Supporting Information for

Mechanistic Details of the Titanium-Mediated Polycondensation Reaction of Polyesters: A DFT Study

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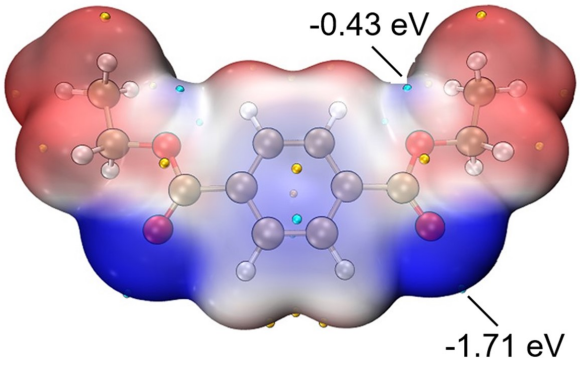

Figure S1. Molecular electrostatic potential (MESP) on the 0.001 a.u. electron density isosurface for the DET molecule.

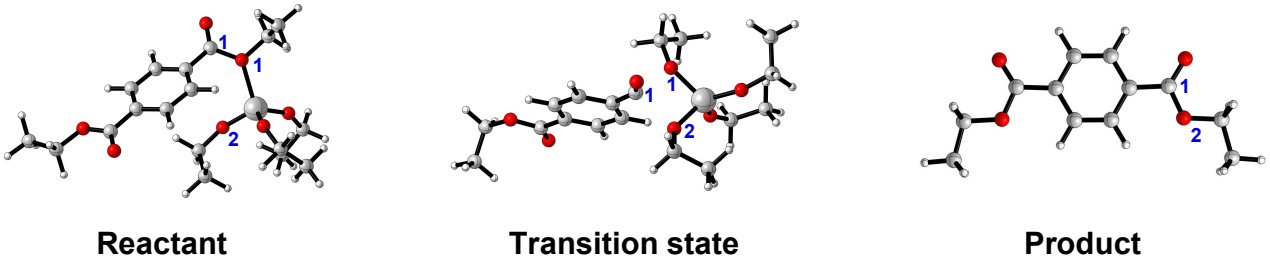

Figure S2. Optimised structure of the reactant, transition state, and product in M2 mechanism over $Ti(OEt)_3^+$ catalyst.

List of Cartesian coordinates

C_2H_5OH
Geometry with 9 atoms:
Thermal correction to Gibbs Free Energy: 0.054277
Total energy: -155.112414

O	1.237738	-0.259215	-0.109759
C	0.085866	0.554463	0.046588
C	-1.212756	-0.240108	-0.021498
H	0.119388	1.291877	-0.773132
H	0.125070	1.131638	0.993262
H	-1.272645	-0.964567	0.808815
H	-2.088741	0.425275	0.048609
H	-1.272968	-0.800279	-0.968409
H	1.249326	-0.896363	0.618393

Int1
Geometry with 30 atoms:
Thermal correction to Gibbs Free Energy: 0.197627
Total energy: -766.971469

C	2.826509	-0.547521	-0.232955
O	3.624852	0.525075	-0.303979
C	5.051676	0.305596	-0.357762
C	5.628844	0.070869	1.027228
O	3.232184	-1.691806	-0.227427
H	5.453651	1.221326	-0.812498
H	5.256524	-0.544811	-1.025091
H	5.228236	-0.856386	1.462413
H	5.389717	0.911130	1.697151
H	6.724337	-0.021136	0.962453
O	-3.217672	1.923386	0.044660
C	-2.808681	0.780512	0.026796
C	-1.359260	0.412167	-0.040114
C	-0.928431	-0.924935	-0.050603
C	0.432552	-1.215698	-0.112259
C	1.377208	-0.178420	-0.165802
C	0.946293	1.158675	-0.155100
C	-0.414672	1.449470	-0.091987
H	-0.765311	2.482829	-0.082149
H	1.681197	1.962885	-0.195320
H	0.783065	-2.249091	-0.120512
H	-1.663176	-1.729318	-0.009880
O	-3.610074	-0.289451	0.065150
C	-5.031371	-0.050576	0.133496
C	-5.725134	-1.395007	0.143616
H	-5.328496	0.563543	-0.731849
H	-5.247344	0.535118	1.041750
H	-5.494004	-1.961771	-0.771458
H	-6.814997	-1.250958	0.196700
H	-5.410922	-1.991771	1.013742

Int2
Geometry with 63 atoms:
Thermal correction to Gibbs Free Energy: 0.451385
Total energy: -2234.766524

C	-5.231435	-0.011341	0.323783
O	-5.406243	-1.322289	0.114195
C	-6.693048	-1.894639	0.435256
C	-7.696949	-1.665752	-0.681052
O	-6.087843	0.719506	0.778347
H	-7.047054	-1.465525	1.384578
H	-6.489162	-2.964283	0.581036
H	-7.903988	-0.592504	-0.802881
H	-8.642427	-2.176615	-0.440460
H	-7.318472	-2.066173	-1.634188
O	0.933751	1.106564	-1.482360
C	0.079487	1.847976	-1.020041
C	-1.308682	1.402200	-0.709194
C	-1.625297	0.048487	-0.901794
C	-2.893885	-0.425659	-0.579048
C	-3.859981	0.450972	-0.058425
C	-3.543124	1.805962	0.129832
C	-2.274656	2.281587	-0.194084
H	-2.022251	3.330791	-0.039399
H	-4.303576	2.473728	0.537742
H	-3.138734	-1.479138	-0.714670
H	-0.851918	-0.629355	-1.263180
O	0.296810	3.127316	-0.733668
C	2.333368	3.553911	0.522523
C	1.648937	3.641110	-0.829279
H	1.531931	4.680448	-1.166193

