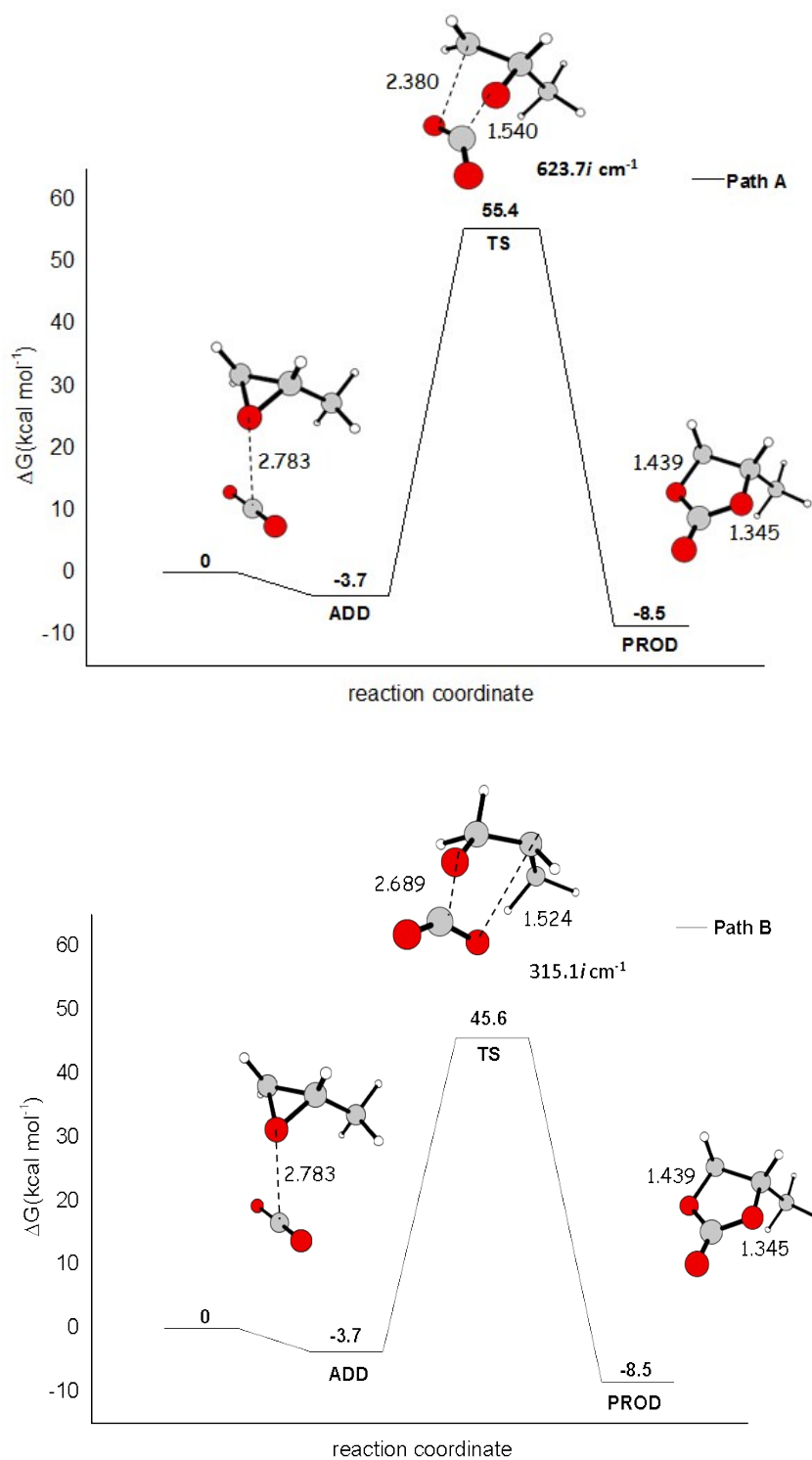


# Electronic Supplementary Information

## **On the ability of zinc pyrrolidine complex to catalyze the synthesis of cyclic carbonates from carbon dioxide and epoxides: A mechanistic theoretical investigation**

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**Figure S1.** M06L zero-point-corrected free energy profiles for the uncatalyzed attack of CO<sub>2</sub> on the less substituted carbon (Path A) and more substituted carbon (Path B) of PO. Energies are relative to the reactants' asymptote. The most significant distances (Å) are reported. Red=oxygen.

## Reaction with Zn-1 and co-cat

### Zn-1

8      -1.081908    -0.066101    -0.410103

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.544354	0.861024	0.972872
6	-0.376535	1.603134	0.299671
6	-0.152367	0.805471	-1.026105
6	-1.491855	0.099068	-1.210071
1	-1.344910	0.584546	2.012556
1	-2.434925	1.506055	0.935007
1	0.538499	1.550314	0.900561
1	0.148693	1.456056	-1.853795
1	-2.255294	0.811251	-1.559955
1	-1.448963	-0.754970	-1.894811
7	-1.732413	-0.356993	0.164294
6	-3.003822	-1.067945	0.399055
1	-2.951451	-1.996823	-0.179374
1	-3.012680	-1.343607	1.460038
6	-4.242966	-0.292513	0.040529
6	-4.751007	-0.338136	-1.263254
6	-4.895557	0.508273	0.984838
6	-5.876528	0.402215	-1.618182
1	-4.260141	-0.969721	-2.002548
6	-6.021673	1.251197	0.634871
1	-4.519804	0.540436	2.006348
6	-6.513347	1.201209	-0.668889
1	-6.260238	0.351336	-2.633645
1	-6.518000	1.865599	1.381269
1	-7.392802	1.777403	-0.942401
7	-0.764510	2.972212	0.006889
6	0.101657	3.907565	-0.107781
1	-0.313372	4.908531	-0.272023
6	1.573386	3.891737	-0.020080
6	2.224231	5.098102	0.272245
7	2.241575	2.740002	-0.233352
6	3.608505	5.110051	0.390530
1	1.641321	6.004154	0.413817
6	3.571684	2.774525	-0.125451
6	4.300987	3.920167	0.190899
1	4.136349	6.028697	0.628193
1	4.089362	1.832176	-0.303876
1	5.382360	3.875834	0.266780
7	0.815839	-0.228264	-0.751642
6	2.001093	-0.233976	-1.224718
1	2.371270	0.549339	-1.893679
6	2.887445	-1.340430	-0.854624
6	4.183355	-1.448857	-1.354732
7	2.359741	-2.244951	-0.004940
6	4.961202	-2.534099	-0.959235
1	4.565887	-0.697708	-2.039815
6	3.108967	-3.279435	0.368607
6	4.417642	-3.465404	-0.081898
1	5.974188	-2.649092	-1.331539
1	2.642864	-3.985046	1.052779
1	4.988650	-4.325015	0.251109
30	0.140287	-1.812979	0.473061
17	-0.693945	-3.513628	-0.788165
17	0.291712	-1.621789	2.723686

