

Computational study of the catalytic olefination reaction

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1 Sum of electronic and thermal Free Energies= -380.785129 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.463895	0.947075	-0.351947
2	6	0	-1.537713	-1.389020	-0.192194
3	6	0	-2.547053	-0.484150	0.124596
4	6	0	-2.240750	0.867793	0.275660
5	6	0	-0.931709	1.305710	0.116534
6	6	0	0.099354	0.401440	-0.176819
7	6	0	-0.223035	-0.953676	-0.340525
8	1	0	-1.771200	-2.440516	-0.328920
9	1	0	-3.569547	-0.828532	0.246386
10	1	0	-3.023674	1.581612	0.512921
11	1	0	-0.698642	2.361866	0.225428
12	1	0	0.547441	-1.667097	-0.613568
13	7	0	2.606132	0.422927	-0.096522
14	7	0	2.683496	-0.859362	0.392966
15	1	0	1.519215	1.965180	-0.736052
16	1	0	1.909175	-1.127523	1.000030
17	1	0	3.561904	-0.960982	0.886833

CCl₄ Sum of electronic and thermal Free Energies= -1878.799847

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.000377	-0.000023	-0.000178
2	17	0	0.441228	1.703514	-0.266412
3	17	0	0.784946	-1.015806	-1.232600
4	17	0	-1.767059	-0.181005	-0.118733
5	17	0	0.541018	-0.506695	1.617809

TS1 Sum of electronic and thermal Free Energies= -2259.517721 a. u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.261017	1.554242	-0.534519
2	6	0	3.381570	-0.933766	1.337973
3	6	0	3.829139	-1.735049	0.286807
4	6	0	3.452083	-1.442623	-1.022073
5	6	0	2.624975	-0.355507	-1.281235
6	6	0	2.162781	0.449596	-0.230146
7	6	0	2.554465	0.152076	1.085957
8	1	0	3.680499	-1.156408	2.357397
9	1	0	4.476372	-2.582830	0.488900
10	1	0	3.802698	-2.061207	-1.842037
11	1	0	2.337299	-0.124369	-2.303471
12	1	0	2.212057	0.784641	1.898318
13	7	0	0.762787	2.295089	0.405916
14	7	0	-0.051586	3.284820	0.057867
15	1	0	1.057162	1.770156	-1.589409
16	1	0	-0.000525	3.669407	-0.882853
17	1	0	-0.236940	3.947515	0.797315
18	6	0	-1.199513	0.051185	-0.069673
19	17	0	-3.950596	-1.745537	0.219510
20	17	0	-0.853201	-0.810814	-1.462005
21	17	0	-0.708082	-0.569023	1.398246
22	17	0	-2.176717	1.375540	-0.132763

2 Sum of electronic and thermal Free Energies= -2259.565705 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.753465	0.937661	-0.387054
2	6	0	3.433130	-1.172535	1.333167
3	6	0	4.080363	-1.717905	0.228038
4	6	0	3.660120	-1.390456	-1.059510
5	6	0	2.593364	-0.518927	-1.243273
6	6	0	1.925474	0.003971	-0.133156
7	6	0	2.354637	-0.311172	1.159891
8	1	0	3.765829	-1.415003	2.336860
9	1	0	4.916755	-2.394885	0.369092
10	1	0	4.164723	-1.809149	-1.923696
11	1	0	2.273866	-0.258375	-2.247485
12	1	0	1.862109	0.109933	2.028720
13	7	0	0.921681	2.052339	0.540298
14	7	0	1.365037	3.096322	0.077014
15	1	0	0.774970	1.279837	-1.428217
16	1	0	1.582490	3.242881	-0.919225
17	1	0	1.538386	3.869903	0.724714
18	6	0	-0.669548	0.338348	-0.166234
19	17	0	-4.915528	-1.306319	0.251282
20	17	0	-0.890662	-0.966474	-1.351976
21	17	0	-0.903331	-0.289059	1.476798
22	17	0	-1.859430	1.639518	-0.473348