H	2.195273	3.068656	-1.590646
H	3.352107	3.965483	0.447136
H	2.399942	2.506727	0.846669
H	1.779235	4.129778	1.279811
Ti	2.119226	-0.519908	0.136947
O	1.373405	-1.680521	-1.045448
C	1.404359	-1.886057	-2.438702
C	2.826390	-2.076110	-2.952538
H	3.291285	-2.960622	-2.488028
H	3.436695	-1.195123	-2.696815
H	2.836215	-2.210152	-4.046163
H	0.933307	-1.017981	-2.936877
H	0.788696	-2.774081	-2.676627
O	3.539542	0.415274	-0.478995
C	4.924303	0.525163	-0.249519
C	5.238665	0.843413	1.207243
H	4.769056	1.794497	1.503608
H	6.326463	0.925414	1.363276
H	4.846456	0.044915	1.855845
H	5.323743	1.320064	-0.907756
H	5.424334	-0.417567	-0.543707
O	1.016073	0.437391	1.240454
C	0.561606	0.291949	2.562843
C	-0.855283	-0.266157	2.609068
H	-1.550276	0.389256	2.062585
H	-1.203391	-0.360543	3.650728
H	-0.888566	-1.261534	2.137557
H	0.593401	1.282059	3.057968
H	1.248352	-0.373793	3.122194
O	2.840401	-1.676223	1.310017
C	3.202656	-3.038033	1.259036
C	4.612105	-3.216555	0.710181
H	4.893740	-4.281819	0.700757
H	5.341857	-2.666514	1.325004
H	4.670928	-2.831635	-0.320431
H	2.477756	-3.581211	0.622595
H	3.131679	-3.458382	2.279236

Int3
Geometry with 63 atoms:
Thermal correction to Gibbs Free Energy:
0.450022
Total energy: -2234.770189

C	-4.164302	-0.177876	0.472927
O	-4.950182	-0.190604	-0.610793
C	-6.125212	-1.030946	-0.587949
C	-7.281090	-0.351182	0.124463
O	-4.382020	-0.835581	1.471493
H	-5.867878	-1.987872	-0.109921
H	-6.353983	-1.210885	-1.647287
H	-7.506348	0.621957	-0.338423
H	-7.044048	-0.193872	1.186837
H	-8.180474	-0.983335	0.059141
O	0.973693	3.433877	-1.272816
C	0.709227	2.848162	-0.241461
O	1.549109	2.750341	0.793258
C	2.880319	3.288372	0.637210
C	3.773079	2.352582	-0.160026
H	2.809493	4.280060	0.164958
H	3.245177	3.409911	1.666454
H	3.409384	2.254915	-1.192469
H	4.798079	2.755215	-0.183434
H	3.781429	1.355410	0.301185
C	-0.590223	2.149938	0.005147
C	-0.872083	1.504988	1.218811
C	-2.052189	0.781749	1.363919
C	-2.966876	0.699659	0.303057
C	-2.708016	1.386772	-0.894664
C	-1.525013	2.106832	-1.039613
H	-1.294815	2.620554	-1.973933
H	-3.422925	1.328247	-1.715494
H	-2.267714	0.247435	2.290359
H	-0.148281	1.545299	2.031412
Ti	1.655807	-1.122744	0.049538
O	2.492198	-0.334983	1.437128
C	2.382207	0.106589	2.767116
C	1.383081	-0.720005	3.566638
H	1.296234	-0.339068	4.596696
H	1.700316	-1.774449	3.607303
H	0.391112	-0.687713	3.089788
H	2.084816	1.171233	2.760550
H	3.382164	0.053875	3.237677
O	1.371541	0.090599	-1.241998
C	1.175106	0.354729	-2.607761
C	2.080207	-0.499775	-3.484483
H	3.138998	-0.290406	-3.263019
H	1.897731	-0.292276	-4.551026

H	1.899879	-1.569205	-3.293022
H	1.363416	1.429519	-2.779596
H	0.113443	0.171519	-2.859254
O	2.721443	-2.404908	-0.651044
C	4.097432	-2.565113	-0.916510
C	4.920233	-2.610602	0.364969
H	4.614789	-3.465027	0.990351
H	4.761450	-1.688308	0.945417
H	5.993668	-2.710395	0.137253
H	4.447211	-1.736776	-1.562814
H	4.235069	-3.498683	-1.494008
O	0.120641	-1.905953	0.532708
C	-1.142143	-2.413107	0.182890
C	-1.490394	-2.107762	-1.268474
H	-0.766771	-2.586317	-1.947985
H	-1.458374	-1.022391	-1.440919
H	-2.500798	-2.471522	-1.514678
H	-1.902325	-1.976489	0.854974
H	-1.148338	-3.506111	0.356364

Int5
Geometry with 57 atoms:
Thermal correction to Gibbs Free Energy:
0.398707
Total energy: -2156.075404

