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Kinetic investigations of Cl atoms initiated photo oxidation reactions of cyclic unsaturated hydrocarbons in the gas phase: an experimental and theoretical study

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Table S-1: Optimized geometries of the reactant, pre-reactive complexes, transition states and products for the reaction of Cl atoms with cyclohexene at MP2/6-31G(d,p) level of theory.

Table S-1-1: Optimized parameters of cyclohexene.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.00762	0.677408	1.303849
2	6	0	0.007617	1.506742	0.038783
3	6	0	0.392279	0.659805	-1.18419
4	6	0	0.007617	-0.67741	1.303849
5	6	0	-0.39228	-0.65981	-1.18419
6	6	0	-0.00762	-1.50674	0.038783
7	1	0	-0.98896	1.962812	-0.11568
8	1	0	0.71257	2.347663	0.160003
9	1	0	0.208105	1.226059	-2.11247
10	1	0	1.474049	0.4357	-1.14593
11	1	0	-1.47405	-0.4357	-1.14593
12	1	0	-0.20811	-1.22606	-2.11247
13	1	0	0.988958	-1.96281	-0.11568
14	1	0	-0.71257	-2.34766	0.160003
15	1	0	0.024813	-1.20829	2.26341
16	1	0	-0.02481	1.208286	2.26341

Table S-1-2: Optimized parameters of pre-reactive complex RC1a.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.661037	1.208174	-0.14249
2	6	0	2.154701	1.323955	-0.08302
3	6	0	2.804641	0.031859	0.410762
4	6	0	0.00455	0.015959	-0.05943
5	6	0	2.195247	-1.17699	-0.29398
6	6	0	0.71271	-1.29898	0.050291
7	1	0	2.526688	1.580249	-1.07898
8	1	0	2.418227	2.162045	0.566995
9	1	0	3.882934	0.073584	0.250074
10	1	0	2.645718	-0.06402	1.488643
11	1	0	2.29933	-1.05588	-1.37405
12	1	0	2.718811	-2.09276	-0.01532
13	1	0	0.591898	-1.67137	1.074216
14	1	0	0.221596	-2.02602	-0.59954
15	1	0	-1.07894	0.01694	-0.03317
16	1	0	0.079919	2.120836	-0.19913
17	17	0	-3.97079	0.019558	0.036908

Table S-1-3: Optimized parameters of transition state TS1a.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.38453	-0.20198	1.112523
2	6	0	0.377769	-1.40332	0.61529
3	6	0	1.20769	-1.07782	-0.63329
4	6	0	0.003506	1.088388	0.815086
5	6	0	2.022056	0.205084	-0.41308
6	6	0	1.089803	1.403419	-0.1703
7	1	0	1.039758	-1.73265	1.440518
8	1	0	-0.32943	-2.22493	0.425473
9	1	0	1.874812	-1.92334	-0.86697
10	1	0	0.523386	-0.94182	-1.48705
11	1	0	2.683738	0.074267	0.462342
12	1	0	2.66925	0.410766	-1.28094
13	1	0	0.598096	1.706688	-1.11426
14	1	0	1.651978	2.284705	0.182506
15	1	0	-0.54394	1.915832	1.276015
16	1	0	-1.12363	-0.35345	1.905108
17	17	0	-2.0554	0.041251	-0.52354

Table S-1-4: Optimized parameters of transition state TS2a.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.03679	-0.86314	1.067805
2	6	0	0.994212	-1.47445	0.167222
3	6	0	1.467613	-0.493	-0.91493
4	6	0	-0.39621	0.475084	0.990566
5	6	0	1.763429	0.872025	-0.27841
6	6	0	0.475056	1.495439	0.286756
7	1	0	1.847901	-1.80631	0.790902
8	1	0	0.568883	-2.38983	-0.27991
9	1	0	2.36396	-0.89408	-1.41444
10	1	0	0.67569	-0.38366	-1.6738
11	1	0	2.498687	0.737634	0.5359
12	1	0	2.215108	1.559259	-1.01143
13	1	0	-0.11263	1.977412	-0.50893
14	1	0	0.71731	2.28251	1.022625
15	1	0	-1.12264	0.852261	1.715783
16	1	0	-0.59285	-1.51461	1.748553
17	17	0	-2.03902	-0.02896	-0.51996