### Substrate

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.146434	-0.027714	0.514099
6	1.033014	0.620710	-0.052715
8	0.834973	-0.788951	-0.254138
1	-0.192673	-0.292798	1.586620
1	1.909553	0.862942	0.576342
1	0.965996	1.218006	-0.980862
6	-1.524928	0.097601	-0.160921
1	-2.078662	-0.805701	-0.011511
1	-2.059317	0.918808	0.269134
1	-1.394589	0.266766	-1.209394

### INT

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.509650	1.251774	0.906313
6	0.845753	1.731330	0.354974
6	0.979917	0.967684	-1.001142
6	-0.475288	0.654133	-1.335188
1	-0.451418	0.843510	1.920407
1	-1.208927	2.100378	0.900413
1	1.676491	1.439932	1.006364
1	1.518417	1.552469	-1.754438
1	-0.992614	1.564079	-1.676032
1	-0.595507	-0.139428	-2.080822
7	-0.946366	0.191489	-0.023250
6	-2.375696	-0.169322	0.060806
1	-2.530003	-1.002619	-0.632825
1	-2.541270	-0.557251	-1.072732
6	-3.330982	0.953154	-0.237324
6	-3.717421	1.230327	-1.554071
6	-3.846914	1.747811	0.791360
6	-4.589746	2.279803	-1.836726
1	-3.342835	0.602596	-2.361632
6	-4.722054	2.797195	0.515464
1	-3.572039	1.525518	1.821510
6	-5.092587	3.068319	-0.801189
1	-4.884099	2.477386	-2.864107
1	-5.120206	3.398449	1.328878
1	-5.776996	3.883600	-1.019268
7	0.810680	3.165285	0.124354
6	1.879901	3.865731	0.050889
1	1.720281	4.941533	-0.084710
6	3.305159	3.502083	0.150302
6	4.225691	4.533281	0.385347
7	3.681647	2.215296	0.005193
6	5.574724	4.224045	0.507447
1	3.874835	5.557647	0.476077
6	4.981933	1.938694	0.124378
6	5.964369	2.895159	0.378887
1	6.306769	5.003593	0.694608
1	5.260380	0.891619	0.007008
1	7.005347	2.600723	0.462519
7	1.612941	-0.296142	-0.717667
6	2.793948	-0.605354	-1.087314
1	3.419315	0.065740	-1.684556
6	3.321155	-1.913184	-0.689807
6	4.587289	-2.346493	-1.076888
7	2.500812	-2.662000	0.075693

### CO<sub>2</sub>

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.000071	0.000136	-0.000050
8	1.081961	0.065999	0.410140

6	5.021024	-3.600029	-0.653118
1	5.213430	-1.711874	-1.697360
6	2.921384	-3.860087	0.474964
6	4.176595	-4.370585	0.137518
1	6.001861	-3.967718	-0.937532
1	2.226786	-4.431211	1.086733
1	4.474958	-5.351731	0.490369
30	0.399260	-1.702415	0.306171
17	-0.624321	-2.997138	-1.271159
17	0.120442	-1.906073	2.541881
6	-6.429796	-0.457406	0.156895
6	-6.591010	-1.723048	-0.550047
8	-5.419117	-1.471376	0.224446
1	-6.123309	0.408609	-0.435434
1	-6.428919	-1.774353	-1.626825
1	-7.258876	-2.482271	-0.141198
6	-7.152586	-0.151536	1.430216
1	-6.519101	0.433892	2.104037
1	-8.053181	0.436772	1.228821
1	-7.447178	-1.069902	1.945346

1	-4.180230	-2.912852	-0.661168
1	-5.341570	-2.811398	-2.880259
30	-1.489760	-1.525165	0.644018
17	-3.100223	-1.538332	2.226901
17	-0.244155	-3.338448	0.030164
6	1.103190	-1.293162	3.146597
6	-0.129038	-0.774507	3.732709
8	0.050520	-0.762100	2.311265
1	1.975416	-0.636039	3.159823
1	-0.152014	0.214288	4.187642
1	-0.888876	-1.473790	4.078023
6	1.384214	-2.755848	3.046709
1	1.943732	-2.989500	2.136550
1	1.978948	-3.076619	3.907424
1	0.455563	-3.331560	3.022372

### INT1

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	2.748499	-0.031912	-1.908105
6	1.485730	0.843544	-1.809998
6	0.831136	0.419447	-0.463763
6	1.955235	-0.349828	0.233328
1	2.887149	-0.500784	-2.890227
1	3.626777	0.607647	-1.708737
1	0.782020	0.643142	-2.625340
1	0.530844	1.292624	0.112884
1	2.638070	0.378286	0.711152
1	1.591161	-1.041164	1.002405
7	2.556071	-1.056023	-0.884543
6	3.711271	-1.899328	-0.578474
1	3.367147	-2.676147	0.114815
1	4.002970	-2.398672	-1.510464
6	4.892542	-1.170944	0.012864
6	4.990412	-0.985032	1.396712
6	5.880091	-0.613942	-0.807513
6	6.043945	-0.259073	1.948449
1	4.232368	-1.421241	2.045912
6	6.936099	0.113730	-0.261182
1	5.821523	-0.760253	-1.885139
6	7.019017	0.294400	1.118956
1	6.106943	-0.129158	3.025528
1	7.696227	0.536843	-0.912544
1	7.843113	0.858596	1.546985
7	1.858385	2.251514	-1.823835
6	0.991296	3.193706	-1.768929
1	1.410552	4.206855	-1.758191
6	-0.480111	3.180214	-1.692022
6	-1.140863	4.387107	-1.426297
7	-1.140036	2.017192	-1.860087
6	-2.525339	4.383025	-1.291755
1	-0.568213	5.304536	-1.316453
6	-2.465836	2.030954	-1.731822
6	-3.204779	3.178640	-1.438148
1	-3.062045	5.300994	-1.070632
1	-2.967947	1.071243	-1.854904
1	-4.282027	3.117790	-1.322218
6	-0.333108	-0.449817	-0.564365
6	-0.429680	-1.302079	-1.516565
1	0.310451	-1.373617	-2.317767
6	-1.569911	-2.217780	-1.566872
6	-1.729628	-3.147975	-2.592176
7	-2.458661	-2.099773	-0.562424
6	-2.846616	-3.978604	-2.569628
1	-0.991002	-3.214438	-3.385192
6	-3.529012	-2.891882	-0.545679
6	-3.763555	-3.850010	-1.531993
7	-2.997930	-4.715240	-3.352073
6	-4.214582	-2.748751	0.286263
1	-4.646561	-4.476997	-1.480039
30	-1.826181	-0.647425	0.965726
17	-3.843427	0.403919	1.129134
17	-0.978354	-2.111602	2.500461