C	-5.557368	0.829541	0.035960
O	-6.532095	-0.001079	-0.363923
C	-7.873207	0.489282	-0.269488
O	-5.774434	1.945991	0.461505
H	-8.123806	0.738303	0.772823
H	-8.520289	-0.317428	-0.633560
O	0.590358	-0.517533	-1.279807
C	-0.159936	-1.298623	-0.446301
O	-0.170285	-2.641101	-0.791378
C	1.102561	-3.204522	-1.099709
H	1.844604	-2.969415	-0.319470
H	0.957695	-4.291001	-1.159419
C	-1.598430	-0.802791	-0.323603
C	-1.800126	0.497472	0.168329
C	-3.088653	1.010334	0.277923
C	-4.196512	0.231851	-0.101235
C	-3.992686	-1.067462	-0.589668
C	-2.697937	-1.581395	-0.698442
H	-2.534574	-2.590640	-1.076192
H	-4.850012	-1.674202	-0.883190
H	-3.259154	2.019128	0.658172
H	-0.936479	1.097700	0.464017
Ti	2.044192	0.258464	-0.289019
O	0.536115	-1.103084	0.807572
C	0.195491	-1.864457	1.965220
C	1.097047	-1.408104	3.095008
H	0.894634	-1.990740	4.006299
H	0.929618	-0.342429	3.313820
H	2.151078	-1.537466	2.807897
H	0.331096	-2.937080	1.747312
H	-0.870247	-1.700736	2.204538
O	3.310145	-0.810523	0.439953
C	4.705759	-0.905001	0.238437
C	5.025621	-1.686179	-1.028640
H	4.597798	-2.700057	-0.976829
H	6.114820	-1.771602	-1.172056
H	4.593965	-1.170181	-1.900593
H	5.147079	-1.401473	1.122429
H	5.149088	0.107381	0.181566
O	2.953158	1.053737	-1.603523
C	3.597697	2.264159	-1.934732
C	2.624371	3.434950	-1.932256
H	1.828572	3.276448	-2.677569
H	3.147065	4.374514	-2.172184
H	2.153964	3.530040	-0.941656
H	4.065085	2.148716	-2.929760
H	4.416011	2.444710	-1.212132
O	1.588006	1.609693	0.796665
C	1.933340	2.316163	1.963843
C	3.366977	2.041061	2.396760
H	4.069800	2.338063	1.601327
H	3.508099	0.966712	2.590518
H	3.613569	2.604113	3.310777
H	1.228006	2.036111	2.769156
H	1.790116	3.396097	1.772132
H	-8.002304	1.390241	-0.888272
H	1.481079	-2.826516	-2.062446

Int7
Geometry with 55 atoms:
Thermal correction to Gibbs Free Energy:

0.385253
Total energy: -2080.015466

C	-5.356654	0.237394	0.027535
O	-5.489608	-1.089592	0.060558
C	-6.829002	-1.620679	0.169507
O	-6.287649	1.012473	0.084191
H	-7.417059	-1.267661	-0.692801
H	-7.296490	-1.209778	1.078561
O	1.068100	1.229654	-0.553170
C	0.110758	2.019124	-0.391627
C	-1.285389	1.563359	-0.288458
C	-1.558341	0.182821	-0.279534
C	-2.873557	-0.261077	-0.175418
C	-3.922976	0.667658	-0.085647
C	-3.648329	2.044671	-0.097633
C	-2.336555	2.495353	-0.195527
H	-2.118051	3.563442	-0.202816
H	-4.477735	2.749725	-0.027734
H	-3.092927	-1.328457	-0.162357
H	-0.742847	-0.539113	-0.340473
O	0.307124	3.299400	-0.316284
C	2.374452	3.693305	0.957045
C	1.669527	3.837500	-0.377409
H	1.512366	4.887248	-0.651656
H	2.202374	3.323288	-1.189359
H	1.788251	4.163059	1.760744
H	3.348163	4.203190	0.895940
Ti	2.320607	-0.256757	-0.191522
O	3.449278	-0.500327	-1.513932
C	4.762958	-0.818717	-1.935827
C	5.722633	-0.916861	-0.760542
H	6.737039	-1.153830	-1.116611
H	5.400865	-1.708885	-0.066005
H	5.086749	-0.038437	-2.646229
H	4.716464	-1.773690	-2.488065
O	3.220712	0.094646	1.277536
C	3.761553	-0.353336	2.507247
C	3.356731	-1.787268	2.808863
H	3.728914	-2.465349	2.024967
H	2.260597	-1.878761	2.849874
H	3.409772	0.332364	3.297316
H	4.859767	-0.257062	2.447043
O	1.432826	-1.757562	0.043526
C	1.320267	-3.153753	-0.164078
C	2.408780	-3.677674	-1.087370
H	2.363886	-3.172859	-2.064423
H	2.284779	-4.760574	-1.242360
H	0.318149	-3.349880	-0.583539
H	1.369503	-3.645309	0.823334
H	3.404707	-3.498465	-0.652692
H	3.776027	-2.105054	3.775905
H	2.557400	2.638463	1.208503
H	5.754629	0.033945	-0.206764
C	-6.724253	-3.128986	0.211710
H	-6.249422	-3.514600	-0.703482
H	-6.131181	-3.456242	1.079457
H	-7.729937	-3.568588	0.292785

Int8
Geometry with 55 atoms:
Thermal correction to Gibbs Free Energy:
0.388919
Total energy: -2079.944030

C	4.741524	-1.158527	-0.077137
O	5.743025	-0.301672	-0.304997
C	7.084248	-0.833312	-0.293930
O	4.909839	-2.341830	0.136472
H	7.265738	-1.314387	0.680672
O	-1.426977	0.567062	-1.041890
C	-0.561255	1.234028	-0.192814
O	-0.500131	2.575746	-0.391938
C	-1.741278	3.296618	-0.522594
H	-2.346004	3.140801	0.386495
C	0.840497	0.644204	-0.170081
C	0.993117	-0.729176	0.076648
C	2.263539	-1.296103	0.105847
C	3.399002	-0.499649	-0.115335
C	3.244362	0.872163	-0.362433
C	1.969640	1.441785	-0.387237
H	1.847147	2.507794	-0.576391
H	4.124318	1.492587	-0.534209
H	2.394259	-2.362126	0.298521
H	0.116758	-1.355424	0.249421
Ti	-2.689222	-0.212262	0.088565
O	-1.256408	0.938149	1.095886
C	-0.750145	1.433981	2.355282
C	-1.797623	1.181990	3.416779