Table S-1-5: Optimized parameters of transition state TS1.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.20475	0.02673	-0.00386
2	6	0	0.393215	-1.32742	0.079341
3	6	0	1.881449	-1.18237	-0.31381
4	6	0	0.323104	1.201457	-0.10754
5	6	0	2.501177	0.037849	0.372997
6	6	0	1.83947	1.337385	-0.09661
7	1	0	0.288984	-1.72376	1.09609
8	1	0	-0.11876	-2.01868	-0.59835
9	1	0	2.418734	-2.09897	-0.04661
10	1	0	1.946457	-1.06108	-1.4016
11	1	0	2.367175	-0.05828	1.457854
12	1	0	3.578486	0.077161	0.179018
13	1	0	2.17681	1.603686	-1.10696
14	1	0	2.118006	2.16808	0.561699
15	1	0	-0.28445	2.100024	-0.19747
16	1	0	-1.75488	0.027605	0.023672
17	17	0	-3.1258	0.024848	0.026447

Table S-1-6: Optimized parameters of transition state TS2.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.350894	1.220954	0.497928
2	6	0	-0.23956	-0.10877	0.781211
3	6	0	0.413081	-1.26583	0.054766
4	6	0	1.497193	1.356921	-0.13997
5	6	0	1.938819	-1.1004	0.100537
6	6	0	2.340398	0.198413	-0.60154
7	1	0	-0.4778	-0.28161	1.836405
8	1	0	-1.41638	-0.04279	0.321068
9	1	0	0.100278	-2.21958	0.489242
10	1	0	0.092186	-1.25735	-0.99452
11	1	0	2.271337	-1.06422	1.145187
12	1	0	2.425632	-1.96019	-0.37213
13	1	0	2.232688	0.088777	-1.69018
14	1	0	3.396656	0.426567	-0.41798
15	1	0	1.877791	2.359536	-0.32929
16	1	0	-0.19075	2.098334	0.844286
17	17	0	-2.83039	0.002633	-0.29351

Table S-1-7: Optimized parameters of transition state TS3.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.64892	1.428529	0.31291
2	6	0	0.169691	0.40029	1.011198
3	6	0	-0.44642	-0.98719	1.031852
4	6	0	-1.6994	1.112844	-0.41967
5	6	0	-1.05406	-1.31236	-0.33255
6	6	0	-2.14644	-0.29963	-0.68142
7	1	0	1.188003	0.313247	0.399759
8	1	0	0.529702	0.735373	1.989865
9	1	0	0.304809	-1.72995	1.318798
10	1	0	-1.2339	-1.00069	1.799636
11	1	0	-0.26384	-1.2677	-1.09128
12	1	0	-1.461	-2.32873	-0.34074
13	1	0	-3.05708	-0.49642	-0.09689
14	1	0	-2.43489	-0.39329	-1.73508
15	1	0	-2.28913	1.912919	-0.86533
16	1	0	-0.36532	2.470898	0.438878
17	17	0	2.590351	-0.01592	-0.43244

Table S-1-8: Optimized parameters of transition state TS4.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.82875	1.254132	-0.1239
2	6	0	-0.31982	1.311116	0.010007
3	6	0	0.171088	-0.01334	0.540032
4	6	0	-2.5286	0.118966	-0.09516
5	6	0	-0.38492	-1.19963	-0.19759
6	6	0	-1.90647	-1.24612	0.05093
7	1	0	0.131752	1.521173	-0.96886
8	1	0	-0.03322	2.130426	0.677427
9	1	0	1.510693	-0.02552	0.293443
10	1	0	0.174861	-0.10661	1.630016
11	1	0	-0.20129	-1.07317	-1.27099
12	1	0	0.086745	-2.13325	0.122891
13	1	0	-2.11167	-1.63908	1.055793
14	1	0	-2.36958	-1.94471	-0.6562
15	1	0	-3.61311	0.168115	-0.17856
16	1	0	-2.34969	2.2036	-0.2378
17	17	0	2.915253	-0.02657	-0.09254