### TS1

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	2.117452	1.426057	-1.808505
6	0.948214	2.016268	-0.997996
6	0.488169	0.843031	-0.085159
6	1.683362	-0.110655	-0.151977
1	2.051545	1.624809	-2.885237
1	3.054955	1.875538	-1.434143
1	0.124247	2.335285	-1.642992
1	0.298557	1.184441	0.934202
1	2.471978	0.262662	0.529318
1	1.433526	-1.141087	0.125781
7	2.041469	-0.009772	-1.554715
6	3.185400	-0.812820	-1.985348
1	2.905814	-1.865542	-1.856373
1	3.317938	-0.637867	-3.059793
6	4.469401	-0.528902	-1.247100
6	4.771414	-1.211804	-0.062607
6	5.349556	0.465507	-1.688294
6	5.919486	-0.906381	0.665504
1	4.097254	-1.994382	0.286022
6	6.498696	0.776413	-0.962877
1	5.132018	0.995952	-2.614362
6	6.785120	0.091518	0.217204
1	6.142499	-1.450354	1.579717
1	7.173248	1.549499	-1.321317
1	7.681492	0.330338	0.782835
7	1.413479	3.144109	-0.203770
6	0.607953	3.931638	0.406164
1	1.091131	4.742749	0.963662
6	-0.861460	3.965038	0.512039
6	-1.441660	5.012066	1.242704
7	-1.597502	2.997597	-0.069254
6	-2.823569	5.055951	1.381771
1	-0.808496	5.772053	1.692806
6	-2.921137	3.050978	0.078905
6	-3.583970	4.051622	0.790947
1	-3.298236	5.854758	1.943547
1	-3.484132	2.245929	-0.393947
1	-4.665274	4.035704	0.879936
7	-0.692429	0.096430	-0.497897
6	-1.143810	0.156101	-1.693249
1	-0.715533	0.812908	-2.454653
6	-2.298660	-0.649535	-2.088777
6	-2.877864	-0.527568	-3.350072
7	-2.774925	-1.497357	-1.157234
6	-3.989536	-1.309974	-3.650609
1	-2.463450	0.169290	-4.072136
6	-3.837562	-2.245267	-1.448075
6	-4.479112	-2.183680	-2.685691
1	-4.465150	-1.237727	-4.623444

6	-0.866167	1.655121	3.321306
6	-1.172705	2.437918	2.126625
8	-0.694615	1.087428	2.002686
1	0.098098	1.839615	3.796737
1	-0.472016	3.189987	1.764947
1	-2.215710	2.563459	1.834590
6	-1.928076	1.064923	4.188687
1	-1.608724	0.099452	4.589144
1	-2.130967	1.734162	5.030157
1	-2.851572	0.917470	3.622760

1	-1.747255	-3.213289	-0.494210
6	-1.631479	-2.717870	-3.256897
1	-1.565120	-1.953319	-4.034931
1	-1.511113	-3.697386	-3.729773
1	-2.625958	-2.666127	-2.804278
53	3.295327	-2.456745	-0.647444

**INT2**

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	1.632321	2.258798	1.694920
6	0.821647	0.992004	2.032809
6	0.230942	0.538793	0.667824
6	1.129123	1.259051	-0.337106
1	1.386705	3.121922	2.328716
1	2.701884	2.028339	1.837074
1	0.001332	1.195338	2.730774
1	0.302490	-0.540435	0.551677
1	2.060761	0.671059	-0.434408
1	0.676424	1.362790	-1.330455
7	1.301231	2.553310	0.301657
6	2.170933	3.509605	-0.380404
1	1.782540	3.622534	-1.399752
1	2.052587	4.477966	0.122757
6	3.632474	3.134691	-0.412312
6	4.121243	2.210312	-1.343156
6	4.517858	3.656784	0.537151
6	5.456709	1.813679	-1.321205
1	3.447005	1.795057	-2.090141
6	5.856208	3.268580	0.559662
1	4.147369	4.376042	1.266819
6	6.328303	2.342806	-0.370095
1	5.814664	1.085388	-2.043936
1	6.529629	3.684949	1.304369
1	7.369266	2.032296	-0.351810
7	1.704210	-0.007473	2.618489
6	1.302382	-1.186075	2.915112
1	2.079453	-1.857987	3.297589
6	-0.020467	-1.830888	2.815861
6	-0.086279	-3.226533	2.916322
7	-1.116954	-1.065704	2.637632
6	-1.320219	-3.854852	2.785997
1	0.824263	-3.799421	3.072927
6	-2.292365	-1.683544	2.522991
6	-2.448903	-3.069616	2.576992
1	-1.397490	-4.936981	2.838306
1	-3.156649	-1.038989	2.364426
1	-3.431836	-3.511805	2.449187
7	-1.155938	0.919272	0.429187
6	-1.611839	2.009459	0.927349
1	-1.017547	2.648801	1.585262
6	-2.978040	2.442511	0.638700
6	-3.505896	3.615210	1.177150
7	-3.693127	1.639897	-0.170531
6	-4.816640	3.961537	0.862741
1	-2.895139	4.236415	1.825184
6	-4.948248	1.971917	-0.467588
6	-5.552989	3.127171	0.027822
1	-5.255767	4.869586	1.263936
1	-5.480075	1.286538	-1.123692
1	-6.577280	3.360599	-0.240754
30	-2.491608	-0.039740	-0.975648
17	-4.070697	-1.651811	-0.574844
17	-2.160068	0.883353	-3.042781
6	-0.568765	-2.523850	-2.225975
6	-0.770122	-2.852940	-0.817744
8	-0.776798	-1.477455	-1.247895
1	0.465810	-2.522509	-2.574050
1	0.089038	-3.109829	-0.196607

**TS2**

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	2.246332	-1.847711	-1.968168
6	1.259195	-0.672487	-2.092237
6	0.618680	-0.554773	-0.673711
6	1.579414	-1.376611	0.188192
1	2.173598	-2.574302	-2.788023
1	3.271341	-1.435173	-1.967737
1	0.476415	-0.868959	-2.831549
1	0.571589	0.486290	-0.337596
1	2.455775	-0.748670	0.437883
1	1.128520	-1.724459	1.122538
7	1.895001	-2.482065	-0.702444
6	2.836649	-3.476807	-0.193440
1	2.373210	-3.937833	0.687832
1	2.930426	-4.256941	-0.959323
6	4.201926	-2.946112	0.169179
6	4.435309	-2.400462	1.437084
6	5.243761	-2.932133	-0.764772
6	5.673937	-1.853124	1.763937
1	3.633130	-2.407162	2.173832
6	6.485991	-2.387143	-0.443124
1	5.077687	-3.359541	-1.752812
6	6.703046	-1.844026	0.822587
1	5.836131	-1.433336	2.753048
1	7.284722	-2.386157	-1.180402
1	7.670121	-1.417448	1.074997
7	1.978133	0.539687	-2.456127
6	1.364256	1.632087	-2.720327
1	2.013588	2.487675	-2.939152
6	-0.068953	1.973889	-2.786665
6	-0.411007	3.325301	-2.929397
7	-0.997021	0.999056	-2.717642
6	-1.752307	3.682963	-2.978328
1	0.373725	4.075607	-2.976413
6	-2.279357	1.358903	-2.772186
6	-2.711604	2.678911	-2.898038
1	-2.043773	4.725368	-3.068998
1	-3.003896	0.547839	-2.696367
1	-3.772620	2.907407	-2.913789
7	-0.714471	-1.110151	-0.512032
6	-1.166475	-2.010398	-1.296799
1	-0.608642	-2.387152	-2.159673
6	-2.508579	-2.551576	-1.076243
6	-3.080224	-3.486066	-1.939407
7	-3.157703	-2.075250	-0.000018
6	-4.373448	-3.929399	-1.677323
1	-2.517958	-3.848382	-2.795211
6	-4.392706	-2.503616	0.250062
6	-5.044603	-3.428636	-0.566091
1	-4.848818	-4.654607	-2.330552
1	-4.861540	-2.092249	1.141654
1	-6.053590	-3.746664	-0.326581
30	-1.979421	-0.546216	1.189865
17	-3.378498	1.234301	0.629951
17	-2.758469	-1.658460	3.153274
6	-0.240118	1.305906	2.788799
6	-0.550585	2.612741	2.310298
8	-0.320804	0.232418	2.041647
1	0.531407	1.282452	3.574502
1	-0.338431	3.485794	2.914095
1	-1.225165	2.708570	1.463417
6	-1.643771	1.667121	3.726574
1	-1.869489	0.620196	3.954501
1	-1.398669	2.235078	4.621748