H	-1.433587	1.540597	4.390933
H	-2.011393	0.105084	3.501534
H	-2.731963	1.712137	3.176298
H	-0.536214	2.505623	2.225721
H	0.193066	0.908019	2.570021
O	-4.212941	0.041175	-0.701162
C	-5.427627	-0.317599	-1.340114
C	-5.523907	-1.819331	-1.546567
H	-4.692366	-2.176190	-2.173557
H	-6.471568	-2.069057	-2.047864
H	-5.490613	-2.347639	-0.581234
H	-5.463910	0.222919	-2.301140
H	-6.254767	0.056558	-0.713414
O	-2.332234	-1.904947	0.086914
C	-2.293378	-3.298923	-0.178763
C	-2.934650	-4.072347	0.959382
H	-3.991278	-3.786087	1.075530
H	-2.409109	-3.874717	1.906022
H	-2.885330	-5.151926	0.749241
H	-1.235231	-3.579871	-0.312203
H	-2.817582	-3.475393	-1.132100
H	7.159752	-1.616293	-1.065767
H	-2.303224	2.890419	-1.377754
C	8.037289	0.313409	-0.550390
H	9.073759	-0.056866	-0.550378
H	7.835338	0.779907	-1.526895
H	7.943389	1.082880	0.231307
C	-1.401790	4.758451	-0.715610
H	-0.790659	4.898358	-1.620351
H	-2.326463	5.344884	-0.825396
H	-0.842156	5.147751	0.148636

TS1
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
0.266114
Total energy: -922.020506

C	-3.380994	-0.000051	0.764814
O	-4.160886	-0.000011	-0.322867
C	-5.587964	-0.000023	-0.113729
C	-6.253430	0.000115	-1.472532
O	-3.817427	-0.000100	1.898003
H	-5.858388	0.887600	0.480866
H	-5.858397	-0.887764	0.480688
H	-7.347386	0.000103	-1.351495
H	-5.967819	-0.893461	-2.048722
H	-5.967817	0.893808	-2.048540
O	2.757568	0.000073	-1.547852
C	2.281697	0.000033	-0.444436
C	0.827107	0.000005	-0.096489
C	-0.090859	0.000096	-1.155033
C	-1.461868	0.000078	-0.895410
C	-1.923703	-0.000030	0.429346
C	-0.999239	-0.000121	1.488286
C	0.367854	-0.000106	1.229532
H	1.084947	-0.000184	2.049590
H	-1.373169	-0.000206	2.513517
H	-2.177707	0.000149	-1.717809
H	0.281335	0.000181	-2.180937
O	3.017400	1.101400	0.668240
C	3.908897	2.038824	0.067023
C	3.148219	3.278717	-0.369444
H	4.417042	1.569213	-0.793779
H	4.675913	2.281711	0.820754
H	2.403748	3.021355	-1.139130
H	3.837864	4.025443	-0.793777
H	2.621640	3.732092	0.484886
O	3.017424	-1.101442	0.668181
C	3.908921	-2.038812	0.066891
C	3.148249	-3.278681	-0.369659
H	4.675950	-2.281751	0.820592
H	4.417055	-1.569137	-0.793884
H	2.621682	-3.732121	0.484645
H	2.403765	-3.021269	-1.139316
H	3.837893	-4.025372	-0.794054
H	3.401900	-0.000013	0.981317

TS2
Geometry with 72 atoms:
Thermal correction to Gibbs Free Energy:
0.524007
Total energy: -2389.819006

C	5.505331	-0.417640	-0.226906
O	5.721244	0.887012	-0.018539
C	7.087723	1.346034	-0.057436
C	7.081096	2.836309	0.204315

O	6.396424	-1.213588	-0.444773
H	7.516382	1.099563	-1.042301
H	7.668079	0.794561	0.699921
H	6.646250	3.058339	1.191036
H	6.495993	3.366214	-0.563058
H	8.111358	3.223002	0.183907
O	-0.967065	-1.049432	-0.109737
C	-0.092242	-1.907383	0.029872
C	1.369495	-1.557024	-0.056456
C	1.717645	-0.213158	0.138765
C	3.056642	0.174039	0.088596
C	4.056493	-0.779715	-0.159860
C	3.700438	-2.124942	-0.353214
C	2.364104	-2.514585	-0.300091
H	2.087369	-3.556828	-0.461027
H	4.487841	-2.855145	-0.547665
H	3.330836	1.218455	0.241601
H	0.929074	0.512655	0.346329
O	-0.354757	-3.248127	-0.824313
C	-2.790302	-3.407165	-1.182233
C	-1.420866	-3.185338	-1.798502
H	-1.175542	-3.951978	-2.548367
H	-1.361802	-2.196438	-2.277249
H	-3.044046	-2.589763	-0.491711
H	-2.828849	-4.369923	-0.646639
H	-3.551193	-3.434332	-1.978465
O	-0.275297	-2.880829	1.288646
C	-1.271901	-2.485940	2.260583
C	-0.705740	-1.431362	3.191545
H	-1.529040	-3.413406	2.793778
H	-2.164203	-2.108402	1.738148
H	-0.497536	-0.506034	2.634233
H	-1.443836	-1.197684	3.975258
H	0.217309	-1.786928	3.675263
H	-0.550134	-3.583541	0.319877
Ti	-2.298407	0.670671	0.029497
O	-1.026875	1.307537	1.196120
C	-0.961124	2.407814	2.067295
C	0.227968	3.299043	1.731303
H	0.291561	4.147863	2.431746
H	0.132308	3.699376	0.709414
H	1.169620	2.729672	1.789368
H	-0.869904	2.037920	3.107835
H	-1.901365	2.988512	2.007975
O	-2.031586	0.761883	-1.781354
C	-0.884452	0.804361	-2.591358
C	-0.106742	2.103448	-2.410894
H	0.191813	2.218045	-1.356686
H	-0.728515	2.970686	-2.684549
H	0.801712	2.111269	-3.034674
H	-1.190831	0.688962	-3.648852
H	-0.229690	-0.055540	-2.349920
O	-3.548310	-0.517736	0.690720
C	-4.938090	-0.386685	0.860004
C	-5.691186	-0.637964	-0.441499
H	-6.779996	-0.551611	-0.291637
H	-5.470115	-1.644257	-0.831419
H	-5.385564	0.099799	-1.201486
H	-5.174096	0.629555	1.232231
H	-5.269546	-1.106729	1.633521
O	-3.385321	2.123611	0.098042
C	-3.731736	3.144221	-0.800922
C	-2.920569	4.410216	-0.552656
H	-1.846478	4.204335	-0.682089
H	-3.077739	4.781565	0.472537
H	-3.210995	5.203871	-1.260243
H	-4.812732	3.360614	-0.699865
H	-3.558381	2.786797	-1.835023