3 Sum of electronic and thermal Free Energies= -1798.791097 a. u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.240034	-0.325749	-0.882392
2	6	0	-3.131766	-0.907002	0.808723
3	6	0	-3.891502	0.130258	0.273748
4	6	0	-3.316859	1.010377	-0.639909
5	6	0	-1.984539	0.857633	-1.010570
6	6	0	-1.212901	-0.169329	-0.463339

7	6	0	-1.799386	-1.060452	0.438567
8	1	0	-3.576255	-1.604104	1.511898
9	1	0	-4.931870	0.247552	0.560679
10	1	0	-3.905635	1.814335	-1.069952
11	1	0	-1.543518	1.542719	-1.728644
12	1	0	-1.224696	-1.883812	0.851051
13	7	0	0.422661	-1.750362	-1.271093
14	7	0	1.138667	-2.551310	-0.664955
15	1	0	0.386121	0.207383	-1.827627
16	1	0	1.636963	-2.146440	0.148002
17	6	0	1.255887	0.344084	0.091410
18	17	0	0.929546	2.102565	0.150180
19	17	0	1.162406	-0.297531	1.759712
20	17	0	2.924270	0.115858	-0.532862

TS2 Sum of electronic and thermal Free Energies= -1798.744299 a. u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.069728	-0.196177	-0.816472
2	6	0	-3.287445	-0.941550	0.833026
3	6	0	-4.084419	0.050516	0.266675
4	6	0	-3.532143	0.951702	-0.640485
5	6	0	-2.184976	0.863423	-0.978396
6	6	0	-1.385614	-0.131710	-0.412714
7	6	0	-1.940909	-1.035186	0.495035
8	1	0	-3.712500	-1.646992	1.539890
9	1	0	-5.135122	0.120986	0.530087
10	1	0	-4.148813	1.724722	-1.087837
11	1	0	-1.756587	1.567095	-1.686636
12	1	0	-1.327832	-1.812424	0.941163
13	7	0	0.258484	-1.888225	-1.060312
14	7	0	1.238242	-2.485821	-0.782364
15	1	0	0.219018	0.137020	-1.843705
16	1	0	2.068210	-1.936078	-0.363742
17	6	0	0.955645	0.539197	0.058118
18	17	0	1.657655	1.984830	-0.538017
19	17	0	0.726095	0.488361	1.752894
20	17	0	3.243152	-0.598914	0.081639

4+N₂+HCl Sum of electronic and thermal Free Energies= -1798.886519 a. u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.678680	-0.641339	-0.867429
2	6	0	2.284076	-0.681585	1.510303
3	6	0	3.237885	-1.311132	0.715027
4	6	0	2.904620	-1.707118	-0.579116
5	6	0	1.623913	-1.480061	-1.068943
6	6	0	0.648447	-0.868483	-0.268883
7	6	0	0.999091	-0.459425	1.024839
8	1	0	2.540339	-0.352786	2.512635
9	1	0	4.239319	-1.482178	1.097482
10	1	0	3.644816	-2.188199	-1.210799
11	1	0	1.372817	-1.780575	-2.082452
12	1	0	0.277327	0.054672	1.649382
13	7	0	3.336715	1.598207	-1.192193
14	7	0	2.365899	1.955250	-0.815178
15	1	0	-0.683548	-0.456833	-1.938869
16	1	0	0.355568	2.427081	0.091376
17	6	0	-1.881893	-0.663009	-0.291897
18	17	0	-3.322991	-0.344584	-1.217051
19	17	0	-2.204149	-1.025025	1.372952
20	17	0	-0.736959	2.885935	0.602302

CuCl CCl₄ Sum of electronic and thermal Free Energies= -3979.297653 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.602579	0.059849	0.000120
2	17	0	0.123518	-1.059817	-0.017327
3	17	0	3.019191	-0.988109	-0.012937
4	17	0	1.553367	1.040408	1.465086
5	17	0	1.555957	1.080153	-1.438137
6	29	0	-1.760896	-0.163919	0.004421
7	17	0	-3.813768	0.185868	-0.004268