1	-2.518533	2.070919	3.212570
53	1.621907	3.510647	0.588353

### INT3

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	2.967589	0.959272	1.772783
6	1.692447	0.113854	1.938078
6	0.966472	0.232546	0.565063
6	2.073126	0.751078	-0.353171
1	3.135217	1.668778	2.594435
1	3.832929	0.273360	1.737465
1	1.036382	0.506318	2.723087
1	0.583301	-0.730821	0.223181
1	2.695275	-0.107409	-0.671357
1	1.685531	1.248389	-1.249409
7	2.768870	1.683226	0.520022
6	3.944374	2.348044	-0.036566
1	3.618177	2.867120	-0.945752
1	4.259274	3.115598	0.682215
6	5.109621	1.440001	-0.345586
6	5.161145	0.715666	-1.542618
6	6.134321	1.256390	0.589369
6	6.206134	-0.170858	-1.796380
1	4.375744	0.854314	-2.283777
6	7.183748	0.373963	0.339792
1	6.106300	1.818255	1.522394
6	7.220390	-0.344284	-0.854694
1	6.230051	-0.725345	-2.730811
1	7.972156	0.246241	1.076986
1	8.036333	-1.034356	-1.052016
7	2.048575	-1.264560	2.238266
6	1.174378	-2.129024	2.599081
1	1.570718	-3.133002	2.796232
6	-0.283547	-2.046002	2.791796
6	-0.954129	-3.196170	3.232672
7	-0.929626	-0.899178	2.507849
6	-2.337590	-3.166321	3.356139
1	-0.389739	-4.098397	3.455325
6	-2.257423	-0.890573	2.619450
6	-3.009527	-1.992142	3.030082
1	-2.883423	-4.046292	3.683836
1	-2.751775	0.044457	2.354546
1	-4.091416	-1.925676	3.084139
7	-0.150090	1.157611	0.521657
6	-0.211674	2.166192	1.302264
1	0.548948	2.384421	2.060102
6	-1.361398	3.069646	1.228912
6	-1.458021	4.205261	2.033710
7	-2.319694	2.719442	0.355777
6	-2.592101	5.004547	1.922400
1	-0.657418	4.449152	2.726648
6	-3.401762	3.485627	0.253267
6	-3.584992	4.638978	1.018121
1	-2.698973	5.896795	2.531936
1	-4.143568	3.155247	-0.471678
1	-4.486294	5.231660	0.901388
30	-1.645587	1.001975	-1.110002
17	-3.877079	0.183084	-0.933223
17	-1.343668	2.834530	-2.625147
6	-0.937225	-1.280752	-2.851335
6	-1.759588	-2.425680	-2.276720
8	-0.514510	-0.386326	-1.897610
1	-0.050797	-1.732709	-3.347883
1	-2.027038	-3.191455	-3.009267
1	-2.644917	-2.057397	-1.752768
6	-1.791636	-0.639778	-3.954749
1	-1.235464	0.188007	-4.404299
1	-2.061283	-1.352896	-4.743315
1	-2.712914	-0.226684	-3.525858
53	-0.639622	-3.518989	-0.707254

### TS3

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	3.877996	-0.386041	1.178788
6	2.337084	-0.338378	1.105184
6	2.042915	0.213074	-0.352946
6	3.446897	0.360218	-0.974696
1	4.260304	-0.117852	2.170629
1	4.200449	-1.416426	0.950833
1	1.942593	0.394108	1.818677
1	1.455032	-0.526753	-0.901705
1	3.693413	-0.572869	-1.514404
1	3.518743	1.186996	-1.692772
7	4.319905	0.586226	0.177012
6	5.756906	0.688157	-0.075563
1	5.910744	1.546677	-0.743190
1	6.235127	0.935116	0.880586
6	6.445267	-0.532193	-0.678629
6	6.564030	-0.675493	-2.069507
6	6.957824	-1.551351	0.139002
6	7.167990	-1.804537	-2.630147
1	6.182211	0.108604	-2.719862
6	7.562063	-2.683360	-0.414684
1	6.883234	-1.457012	1.219700
6	7.668017	-2.814216	-1.802652
1	7.247570	-1.895580	-3.710376
1	7.947845	-3.462778	0.237088
1	8.135667	-3.694687	-2.234979
7	1.769355	-1.638782	1.437255
6	0.520258	-1.796121	1.218107
1	-0.111566	-1.020743	0.765121
6	-0.217363	-3.038528	1.547811
6	-1.597812	-3.042588	1.281159
7	0.426409	-4.099838	2.074617
6	-2.338796	-4.186775	1.573384
1	-2.055273	-2.154156	0.852537
6	-0.299463	-5.184748	2.350672
6	-1.678615	-5.285814	2.123607
1	-3.405339	-4.212815	1.368530
1	0.246059	-6.027032	2.776832
1	-2.208495	-6.201742	2.371155
7	1.214791	1.409422	-0.278779
6	1.731013	2.567225	-0.200415
1	2.815153	2.746760	0.852545
6	0.895465	3.783863	-0.105209
6	1.529618	5.031251	-0.200223
7	-0.441754	3.675019	0.057067
6	0.768078	6.197328	-0.147173
1	2.609052	5.071153	-0.314954
6	-1.167675	4.799917	0.109244
6	-0.611060	6.079371	0.004493
1	1.243126	7.172146	-0.220447
1	-2.234447	4.651429	0.257444
1	-1.255675	6.951172	0.055449
30	-1.613388	1.723148	0.775299
17	-0.563165	1.573825	2.785512
17	-3.702924	2.789521	0.780399
6	-2.399051	-0.023950	-1.477024
6	-3.943125	-0.069257	-1.322715
8	-1.759696	0.096880	-0.250386
1	-2.071190	-0.964021	-1.954483
1	-4.489344	0.485974	-2.084909
1	-4.253509	0.241524	-0.328882
6	-2.043761	1.118723	-2.457216
1	-0.954763	1.189054	-2.542219
1	-2.466592	0.938082	-3.454920
1	-2.424498	2.077403	-2.086282
53	-4.838907	-2.126360	-1.537871