TS3
Geometry with 63 atoms:
Thermal correction to Gibbs Free Energy:
0.449018
Total energy: -2234.723203

C	-5.265624	-0.329848	0.280681
O	-5.580298	0.571577	-0.659253
C	-6.973951	0.905903	-0.814016
C	-7.080485	1.944511	-1.909361
O	-6.093395	-0.864229	0.991400
H	-7.358718	1.278223	0.149247
H	-7.533842	-0.011783	-1.057284
H	-8.134803	2.223710	-2.057410
H	-6.688203	1.552329	-2.860329
H	-6.514835	2.851389	-1.645354
O	0.797709	-2.382471	1.480164
C	0.414906	-1.480750	0.749475
C	-1.057535	-1.161264	0.570186

C	-1.977244	-1.807638	1.404697
C	-3.339226	-1.528142	1.299701
C	-3.798207	-0.598456	0.353863
C	-2.874411	0.044516	-0.489105
C	-1.514563	-0.236679	-0.380682
H	-0.797989	0.263988	-1.032089
H	-3.228660	0.765549	-1.226400
H	-4.064632	-2.024773	1.946669
H	-1.605652	-2.527868	2.135281
O	1.078081	0.043237	1.161094
C	1.148459	0.340829	2.544993
C	-0.062808	1.133077	3.015774
H	2.074525	0.910833	2.715020
H	1.239463	-0.614008	3.092928
H	-0.135400	2.088353	2.473637
H	-0.992111	0.569536	2.847203
H	0.021439	1.351219	4.092570
O	3.192855	-0.132158	-1.893797
C	4.428537	-0.729542	-2.207134
C	5.554535	0.296088	-2.203444
H	5.637236	0.766244	-1.212032
H	5.355584	1.088197	-2.942594
H	6.516693	-0.180550	-2.450128
H	4.348229	-1.206491	-3.202021
H	4.648481	-1.539626	-1.484656
O	3.532001	1.120040	0.583052
C	4.568956	0.934773	1.515645
C	4.765006	-0.538679	1.849255
H	5.561056	-0.668104	2.599056
H	5.042919	-1.102016	0.944257
H	3.832698	-0.970733	2.245009
H	4.333406	1.511976	2.428785
H	5.499635	1.362419	1.098362
O	1.130522	-1.332536	-0.583604
C	1.317450	-2.540282	-1.343236
C	0.052351	-2.952935	-2.074557
H	0.259241	-3.839694	-2.694385
H	-0.300883	-2.141954	-2.729718
H	-0.754811	-3.206066	-1.371222
H	1.659756	-3.322347	-0.647892
H	2.127882	-2.311680	-2.045630
Ti	2.257270	0.433041	-0.453816
O	1.256599	1.768579	-1.113730
C	0.518789	2.829283	-0.536221
H	0.066734	3.410764	-1.360031
H	-0.311026	2.403238	0.057055
C	1.379674	3.730691	0.337038
H	1.825139	3.155184	1.162786
H	2.199942	4.173472	-0.249650
H	0.771317	4.545111	0.761012

TS4

Geometry with 57 atoms:

Thermal correction to Gibbs Free Energy:

0.396299

Total energy: -2156.067873

C	5.465629	0.355470	-0.038734
O	5.606995	1.682967	0.083822
C	6.919310	2.213114	-0.130628
O	6.386641	-0.386618	-0.311909
H	7.632708	1.789213	0.592172
H	6.837155	3.297581	0.007488
O	-0.824906	-0.764096	1.356221
C	0.027461	-1.494479	0.733863
O	-0.077765	-2.829367	0.771019
C	-1.388526	-3.369039	0.962168
H	-1.273155	-4.459036	0.964185
H	-1.817931	-3.026353	1.914099
C	1.450714	-1.038849	0.576994
C	1.730874	0.329242	0.707924
C	3.027047	0.799550	0.513518
C	4.060767	-0.097449	0.192516
C	3.778569	-1.467348	0.074231
C	2.480449	-1.937681	0.265323
H	2.258349	-3.000435	0.166797
H	4.590394	-2.153564	-0.172875
H	3.245246	1.863987	0.603705
H	0.914729	1.018743	0.928868
Ti	-1.997388	0.163142	-0.104501
O	-0.636530	-1.051865	-0.914843
C	-0.443933	-1.781774	-2.103331
C	0.584661	-1.111599	-3.003870
H	1.556588	-1.037692	-2.491706
H	0.255777	-0.093674	-3.267419
H	0.722526	-1.685843	-3.934442
H	-1.419617	-1.868489	-2.614837
H	-0.118642	-2.804478	-1.832742

O	-3.179775	-0.133332	-1.448547
C	-4.527693	-0.544912	-1.469698
C	-5.465574	0.650987	-1.368844
H	-6.519020	0.327211	-1.379871
H	-5.303096	1.342012	-2.211324
H	-5.270088	1.192872	-0.430674
H	-4.723333	-1.245475	-0.634437
H	-4.712781	-1.103596	-2.406615
O	-3.175923	0.446380	1.225794
C	-3.362267	0.184996	2.594225
C	-2.548502	1.143533	3.453469
H	-2.833636	2.187294	3.245063
H	-1.478186	1.020311	3.228875
H	-2.712233	0.943862	4.524881
H	-3.064784	-0.857596	2.809881
H	-4.440393	0.275944	2.825145
O	-1.264938	1.785172	-0.373899
C	-1.695782	3.104844	-0.118613
C	-2.568713	3.631104	-1.249415
H	-2.015794	3.620110	-2.202333
H	-2.891584	4.664460	-1.044222
H	-3.462783	2.998757	-1.363992
H	-0.800612	3.742272	0.005722
H	-2.253278	3.129804	0.836870
H	7.268851	1.983443	-1.148563
H	-2.046176	-3.062971	0.133493