TS3 Sum of electronic and thermal Free Energies= -4360.057464 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.450750	1.792927	0.494896
2	6	0	-4.776369	-0.595592	-1.284265
3	6	0	-5.343981	-1.269237	-0.201760
4	6	0	-4.967289	-0.932405	1.095695
5	6	0	-4.027040	0.071593	1.309841
6	6	0	-3.451074	0.750810	0.230016
7	6	0	-3.838580	0.406867	-1.073239
8	1	0	-5.068079	-0.852822	-2.298163
9	1	0	-6.078021	-2.051186	-0.370839
10	1	0	-5.405192	-1.450044	1.943645
11	1	0	-3.734848	0.331286	2.324456
12	1	0	-3.398116	0.933951	-1.913462
13	7	0	-1.851325	2.409086	-0.455290
14	7	0	-0.885304	3.311741	-0.120396
15	1	0	-2.235774	2.018653	1.546995
16	1	0	-1.000418	3.754024	0.790392
17	1	0	-0.770622	3.996954	-0.855691
18	6	0	0.093008	-0.464322	0.000063
19	17	0	2.231574	-2.064713	-0.132488
20	17	0	-0.556060	-1.085981	1.425571
21	17	0	-0.614745	-0.905876	-1.461229
22	17	0	1.046359	0.889146	0.063986
23	29	0	3.632469	-0.496750	-0.022115
24	17	0	4.603362	1.350676	0.108649

5 Sum of electronic and thermal Free Energies= -4360.065317 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.217529	1.586923	0.533847
2	6	0	-4.892516	-0.273405	-1.365087
3	6	0	-5.519750	-0.959797	-0.324178

4	6	0	-5.072674	-0.796247	0.984667
5	6	0	-4.000242	0.047843	1.252904
6	6	0	-3.361690	0.736409	0.213086
7	6	0	-3.821022	0.569428	-1.102663
8	1	0	-5.242677	-0.397015	-2.385220
9	1	0	-6.356629	-1.618418	-0.535057
10	1	0	-5.559236	-1.324704	1.798430
11	1	0	-3.654881	0.178677	2.275113
12	1	0	-3.333721	1.106985	-1.909493
13	7	0	-1.578183	2.237160	-0.385098
14	7	0	-0.534348	2.978971	-0.011918
15	1	0	-1.955034	1.702828	1.591625
16	1	0	-0.491027	3.319038	0.946526
17	1	0	-0.231276	3.636342	-0.716719
18	6	0	-0.180336	-0.360523	0.103170
19	17	0	2.825183	-2.331581	-0.205928
20	17	0	-0.604612	-1.181685	1.517507
21	17	0	-0.741795	-0.970344	-1.362419
22	17	0	1.109179	0.657434	0.116285
23	29	0	3.425225	-0.307369	-0.070914
24	17	0	4.275294	1.619897	0.051963

TS4 Sum of electronic and thermal Free Energies= -4360.064145 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.172758	1.542383	0.527987
2	6	0	-4.896166	-0.255834	-1.357617
3	6	0	-5.520862	-0.943185	-0.315884
4	6	0	-5.055996	-0.800378	0.989331
5	6	0	-3.967865	0.024106	1.253401
6	6	0	-3.331652	0.713493	0.212175
7	6	0	-3.808839	0.567748	-1.100038
8	1	0	-5.261095	-0.363391	-2.374299
9	1	0	-6.370881	-1.585884	-0.523134
10	1	0	-5.541503	-1.329271	1.803328
11	1	0	-3.608669	0.140049	2.272554
12	1	0	-3.324293	1.106871	-1.907357
13	7	0	-1.560437	2.228696	-0.392628

14	7	0	-0.539220	2.981364	-0.025765
15	1	0	-1.900249	1.654214	1.583027
16	1	0	-0.446764	3.284873	0.941269
17	1	0	-0.202852	3.617558	-0.734535
18	6	0	-0.219336	-0.304245	0.112485
19	17	0	2.788863	-2.336678	-0.233481
20	17	0	-0.606901	-1.159707	1.524547
21	17	0	-0.756870	-0.943987	-1.355398
22	17	0	1.105415	0.682390	0.118689
23	29	0	3.416290	-0.322986	-0.075522
24	17	0	4.300219	1.587784	0.070761