INT4

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	3.261921	-0.728589	1.764330
6	1.842265	-0.184493	1.868706
6	1.578072	0.394333	0.447268
6	2.969180	0.405592	-0.210582
1	3.772812	-0.802729	2.730471
1	3.236748	-1.739603	1.311892
1	1.855035	0.646481	2.589317
1	0.912230	-0.269364	-0.109725
1	3.039008	-0.443365	-0.914292
1	3.168540	1.322849	-0.776223
7	3.893297	0.267334	0.912293
6	5.291657	0.023883	0.551815
1	5.641592	0.910091	0.007957
1	5.858323	-0.027503	1.489304
6	5.545485	-1.211402	-0.276256
6	5.544141	-1.140734	-1.673931
6	5.735278	-2.459374	0.328563
6	5.725558	-2.284075	-2.449427
1	5.402158	-0.174664	-2.156392
6	5.916363	-3.606690	-0.441821
1	5.745793	-2.528508	1.415351
6	5.910950	-3.521370	-1.833734
1	5.722084	-2.209580	-3.533514
1	6.063886	-4.567453	0.044164
1	6.052787	-4.414903	-2.435550
7	0.899526	-1.168318	2.357148
6	-0.339044	-0.969599	2.112546
1	-0.701109	-0.094618	1.541042
6	-1.408897	-1.872510	2.564943
6	-2.735496	-1.479709	2.346671
7	-1.079779	-3.038871	3.156176
6	-3.764598	-2.321784	2.753779
1	-2.938325	-0.525125	1.862135
6	-2.081216	-3.832006	3.535575
6	-3.433824	-3.527055	3.361094
1	-4.802072	-2.043339	2.591898
1	-1.791947	-4.771207	4.006462
1	-4.197920	-4.223560	3.692146
7	0.929551	1.697772	0.418384
6	1.414768	2.671826	1.089944
1	2.307462	2.576012	1.722920
6	0.761550	3.979135	1.028479
6	1.190527	5.054663	1.806072
7	-0.285109	4.068207	0.188051
6	0.495939	6.257878	1.720408
1	2.046298	4.939494	2.465185
6	-0.948410	5.219905	0.111647
6	-0.596023	6.342034	0.863567
1	0.801282	7.113262	2.314979
1	-1.779002	5.232215	-0.590738
1	-1.168442	7.258649	0.768955
30	-0.916359	2.129045	-0.871116
17	-2.682120	1.830079	0.668566
17	-1.614239	3.543406	-2.680821
6	-1.353425	-0.463110	-2.266769
6	-1.597474	-1.330104	-1.041625
8	-0.435721	0.477563	-1.819453
1	-0.887033	-1.092502	-3.052228
1	-2.130224	-0.771777	-0.267090
1	-0.669989	-1.750906	-0.650403
6	-2.634898	0.132268	-2.828222
1	-2.399275	0.827354	-3.637778
1	-3.311200	-0.641293	-3.209132
1	-3.159919	0.698746	-2.048283
53	-2.866404	-3.161333	-1.375433

INT5

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-2.555435	-2.089447	-1.947934
6	-1.426404	-1.069888	-2.038296
6	-1.486528	-0.342906	-0.659378
6	-2.825723	-0.806905	-0.061055
1	-2.939327	-2.400807	-2.925538
1	-2.194796	-2.993363	-1.418734
1	-1.693476	-0.343935	-2.820407
1	-0.658177	-0.666631	-0.024547
1	-2.625590	-1.574502	0.709372
1	-3.382815	0.005595	0.417056
7	-3.560187	-1.348486	-1.201716
6	-4.791434	-2.069356	-0.871891
1	-5.462213	-1.574511	-0.383620
1	-5.257744	-2.357653	-1.821783
6	-4.617974	-3.283706	0.005716
6	-4.684216	-3.174127	1.399451
6	-4.332717	-4.535172	-0.552342
6	-4.467272	-4.282736	2.215723
1	-4.913108	-2.207266	1.845918
6	-4.115492	-5.647446	0.258543
1	-4.284501	-4.635311	-1.635735
6	-4.181180	-5.522870	1.646061
1	-4.522485	-4.179119	3.296017
1	-3.897790	-6.612138	-0.192140
1	-4.011854	-6.388769	2.280201
7	-0.162800	-1.669481	-2.409212
6	0.899348	-1.002617	-2.164243
1	0.879902	-0.011724	-1.673557
6	2.247481	-1.472935	-2.519125
6	3.317190	-0.582413	-2.364240
7	2.404621	-2.732027	-2.975008
6	4.599851	-1.003355	-2.698747
1	3.127578	0.421627	-1.986019
6	3.642877	-3.117467	-3.281177
6	4.770920	-2.300834	-3.166470
1	5.446951	-0.332411	-2.588149
1	3.747269	-4.141213	-3.639611
1	5.751408	-2.682470	-3.434289
7	-1.364477	1.106816	-0.739192
6	-2.205728	1.769176	-1.438176
1	-3.014149	1.288062	-2.006077
6	-2.101745	3.225934	-1.492632
6	-2.922688	3.991551	-2.320920
7	-1.156975	3.772762	-0.706524
6	-2.739879	5.370875	-2.349161
1	-3.679557	3.506417	-2.930616
6	-0.982771	5.092474	-0.740087
6	-1.748647	5.931831	-1.550918
1	-3.359159	5.995590	-2.985246
1	-0.210760	5.477216	-0.077350
1	-1.568713	7.001536	-1.544624
30	0.150966	2.306282	0.477398
17	1.967045	2.577186	-0.988732
17	0.208691	3.998881	2.182302
6	1.479604	0.184740	2.124889
6	2.065264	-0.631126	0.983192
8	0.297467	0.683270	1.590824
1	1.242746	-0.501427	2.963622
1	2.396196	0.018584	0.168190
1	1.363433	-1.382727	0.618481
6	2.437722	1.250230	2.632168
1	1.963174	1.844777	3.416682
1	3.356579	0.808474	3.034281
1	2.707597	1.930608	1.814213
53	3.885775	-1.853691	1.484452
6	-1.636993	1.408651	3.130519

8	-2.305071	1.647589	2.197206
8	-1.081779	1.179219	4.134492

8	1.981279	-1.460538	3.559546
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### TS4