TS5
Geometry with 57 atoms:
Thermal correction to Gibbs Free Energy:
0.399404
Total energy: -2156.070732

C	-5.553631	0.016382	0.010984
O	-5.912495	-0.962439	0.853258
C	-7.295346	-1.333159	0.857449
O	-6.338069	0.579525	-0.724438
H	-7.926808	-0.473436	1.127945
H	-7.395943	-2.129270	1.604399
O	0.834848	0.804374	1.101381
C	0.092467	1.297361	0.176032
O	0.390335	2.471595	-0.374951
C	1.768931	2.905300	-0.338259
H	2.059845	3.053740	0.712891
C	-1.374699	0.994803	0.142041
C	-1.868125	-0.023908	0.968406
C	-3.220596	-0.356578	0.940507
C	-4.094620	0.331343	0.082223
C	-3.597733	1.354365	-0.741575
C	-2.245558	1.688008	-0.711642
H	-1.858526	2.484338	-1.347879
H	-4.288515	1.881892	-1.401460
H	-3.605804	-1.150124	1.581130
H	-1.177152	-0.554420	1.624975
Ti	1.981085	-0.693020	0.272327
O	0.692187	0.053760	-1.093890
C	0.794124	0.331312	-2.461755
H	0.138685	-0.335414	-3.051285
H	1.837885	0.203381	-2.799770
O	1.521147	-2.420308	0.023707
C	0.909793	-3.099303	-1.054602
C	-0.608008	-3.009462	-0.977263
H	-1.074340	-3.556774	-1.812399
H	-0.918322	-1.955000	-1.021104
H	-0.972799	-3.439031	-0.030436
H	1.237945	-4.155244	-1.026020
H	1.266362	-2.677593	-2.013822
O	3.377436	-0.307805	-0.821070
C	4.718617	-0.744756	-0.821842
C	4.841252	-2.140579	-1.419663
H	4.234268	-2.852143	-0.837419
H	5.889397	-2.480402	-1.414561
H	4.474044	-2.149990	-2.458373
H	5.107760	-0.740093	0.214076
H	5.320409	-0.021309	-1.402791
O	2.813864	-0.769233	1.872004
C	3.118902	0.089377	2.941970
C	4.226876	1.071840	2.580838
H	4.433897	1.752332	3.422419
H	3.930443	1.674703	1.707954
H	5.156658	0.538094	2.328141
H	3.420906	-0.523046	3.812693
H	2.205213	0.642461	3.228300
H	-7.601929	-1.699021	-0.134123
H	2.401905	2.105436	-0.755337
C	1.869404	4.180231	-1.145339
H	1.214623	4.961175	-0.729369
H	2.906068	4.549200	-1.126216

```
 H   1.582976   4.004144  -2.193590
 H   0.490653   1.376635  -2.659227
```

TS6

Geometry with 64 atoms:

Thermal correction to Gibbs Free Energy: 0.461371

Total energy: -2235.078522

```
 C  -4.711597   0.038300  -0.412375
 O  -4.957091  -1.246311  -0.129350
 C  -6.281064  -1.760186  -0.396523
 O  -5.527328   0.793667  -0.898863
 H  -6.139461  -2.844954  -0.496730
 H  -6.633126  -1.354804  -1.356741
 O   1.664602   0.807313   0.684421
 C   0.721364   1.676695   0.827241
 C  -0.699891   1.270068   0.513882
 C  -1.102969  -0.040780   0.807105
 C  -2.400784  -0.455546   0.516586
 C  -3.311346   0.439585  -0.065553
 C  -2.909202   1.753909  -0.343648
 C  -1.610415   2.170623  -0.054368
 H  -1.297683   3.188530  -0.284632
 H  -3.625041   2.440749  -0.797717
 H  -2.709704  -1.477619   0.734718
 H  -0.405130  -0.750771   1.252953
 O   1.049430   3.014731   0.206259
 C   1.546557   2.627772  -2.151898
 C   2.088253   3.094280  -0.818117
 H   2.950263   2.498528  -0.485741
 H   2.365910   4.156157  -0.826013
 H   0.667941   3.218469  -2.450357
 H   1.268692   1.564334  -2.123413
 O   0.774902   2.362463   2.181191
 C   1.641623   1.800589   3.214541
 H   1.665686   2.589022   3.978505
 H   1.161326   3.249185   1.396537
Ti   2.144950  -0.846251  -0.185786
 O   1.104847  -0.955607  -1.605106
 C  -0.006720  -1.546042  -2.256920
 C  -0.860030  -0.483405  -2.928434
 H  -1.240300   0.233403  -2.186672
 H  -1.720331  -0.954717  -3.429032
 H  -0.596549  -2.109168  -1.512344
 H   0.378472  -2.267615  -2.997852
 O   3.861204  -0.814838  -0.596056
 C   4.854488  -0.888768  -1.603162
 C   4.338408  -0.390974  -2.944157
 H   4.025001   0.662363  -2.871421
 H   3.469622  -0.985439  -3.267040
 H   5.191423  -1.937885  -1.676286
 H   5.718008  -0.288328  -1.267062
 O   1.720884  -2.097941   0.991193
 C   2.114008  -3.150283   1.853382
 C   3.623650  -3.323309   1.889304
 H   4.011408  -3.546437   0.882954
 H   3.895947  -4.150909   2.562661
 H   1.619676  -4.075238   1.508380
 H   1.720971  -2.922152   2.859895
 H   2.650579   1.671841   2.797692
 H   4.110339  -2.403562   2.249702
 H   5.125677  -0.469948  -3.709908
 H   2.327462   2.752208  -2.917699
 H  -0.275826   0.067037  -3.681758
 C   1.078625   0.502608   3.754545
 H   1.140604  -0.301580   3.007851
 H   1.668456   0.195744   4.631652
 H   0.031119   0.629224   4.066401
 C  -7.241873  -1.424465   0.730438
 H  -6.863486  -1.804346   1.691958
 H  -7.384098  -0.336633   0.808822
 H  -8.220866  -1.889004   0.534280
```