6 Sum of electronic and thermal Free Energies= -4360.119222 a. u.

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-1.129459	-0.203859	0.252545
2	6	0	-4.914521	-0.311309	0.726781
3	6	0	-5.287015	-1.111445	-0.350078
4	6	0	-4.316637	-1.621712	-1.210091
5	6	0	-2.974756	-1.330220	-0.994972
6	6	0	-2.603380	-0.507565	0.071262
7	6	0	-3.574332	-0.007922	0.943877
8	1	0	-5.666959	0.076334	1.405510
9	1	0	-6.334257	-1.343313	-0.515777
10	1	0	-4.602503	-2.252217	-2.045478
11	1	0	-2.218406	-1.733067	-1.661922
12	1	0	-3.292916	0.607124	1.790916
13	7	0	-0.858445	-0.399004	1.680043
14	7	0	-0.039812	-1.268865	1.958227
15	1	0	-0.528734	-0.883543	-0.362563
16	1	0	0.538872	-1.793990	1.242587
17	1	0	0.125304	-1.443363	2.953525
18	6	0	-0.663436	1.233394	-0.142253
19	17	0	4.612043	0.857492	-0.065730
20	17	0	-1.145196	1.532490	-1.825371
21	17	0	-1.338121	2.490634	0.916933
22	17	0	1.129151	1.248519	-0.029923
23	29	0	3.230343	-0.711116	-0.132254

24 17 0 1.881457 -2.351058 -0.185423

7 Sum of electronic and thermal Free Energies= -3899.309534 a. u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.418391	0.014730	0.483400
2	6	0	-4.159297	-0.679144	0.595526
3	6	0	-4.246771	-1.778976	-0.255109
4	6	0	-3.097035	-2.290322	-0.852398
5	6	0	-1.863668	-1.697765	-0.604210
6	6	0	-1.775820	-0.586514	0.236094
7	6	0	-2.926998	-0.082951	0.845173
8	1	0	-5.051982	-0.284436	1.069996
9	1	0	-5.209618	-2.242727	-0.445309
10	1	0	-3.157705	-3.152966	-1.508118
11	1	0	-0.965252	-2.100547	-1.064230
12	1	0	-2.861844	0.761854	1.522202
13	7	0	-0.237413	0.217146	1.944011
14	7	0	0.777981	-0.258928	2.456952
15	1	0	0.359968	-0.666996	0.114771
16	1	0	1.401898	-0.691116	1.738616
17	6	0	-0.145482	1.347966	-0.255947
18	17	0	-0.557865	1.227789	-1.970360
19	17	0	-0.926105	2.743825	0.479153
20	17	0	1.692267	1.638816	-0.152717
21	29	0	2.499508	-0.374641	-0.187066
22	17	0	2.792621	-2.430909	-0.001072

TS5 Sum of electronic and thermal Free Energies= -3899.277817 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.225510	0.608524	-0.540270
2	6	0	4.744883	-0.444832	0.486706
3	6	0	4.865873	-1.665312	-0.173787

4	6	0	3.814189	-2.146069	-0.951107
5	6	0	2.640553	-1.409002	-1.068991
6	6	0	2.524481	-0.185970	-0.407300
7	6	0	3.572075	0.295565	0.380015
8	1	0	5.563326	-0.067678	1.091055
9	1	0	5.781208	-2.241458	-0.083654
10	1	0	3.907071	-3.094426	-1.469992
11	1	0	1.823288	-1.780714	-1.680067
12	1	0	3.480166	1.247224	0.892660
13	7	0	1.544428	2.056569	-0.649223
14	7	0	1.140083	2.651905	-1.645426
15	1	0	0.647009	0.245727	-1.400682
16	1	0	0.577118	2.048308	-2.279561
17	6	0	0.411684	0.356330	0.688472
18	17	0	-0.561219	-0.971504	0.749704
19	17	0	0.586270	1.293935	2.058467
20	17	0	-1.895230	1.703404	-0.581991
21	29	0	-2.985784	-0.093359	-0.306961
22	17	0	-3.822676	-1.970793	0.092185