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.328322	3.394555	-1.061739
6	-0.377546	1.870219	-1.156157
6	0.331064	1.413084	0.144558
6	-0.102849	2.481994	1.132673
1	0.496384	3.801277	-1.668933
1	-1.266522	3.808962	-1.452108
1	0.163861	1.473580	-2.026526
1	-0.014649	0.418751	0.433497
1	-1.100530	2.204855	1.511593
1	0.579963	2.566913	1.990034
7	-0.112131	3.721389	0.354571
6	-0.903025	4.819473	0.904295
1	-0.527448	5.013478	1.918068
1	-0.687046	5.715889	0.307629
6	-2.391348	4.578142	0.944310
6	-2.981513	3.908411	2.022559
6	-3.207007	4.950057	-0.130219
6	-4.337344	3.591662	2.013656
1	-2.367408	3.632588	2.878317
6	-4.563176	4.636600	-0.144635
1	-2.768314	5.493024	-0.966441
6	-5.130371	3.948490	0.925332
1	-4.773716	3.057515	2.853815
1	-5.176267	4.922479	-0.995528
1	-6.185402	3.687964	0.910041
7	-1.753776	1.402167	-1.093000
6	-1.978864	0.326507	-1.746714
1	-1.180133	-0.172234	-2.322500
6	-3.269135	-0.374905	-1.745351
6	-3.324421	-1.631536	-2.363761
7	-4.334109	0.186576	-1.142590
6	-4.519426	-2.340121	-2.352098
1	-2.424814	-2.044801	-2.815970
6	-5.468972	-0.505664	-1.146731
6	-5.622516	-1.765913	-1.731198
1	-4.581298	-3.326827	-2.803358
1	-6.314746	-0.028698	-0.648833
1	-6.578593	-2.280269	-1.685578
7	1.748807	1.272854	-0.096383
6	2.555684	2.255192	-0.022033
1	2.244387	3.275540	0.247971
6	3.971162	2.011869	-0.309771
6	4.912564	3.040150	-0.252468
7	4.302463	0.750685	-0.638410
6	6.239076	2.751268	-0.555536
1	4.597106	4.042114	0.028106
6	5.573686	0.475590	-0.923362
6	6.576159	1.448155	-0.902101
1	6.995960	3.530834	-0.518120
1	5.773380	-0.570581	-1.150568
1	7.598507	1.175644	-1.144929
30	2.646979	-0.860699	-0.455840
17	1.329259	-1.068592	-2.358630
17	4.305916	-2.463035	-0.416514
6	0.620643	-2.499320	1.233231
6	-0.720441	-2.076987	0.653121
8	1.427591	-1.348630	1.126015
1	0.495988	-2.713935	2.307132
1	-0.659777	-1.900768	-0.426517
1	-1.132200	-1.204953	1.164202
6	1.230386	-3.699162	0.535157
1	2.225114	-3.897679	0.940192
1	0.607172	-4.591246	0.659226
1	1.351145	-3.499716	-0.536594
53	-2.323753	-3.608617	0.903688
6	2.398073	-0.851327	2.617780
8	3.154801	-0.034451	2.162415

### INT6

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.264232	3.259722	1.133385
6	-0.164700	1.744576	1.321756
6	-0.754087	1.181642	0.001587
6	-0.297231	2.216787	-1.010858
1	-1.114460	3.678729	1.693321
1	0.649055	3.729418	1.521527
1	-0.749379	1.373864	2.176277
1	-0.326787	0.193832	-0.197139
1	0.748560	1.987180	-1.278659
1	-0.894321	2.205492	-1.932332
7	-0.453427	3.485057	-0.305429
6	0.230892	4.639498	-0.889561
1	-0.152935	4.760725	-1.910494
1	-0.077150	5.526764	-0.323208
6	1.735077	4.534393	-0.912154
6	2.387643	3.876917	-1.962501
6	2.507248	5.025127	0.147637
6	3.768023	3.688995	-1.941378
1	1.804696	3.511836	-2.806604
6	3.888217	4.841212	0.173078
1	2.018024	5.561137	0.959455
6	4.521397	4.166003	-0.869495
1	4.256531	3.171321	-2.762480
1	4.470473	5.224652	1.006993
1	5.597722	4.017569	-0.849668
7	1.230003	1.341882	1.392339
6	1.486188	0.353764	2.160748
1	0.689449	-0.152754	2.731513
6	2.826885	-0.235668	2.290977
6	2.931214	-1.520145	2.840040
7	3.894635	0.465664	1.863230
6	4.184642	-2.115266	2.933631
1	2.033518	-2.038990	3.169762
6	5.087633	-0.118366	1.971519
6	5.290864	-1.398833	2.491963
1	4.293354	-3.115673	3.421282
1	5.937034	0.468967	1.624064
1	6.292163	-1.814796	2.546298
7	-2.182820	0.987319	0.112591
6	-3.034717	1.936585	0.083971
1	-2.764287	2.994259	-0.032307
6	-4.455259	1.584268	0.178171
6	-5.446793	2.563164	0.186850
7	-4.747088	0.267351	0.244827
6	-6.779598	2.171325	0.267256
1	-5.166516	3.610765	0.129572
6	-6.026483	-0.103606	0.319322
6	-7.076374	0.814706	0.333916
1	-7.572016	2.913523	0.275395
1	-6.194213	-1.177983	0.361896
1	-8.100462	0.462896	0.393476
30	-3.033532	-1.121535	0.162145
17	-1.783648	-1.431836	2.122786
17	-4.356883	-3.070204	0.075999
6	0.455192	-2.855618	-1.192396
6	1.442506	-1.743616	-0.899543
8	-0.850605	-2.268430	-1.049708
1	0.572220	-3.192751	-2.229223
1	1.387876	-1.423179	0.143946
1	1.302145	-0.895381	-1.570315
6	0.517247	-4.008570	-0.219891
1	-0.285243	-4.720278	-0.424048
1	1.473114	-4.532978	-0.301006
1	0.403241	-3.649087	0.807841
53	3.532308	-2.350700	-1.211967



6	-1.347517	-1.520525	-2.120967
8	-2.468925	-1.000974	-1.820024
8	-0.708109	-1.432217	-3.171612

6	0.452134	-1.795806	-1.262874
8	-0.702087	-1.348156	-1.465556
8	1.380876	-1.924352	-2.105228

**TS5**

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.737560	2.167056	1.276336
6	-0.991743	1.285876	0.268187
6	-1.985908	1.254749	-0.913294
6	-2.496288	2.683385	-0.918875
1	-2.292631	1.528417	1.978191
1	-1.026696	2.764283	1.858009
1	-0.813158	0.277560	0.670404
1	-1.463703	0.983786	-1.835036
1	-1.729965	3.302322	-1.412429
1	-3.436011	2.821965	-1.470772
7	-2.669167	3.002140	0.497820
6	-2.685607	4.429632	0.832126
1	-3.511175	4.884686	0.270143
1	-2.938860	4.513635	1.895775
6	-1.403320	5.170599	0.545329
6	-1.167109	5.723899	-0.719345
6	-0.393490	5.270706	1.511266
6	0.050571	6.330739	-1.021200
1	-1.951480	5.680733	-1.473563
6	0.826182	5.875706	1.214694
1	-0.570253	4.877664	2.511221
6	1.053660	6.402067	-0.055988
1	0.216261	6.748453	-2.010827
1	1.598412	5.939005	1.977170
1	2.007671	6.866714	-0.291983
7	0.226928	1.935442	-0.168588
6	1.320748	1.364070	0.155923
1	1.328390	0.417289	0.727676
6	2.649724	1.897121	-0.174954
6	3.774026	1.242070	0.341811
7	2.741853	2.990959	-0.957131
6	5.042194	1.730802	0.046339
1	3.655432	0.359029	0.967815
6	3.963819	3.447387	-1.225005
6	5.143095	2.863162	-0.753040
1	5.926165	1.230330	0.431252
1	4.010254	4.333647	-1.857781
1	6.107633	3.286857	-1.015097
7	-2.950474	0.193786	-0.660623
6	-4.185740	0.431199	-0.440315
1	-4.606684	1.441948	-0.419806
6	-5.093694	-0.692675	-0.193283
6	-6.453408	-0.504163	0.043743
7	-4.532712	-1.917393	-0.213499
6	-7.253748	-1.621855	0.266760
1	-6.867496	0.499826	0.052848
6	-5.299749	-2.984678	0.000237
6	-6.670219	-2.883377	0.243356
1	-8.316563	-1.507093	0.455646
1	-4.783958	-3.942818	-0.028354
1	-7.257772	-3.779121	0.412655
30	-2.306477	-1.907913	-0.239234
17	-2.080482	-1.678503	2.060213
17	-2.146264	-4.169493	-0.798456
6	1.985625	-2.876447	0.140288
6	2.979211	-2.231330	-0.795134
8	0.740538	-2.146175	0.021941
1	1.796263	-3.898702	-0.212981
1	3.113600	-1.157093	-0.779521
1	3.442103	-2.783240	-1.594811
6	2.279478	-2.881670	1.623353
1	1.369215	-3.176540	2.151316
1	3.080545	-3.580367	1.862299
1	2.578394	-1.886463	1.965761
53	5.454682	-2.397506	0.351475