TS7

Geometry with 55 atoms:

Thermal correction to Gibbs Free Energy: 0.383506

Total energy: -2079.955038

```
 C   4.915635  -0.682495  -0.231197
 O   5.902660  -0.103449   0.453745
 C   7.249176  -0.597921   0.257577
 O   5.062964  -1.608590  -0.999418
 H   7.217504  -1.695965   0.200746
 H   7.783989  -0.301176   1.169718
 O  -0.639767   2.528803   1.488626
 C  -0.205058   1.628582   0.915132
```

C	1.053610	1.001925	0.552710
C	2.182431	1.570586	1.177156
C	3.442907	1.032726	0.928204
C	3.579230	-0.060414	0.061264
C	2.447724	-0.612749	-0.561749
C	1.183500	-0.091419	-0.320637
H	0.313167	-0.532286	-0.802806
H	2.576149	-1.461412	-1.234462
H	4.322499	1.460254	1.408906
H	2.067724	2.419491	1.852579
O	-1.369510	-0.021111	1.326610
C	-0.952091	-0.927305	2.346436
H	-1.396456	-0.596141	3.299698
H	0.145037	-0.845452	2.439014
O	-4.122608	0.372357	-0.025596
C	-5.474223	0.242804	0.371653
C	-5.580169	-0.477455	1.705445
H	-5.145913	-1.487125	1.632148
H	-6.635425	-0.571367	2.005227
H	-6.010611	-0.307536	-0.420510
H	-5.907204	1.255940	0.430377
O	-1.350980	1.458683	-0.849354
C	-1.530613	2.727628	-1.473990
C	-2.716543	2.711630	-2.424742
H	-3.643101	2.469322	-1.880314
H	-2.569285	1.960366	-3.216223
H	-0.596488	2.967977	-2.009706
H	-1.674190	3.487299	-0.684987
Ti	-2.412533	0.062731	-0.214030
O	-2.099263	-1.382979	-1.171226
C	-2.566567	-2.586545	-1.752372
H	-2.281987	-2.579236	-2.818841
H	-2.028736	-3.422105	-1.270840
C	-4.070028	-2.743114	-1.590174
H	-4.599462	-1.904506	-2.068786
H	-4.342839	-2.762265	-0.523243
H	-4.408146	-3.682281	-2.054523
H	-2.835830	3.699227	-2.896114
H	-5.040019	0.077748	2.488076
C	-1.353048	-2.355127	2.016755
H	-2.447938	-2.438155	1.926191
H	-0.901751	-2.674721	1.065522
H	-1.017819	-3.035357	2.814613
C	7.881213	0.004125	-0.984389
H	7.875822	1.103603	-0.931224
H	8.925546	-0.334711	-1.068298
H	7.340999	-0.311990	-1.888845

TS8
Geometry with 55 atoms:
Thermal correction to Gibbs Free Energy:
0.390328
Total energy: -2079.946505

O	-1.249637	0.839049	-1.720448
C	-0.705446	1.417345	-0.644032
O	-1.036302	2.682384	-0.378806
C	-2.388190	3.122130	-0.641048
C	-2.487246	4.568211	-0.209492
H	-2.600093	2.992322	-1.712748
H	-3.078277	2.481194	-0.069503
H	-1.777511	5.193541	-0.772168
H	-3.505308	4.941214	-0.397351
H	-2.271146	4.671038	0.864894
C	0.758006	1.165267	-0.375187
C	1.371311	0.018722	-0.899346
C	2.713548	-0.242256	-0.627757
C	3.455373	0.643977	0.169713
C	2.838658	1.791337	0.690732
C	1.497198	2.052815	0.420646
H	1.018728	2.946457	0.821426
H	3.425947	2.472988	1.308035
H	3.192201	-1.133299	-1.034279
H	0.793469	-0.673271	-1.512247
Ti	-2.280506	-0.622656	-0.996959
O	-1.545053	0.474298	0.457137
C	-1.151510	0.252895	1.819273
C	-2.371827	-0.087912	2.650926
H	-2.073166	-0.265302	3.695102
H	-2.860764	-0.996778	2.270671
H	-3.099875	0.736697	2.627087
H	-0.674709	1.182298	2.167300
H	-0.399100	-0.552185	1.840732
O	-3.877938	-0.855347	-0.341975
C	-5.145941	-0.625382	0.245355
C	-5.681823	-1.900161	0.872064
H	-5.007686	-2.259215	1.664493
H	-5.782116	-2.691506	0.113514

H	-6.672111	-1.711510	1.314722
H	-5.819814	-0.250396	-0.543335
H	-5.028807	0.175550	0.995125
O	-1.311908	-2.063609	-0.872704
C	-1.095389	-3.393528	-0.419623
C	-2.124607	-3.821007	0.610834
H	-3.142075	-3.749154	0.197963
H	-2.066638	-3.184333	1.506934
H	-1.939549	-4.863372	0.912265
H	-0.072520	-3.430632	-0.008674
H	-1.123563	-4.045954	-1.308676
C	4.898736	0.412537	0.491821
O	5.561109	1.147118	1.195462
O	5.383586	-0.693712	-0.081719
C	6.770329	-1.011303	0.161392
C	7.096135	-2.272840	-0.607406
H	6.918659	-1.135667	1.246275
H	7.389364	-0.158030	-0.159166
H	8.149772	-2.546025	-0.444484
H	6.464504	-3.110061	-0.272759
H	6.938551	-2.124720	-1.686814