8 Sum of electronic and thermal Free Energies= -3899.277817 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.225510	0.608524	-0.540270
2	6	0	4.744883	-0.444832	0.486706
3	6	0	4.865873	-1.665312	-0.173787
4	6	0	3.814189	-2.146069	-0.951107
5	6	0	2.640553	-1.409002	-1.068991
6	6	0	2.524481	-0.185970	-0.407300
7	6	0	3.572075	0.295565	0.380015
8	1	0	5.563326	-0.067678	1.091055
9	1	0	5.781208	-2.241458	-0.083654
10	1	0	3.907071	-3.094426	-1.469992
11	1	0	1.823288	-1.780714	-1.680067
12	1	0	3.480166	1.247224	0.892660
13	7	0	1.544428	2.056569	-0.649223
14	7	0	1.140083	2.651905	-1.645426
15	1	0	0.647009	0.245727	-1.400682

16	1	0	0.577118	2.048308	-2.279561
17	6	0	0.411684	0.356330	0.688472
18	17	0	-0.561219	-0.971504	0.749704
19	17	0	0.586270	1.293935	2.058467
20	17	0	-1.895230	1.703404	-0.581991
21	29	0	-2.985784	-0.093359	-0.306961
22	17	0	-3.822676	-1.970793	0.092185

TS6 Sum of electronic and thermal Free Energies= -3899.275350 a. u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.363421	-0.389537	-0.677496
2	6	0	4.933346	0.819799	-0.100292
3	6	0	5.595368	-0.393620	0.067410
4	6	0	4.885913	-1.590232	-0.009250
5	6	0	3.516976	-1.573189	-0.253950
6	6	0	2.852100	-0.356522	-0.421818
7	6	0	3.562952	0.841790	-0.343208
8	1	0	5.481581	1.754524	-0.043110
9	1	0	6.664256	-0.407305	0.255799
10	1	0	5.396860	-2.538902	0.119203
11	1	0	2.964519	-2.506386	-0.315046
12	1	0	3.058673	1.794140	-0.473100
13	7	0	1.110685	0.790912	-1.804954
14	7	0	0.341508	1.702336	-1.727156
15	1	0	1.080064	-1.257802	-1.275241
16	1	0	-0.303490	1.813632	-0.909668
17	6	0	0.536764	-0.331088	0.504813
18	17	0	-0.914839	-1.137969	0.565007
19	17	0	0.891367	0.712648	1.776547
20	17	0	-2.179088	2.009139	0.216038
21	29	0	-3.117500	0.121098	-0.059072
22	17	0	-4.125754	-1.688576	-0.411607

4+N₂+HCl CuCl Sum of electronic and thermal Free Energies= -3899.385163 a. u.

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.628389	-0.992611	0.010173
2	6	0	5.039131	0.678856	-0.021482
3	6	0	5.863981	-0.438193	-0.128463
4	6	0	5.298802	-1.709742	-0.202747
5	6	0	3.918000	-1.859354	-0.162828
6	6	0	3.078946	-0.743913	-0.025142
7	6	0	3.656536	0.531259	0.030426
8	1	0	5.471685	1.673651	0.018426
9	1	0	6.942437	-0.318487	-0.162247
10	1	0	5.933533	-2.585588	-0.295734
11	1	0	3.480389	-2.851712	-0.227695
12	1	0	3.030976	1.414312	0.092432
13	7	0	1.539662	1.359605	-2.664564
14	7	0	0.613521	1.691838	-2.171499
15	1	0	1.288180	-1.859088	-0.551997
16	1	0	-1.191476	2.307345	-1.210041
17	6	0	0.671425	-0.337042	0.668034
18	17	0	-0.994985	-0.847353	0.550957
19	17	0	0.891917	1.025278	1.713795
20	17	0	-2.342296	2.473663	-0.630804
21	29	0	-3.193052	0.537114	-0.145211
22	17	0	-4.536856	-1.012731	0.273643