**INT7**

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-3.088796	2.003706	1.186170
6	-1.963216	1.020811	0.821192
6	-2.447272	0.391885	-0.529295
6	-3.688411	1.200170	-0.877413
1	-3.305703	2.023485	2.259802
1	-2.774613	3.019707	0.880765
1	-1.883917	0.218101	1.572186
1	-1.661357	0.486123	-1.278753
1	-3.380397	2.098164	-1.444233
1	-4.416274	0.656612	-1.492584
7	-4.241024	1.526626	0.432405
6	-5.416312	2.400226	0.435801
1	-6.218596	1.856752	-0.079510
1	-5.724816	2.519577	1.481232
6	-5.224761	3.752193	-0.204502
6	-5.397971	3.914100	-1.584239
6	-4.823241	4.858367	0.552480
6	-5.174286	5.146667	-2.193960
1	-5.717906	3.062687	-2.183490
6	-4.601101	6.094939	-0.051573
1	-4.691794	4.747499	1.627896
6	-4.775005	6.241050	-1.427378
1	-5.314710	5.254593	-3.266118
1	-4.294357	6.945033	0.551643
1	-4.603385	7.204325	-1.899568
7	-0.710437	1.727485	0.667099
6	0.218887	1.401991	1.481306
1	0.071047	0.597225	2.221691
6	1.555779	2.011756	1.504245
6	2.503473	1.463045	2.377550
7	1.832620	3.053490	0.694709
6	3.793282	1.984722	2.399972
1	2.224911	0.626893	3.015276
6	3.070211	3.546483	0.737125
6	4.087523	3.051230	1.559448
1	4.553137	1.560078	3.049929
1	3.270541	4.385984	0.072560
1	5.080509	3.487818	1.525983
7	-2.661936	-1.044656	-0.326905
6	-3.826412	-1.489354	-0.029082
1	-4.695958	-0.831662	0.058578
6	-4.025917	-2.912908	0.238204
6	-5.290064	-3.443394	0.490150
7	-2.917950	-3.674965	0.221829
6	-5.402024	-4.810450	0.728145
1	-6.160419	-2.794467	0.493719
6	-3.027275	-4.982866	0.445166
6	-4.253584	-5.595002	0.706235
1	-6.371845	-5.263199	0.925084
1	-2.100923	-5.551359	0.406214
1	-4.297750	-6.663526	0.885817
30	-1.078258	-2.545889	-0.265111
17	-0.130291	-2.293346	1.808076
17	-0.390901	-4.122359	-1.773120
6	3.529430	-1.294188	-0.604804
6	3.385483	0.178994	-0.997955
8	2.189755	-1.821120	-0.877419
1	4.205812	-1.827872	-1.275658
1	3.745636	0.867072	-0.229086
1	3.852436	0.425432	-1.953331
6	3.871381	-1.544463	0.838064
1	3.869561	-2.613455	1.060421
1	4.868883	-1.139150	1.035630
1	3.151869	-1.050187	1.497719
53	7.111332	0.499777	-0.561207
6	1.348258	-0.815960	-1.079475

8	0.140235	-0.935323	-1.212109
8	1.956325	0.366671	-1.131748

## Reaction with co-cat on carbon less substituted

### INT

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	2.545629	0.140785	-0.415689
6	2.724035	-1.070292	0.371968
8	3.853653	-0.420884	-0.217123
1	2.178278	0.016659	-1.436114
1	2.474764	-2.043118	-0.050362
1	2.672767	-1.006251	1.459331
6	2.274730	1.467315	0.217437
1	2.734602	2.280724	-0.351888
1	1.194236	1.642365	0.251710
1	2.663125	1.496955	1.239451
53	-1.698365	-0.042398	-0.007876

### TS1

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	2.113061	-0.032924	-0.370837
6	1.036071	-0.841372	0.305190
8	3.134873	-0.853917	-0.028890
1	1.914628	0.006908	-1.448999
1	0.846035	-1.801660	-0.128262
1	1.035386	-0.817860	1.377637
6	2.254104	1.395203	0.147144
1	3.149849	1.833931	-0.283419
1	1.406190	2.020438	-0.116196
1	2.367764	1.396842	1.228719
53	-1.287137	0.020138	-0.016742

### INT1

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-2.103701	-0.235656	0.217277
6	-0.794819	-0.495003	0.999181
1	-2.796150	-0.442776	1.091330
1	-0.648001	-1.550011	1.154406
1	-0.687924	0.070038	1.914009
6	-2.284752	1.266459	-0.079051
1	-3.299050	1.423644	-0.434945
1	-2.119637	1.902480	0.794836
1	-1.603734	1.570382	-0.868122
53	1.144792	0.037385	-0.075110
8	-2.302482	-1.021248	-0.811892

### INT2

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.737879	1.060459	-0.396891
6	0.026381	-0.298557	-0.392878
8	1.989192	0.764012	-0.808289
1	0.191616	1.711316	-1.098387
1	0.043982	-0.768831	-1.358774
1	0.363343	-0.960500	0.386249
6	0.698959	1.739669	0.977564
1	1.298036	2.644769	0.934599
1	-0.305202	2.011255	1.292278
1	1.133995	1.088587	1.733324
53	-2.241736	-0.229832	-0.004475

6	4.118738	-0.643572	0.154032
8	3.532241	-1.219379	0.952450
8	4.802881	-0.131321	-0.607044

### TS2

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.918471	1.184648	0.145385
6	0.143280	0.547780	1.051843
1	-1.588004	1.590458	0.935587
1	-0.252123	-0.293831	1.594484
1	0.639562	1.241043	1.713268
6	-0.370933	2.405550	-0.605103
1	-1.194626	2.916858	-1.094458
1	0.125129	3.114748	0.056995
1	0.333051	2.097993	-1.372360
53	1.869177	-0.402028	-0.036407
8	-1.555483	0.312442	-0.650294
6	-3.439813	-0.705362	0.045478
8	-3.560349	-0.193112	1.072286
8	-3.585884	-1.363764	-0.888188