TS9

Geometry with 55 atoms:

Thermal correction to Gibbs Free Energy: 0.391905

Total energy: -2079.946669

C	4.720210	0.220658	0.435983
O	5.195157	-0.853612	-0.206619
C	6.572784	-1.225027	0.021146
O	5.375985	0.891865	1.206252
H	6.616756	-2.291081	-0.240598
O	-1.458403	0.715454	-1.682955
C	-0.883710	1.295646	-0.617111
O	-1.222898	2.561646	-0.341846
C	-2.590193	2.970294	-0.578253
H	-2.773736	2.965297	-1.663210
C	0.594563	1.066701	-0.410856
C	1.221932	-0.004813	-1.058679
C	2.561653	-0.291211	-0.801622
C	3.286667	0.496795	0.106370
C	2.660208	1.582758	0.737657
C	1.321546	1.870075	0.479784
H	0.835980	2.714536	0.969442
H	3.237256	2.193025	1.434227
H	3.049048	-1.129577	-1.299397
H	0.654304	-0.618177	-1.758927
Ti	-2.527173	-0.697316	-0.905003
O	-1.611552	0.340309	0.488484
C	-1.593829	0.543148	1.909179
H	-2.642175	0.533483	2.245925
O	-2.118320	-2.311653	-0.410990
C	-1.418103	-3.458428	0.041843
C	0.082266	-3.297716	-0.122208
H	0.597134	-4.198427	0.245761
H	0.444742	-2.429108	0.446715
H	0.344077	-3.153419	-1.181501
H	-1.797769	-4.320176	-0.532486
H	-1.695868	-3.614051	1.098381
O	-4.182699	-0.331579	-0.489153
C	-5.347018	-0.739867	0.220494
C	-5.118477	-2.020524	1.003208
H	-6.036922	-2.298250	1.542567
H	-4.306828	-1.885921	1.735458
H	-4.841058	-2.845173	0.329365
H	-6.153786	-0.860206	-0.522228
H	-5.627093	0.093971	0.886025
H	6.800123	-1.109788	1.091431
H	-3.267146	2.234254	-0.114729
C	-2.763938	4.346208	0.024470
H	-2.064990	5.063019	-0.432793
H	-3.790698	4.700787	-0.151330
H	-2.583324	4.322979	1.110000
H	-1.194460	1.555399	2.078294
C	-0.764697	-0.523322	2.595370
H	-0.765012	-0.354503	3.683146
H	-1.183818	-1.521750	2.400297
H	0.274776	-0.498425	2.236386
C	7.518514	-0.400931	-0.834663
H	7.473920	0.660571	-0.550364
H	8.551536	-0.755149	-0.692654
H	7.262394	-0.495295	-1.901188

$TiOEt_3^+$

Geometry with 25 atoms:

Thermal correction to Gibbs Free Energy:

0.165939
Total energy: -1312.941934

Ti	0.158558	-0.141938	-1.211496
O	1.524231	0.360419	-0.239412
C	2.195479	0.058356	0.977286
C	3.682495	-0.125814	0.730886
H	4.120433	0.785697	0.295936
H	3.859808	-0.965347	0.040990
H	1.745170	-0.854311	1.405436
H	2.008838	0.890644	1.677108
O	-1.042226	1.091210	-0.855100
C	-1.136751	2.329287	-0.162151
C	-1.637741	2.130944	1.258027
H	-0.934786	1.506362	1.830865
H	-2.623472	1.642391	1.262028
H	-1.824751	2.972594	-0.736790
H	-0.142527	2.810131	-0.162791
O	-0.388541	-1.603729	-0.435242
C	-1.271402	-2.388159	0.350358
C	-2.300651	-1.534487	1.069232
H	-1.810667	-0.842814	1.770018
H	-2.990410	-2.178995	1.635716
H	-0.659790	-2.963266	1.066208
H	-1.758186	-3.110281	-0.327534
H	-2.882471	-0.940057	0.348785
H	-1.726815	3.106297	1.761429
H	4.195069	-0.340365	1.681702
C	2.467789	1.510162	0.955832
C	2.100954	2.859206	0.349826
H	1.678635	2.719599	-0.657768
H	2.986267	3.511054	0.278681
H	1.341777	3.364131	0.968525
H	3.253152	1.019626	0.349253
H	2.886750	1.648368	1.970532
O	-0.622429	1.220003	-1.095193
C	-1.484223	2.332784	-1.126510
C	-2.792603	2.062588	-0.393356
H	-3.451510	2.944677	-0.432118
H	-2.595718	1.812318	0.661043
H	-3.319364	1.210014	-0.851028
H	-1.686121	2.589499	-2.183635
H	-0.968141	3.203335	-0.678367
O	-1.242936	-0.620326	1.125832
C	-2.429873	-1.370803	1.205610
C	-2.450931	-2.525617	0.212068
H	-3.388079	-3.098039	0.300607
H	-1.604349	-3.206494	0.394879
H	-2.366567	-2.147077	-0.819353
H	-3.290466	-0.699013	1.025043
H	-2.533694	-1.755845	2.237708

$TiOEt_4$
Geometry with 33 atoms:
Thermal correction to Gibbs Free Energy:
0.226463
Total energy: -1467.777450

Ti	0.041832	-0.030495	0.015909
O	0.678155	-1.366502	-1.011188
C	1.489207	-2.514062	-0.928309
C	2.868113	-2.192053	-0.365573
H	3.381653	-1.458482	-1.007635
H	3.488953	-3.100046	-0.303147
H	2.774802	-1.753937	0.640764
H	1.582255	-2.951284	-1.940508
H	0.987333	-3.272824	-0.297188
O	1.351151	0.656585	1.047573