H	-1.7771615184	1.8126046469	1.9643379094
H	-1.6792536972	1.9554847106	0.1724078859
O	-1.6259753723	-0.4311120172	1.9739353853
O	-1.4244083709	-1.7583696292	2.4161966254
H	-0.8752574445	-2.1429295564	1.0864882477