### INT3

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.918471	1.184648	0.145385
6	0.143280	0.547780	1.051843
1	-1.588004	1.590458	0.935587
1	-0.252123	-0.293831	1.594484
1	0.639562	1.241043	1.713268
6	-0.370933	2.405550	-0.605103
1	-1.194626	2.916858	-1.094458
1	0.125129	3.114748	0.056995
1	0.333051	2.097993	-1.372360
53	1.869177	-0.402028	-0.036407
8	-1.555483	0.312442	-0.650294
6	-3.439813	-0.705362	0.045478
8	-3.560349	-0.193112	1.072286
8	-3.585884	-1.363764	-0.888188

### TS3

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	1.074035	0.730839	-0.343360
6	0.437555	-0.442301	0.387961
1	0.483792	0.959064	-1.215173
1	0.259954	-0.406228	1.437775
1	0.432566	-1.401507	-0.079852
6	1.206577	1.966853	0.532786
1	1.672781	2.761991	-0.037052
1	0.229245	2.304384	0.858947
1	1.814720	1.760120	1.405662
53	-2.122024	-0.138039	-0.057778
6	3.100788	-0.450597	-0.044427
8	4.248229	-0.627548	-0.412557
8	2.508565	-0.888745	0.958177
8	2.325765	0.329981	-0.858846

### INT4

Atomic Number	Coordinates (Angstroms)						
	X	Y	Z				
				8	4.866123	-0.879138	-0.254896
				53	-2.794993	-0.133497	-0.049617
				6	1.520917	2.109792	0.363085
6	1.590516	-0.456973	0.543124	1	1.831908	2.937257	-0.263482
1	0.742218	-1.014216	0.184025	1	0.444630	2.158861	0.485725
1	1.478526	-0.247511	1.598055	1	1.989953	2.208963	1.335849
8	2.768366	-1.244061	0.364162	6	1.894557	0.795004	-0.279446
8	3.322122	0.704526	-0.421526	1	1.474868	0.717584	-1.273240
6	3.747286	-0.503862	-0.116625				

## Reaction with co-cat on carbon more substituted

### INT

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	2.545629	0.140785	-0.415689
6	2.724035	-1.070292	0.371968
8	3.853653	-0.420884	-0.217123
1	2.178278	0.016659	-1.436114
1	2.474764	-2.043118	-0.050362
1	2.672767	-1.006251	1.459331
6	2.274730	1.467315	0.217437
1	2.734602	2.280724	-0.351888
1	1.194236	1.642365	0.251710
1	2.663125	1.496955	1.239451
53	-1.698365	-0.042398	-0.007876

### TS1

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	1.263651	0.257750	-0.361299
6	1.978193	-0.879489	0.301908
8	3.229316	-0.656287	-0.167078
1	1.242300	0.164507	-1.447428
1	1.512909	-1.851113	0.012231
1	1.852348	-0.800620	1.411288
6	1.518899	1.642268	0.149168
1	0.912193	2.390069	-0.365283
1	1.319473	1.707898	1.224036
1	2.572689	1.887390	-0.012697
53	-1.203979	-0.082472	-0.000456

### INT1

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	1.163661	0.274573	-0.367455
1	1.182228	0.202384	-1.457989
53	-1.171555	-0.089035	0.001756
6	1.456033	1.656637	0.144124
1	2.518148	1.863553	-0.018066
1	0.872553	2.425981	-0.366428
1	1.260681	1.725191	1.220039
6	1.939886	-0.857060	0.275687
1	1.469843	-1.827656	-0.025496
1	1.780469	-0.791534	1.386432
8	3.206375	-0.665494	-0.143212

### INT2

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.104634	0.144929	-0.070587
1	0.294406	0.294427	-1.136962

53	-2.273620	-0.016024	-0.115131
6	0.434732	1.351296	0.761262
1	1.522902	1.463194	0.772920
1	-0.002279	2.269762	0.362330
1	0.094378	1.221025	1.794507
6	0.672999	-1.175052	0.412846
1	0.188741	-2.004500	-0.162055
1	0.334462	-1.321758	1.473838
6	4.269647	0.226071	-0.244422
8	4.855178	-0.779278	-0.127755
8	3.787205	1.283756	-0.382596
8	2.004763	-1.049023	0.240698

### TS2

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.416650	0.140366	-0.655586
1	0.132761	-0.025592	-1.690221
53	-2.256296	-0.034370	0.071596
6	0.743384	1.533597	-0.246539
1	0.815841	1.624540	0.840087
1	1.704851	1.830904	-0.679593
1	-0.003945	2.237013	-0.616272
6	1.020983	-1.015188	0.021465
1	0.512734	-1.974333	-0.157267
1	1.158350	-0.864512	1.104694
6	3.705761	0.000684	0.295059
8	3.313541	0.069202	1.417144
8	4.499639	0.143950	-0.579252
8	2.179625	-0.833550	-0.723192

### INT3

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.933207	-0.823494	-0.024682
6	0.067987	0.260425	-0.640528
8	2.224904	-0.744246	-0.597066
1	0.989210	-0.699895	1.062487
1	-0.036150	0.108140	-1.717579
53	-2.038717	-0.096038	0.076599
6	3.271026	-0.121246	0.186775
8	2.964827	0.268001	1.327772
8	4.341464	-0.085910	-0.444252
1	0.524830	-1.813731	-0.257731
6	0.478957	1.669760	-0.311231
1	0.488409	1.846407	0.767379
1	1.499139	1.826841	-0.679017
1	-0.170077	2.406808	-0.788911

### TS3

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

6	1.179684	-0.144140	1.065953
6	0.578289	0.678956	-0.032910
8	2.195744	-1.001972	0.580158
1	1.585626	0.542662	1.823629
1	0.617200	0.280899	-1.036803
53	-2.023102	-0.250096	-0.105425
6	3.128966	-0.299158	-0.212288
8	2.781495	0.889577	-0.479903
8	4.134866	-0.933747	-0.535683
1	0.445454	-0.785113	1.555413
6	0.279128	2.116368	0.179771
1	-0.194638	2.289127	1.149404
1	1.233326	2.655082	0.179625
1	-0.355826	2.529417	-0.603455

#### INT4

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	1.343744	-0.447831	0.704844
1	0.465609	-1.050796	0.472786
1	1.333466	-0.173843	1.765403
8	2.534663	-1.222279	0.451052
8	2.934070	0.760626	-0.468549
6	3.448832	-0.439837	-0.154661
8	4.585173	-0.778513	-0.382405
53	-2.460199	-0.157822	-0.073305
6	1.084201	2.076494	0.388775
1	1.310372	2.901858	-0.289222
1	0.004172	2.063221	0.563202
1	1.591734	2.251716	1.341749
6	1.497891	0.761490	-0.205460
1	1.005927	0.591812	-1.170501