Table S-1-9: Optimized parameters of Transition state TS5.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.440081	0.985141	-0.77693
2	6	0	0.708039	1.487504	0.439808
3	6	0	-0.02376	0.387997	1.168979
4	6	0	1.557343	-0.31217	-1.08679
5	6	0	0.66696	-0.95199	1.176424
6	6	0	0.990794	-1.42517	-0.24511
7	1	0	1.421852	1.9478	1.142412
8	1	0	0.009716	2.285038	0.156956
9	1	0	-0.48943	0.689272	2.110729
10	1	0	-1.11997	0.185447	0.439127
11	1	0	1.609882	-0.82328	1.732659
12	1	0	0.069666	-1.69646	1.711927
13	1	0	0.085736	-1.82071	-0.72373
14	1	0	1.706764	-2.25372	-0.19889
15	1	0	2.072877	-0.58912	-2.00468
16	1	0	1.879315	1.733866	-1.43307
17	17	0	-2.31077	-0.04035	-0.41128

Table S-1-10: Optimized parameters of Transition State TS6.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.55772	-0.31202	-1.08663
2	6	0	0.990996	-1.42513	-0.24521
3	6	0	0.666882	-0.95211	1.176313
4	6	0	1.440332	0.985246	-0.77668
5	6	0	-0.02388	0.387863	1.168891
6	6	0	0.70794	1.487481	0.439903
7	1	0	0.086034	-1.82061	-0.72406
8	1	0	1.706962	-2.25368	-0.19894
9	1	0	0.069522	-1.69665	1.711641
10	1	0	1.609698	-0.82344	1.732717
11	1	0	-1.12	0.185317	0.438822
12	1	0	-0.48973	0.689018	2.110588
13	1	0	1.42153	1.947878	1.142668
14	1	0	0.00957	2.284921	0.156899
15	1	0	1.87973	1.734049	-1.43261
16	1	0	2.073524	-0.58886	-2.0044
17	17	0	-2.31099	-0.04035	-0.41134

Table S-1-11: Optimized parameters of Transition State TS7.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.52856	0.11887	-0.09542
2	6	0	-1.90636	-1.24613	0.0511
3	6	0	-0.38486	-1.19957	-0.1976
4	6	0	-1.82877	1.254049	-0.12402
5	6	0	0.171203	-0.01334	0.540076
6	6	0	-0.31989	1.311179	0.010326
7	1	0	-2.11138	-1.63871	1.056152
8	1	0	-2.36949	-1.94505	-0.65568
9	1	0	0.086893	-2.13321	0.122695
10	1	0	-0.20136	-1.073	-1.27101
11	1	0	0.174991	-0.10675	1.630061
12	1	0	1.510504	-0.02536	0.293369
13	1	0	0.131901	1.521666	-0.96835
14	1	0	-0.03361	2.130335	0.678074
15	1	0	-2.34972	2.203478	-0.23822
16	1	0	-3.61305	0.167937	-0.1792
17	17	0	2.915162	-0.02657	-0.09263

Table S-1-12: Optimized parameters of Transition State TS8.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.497078	1.356947	-0.13991
2	6	0	2.340475	0.198491	-0.60129
3	6	0	1.938839	-1.10039	0.100644
4	6	0	0.350657	1.220942	0.497689
5	6	0	0.413113	-1.26577	0.054477
6	6	0	-0.23957	-0.10888	0.78109
7	1	0	2.233016	0.088845	-1.68995
8	1	0	3.396674	0.426745	-0.41751
9	1	0	2.425712	-1.9601	-0.37212
10	1	0	2.271187	-1.06436	1.145388
11	1	0	0.092481	-1.25694	-0.99487
12	1	0	0.100089	-2.21963	0.488556
13	1	0	-0.47748	-0.28175	1.836364
14	1	0	-1.41668	-0.04309	0.321287
15	1	0	-0.19109	2.098236	0.843929
16	1	0	1.877664	2.359583	-0.32916
17	17	0	-2.8303	0.002614	-0.29342

Table S-1-13: Optimized parameters of Transition State TS9.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.699	1.112998	-0.41963
2	6	0	-2.14626	-0.2994	-0.68144
3	6	0	-1.05397	-1.31229	-0.33273
4	6	0	-0.64867	1.428485	0.313216
5	6	0	-0.44642	-0.98738	1.031778
6	6	0	0.169747	0.400052	1.011353
7	1	0	-3.05676	-0.49606	-0.09664
8	1	0	-2.43502	-0.39301	-1.73501
9	1	0	-1.46097	-2.32864	-0.34116
10	1	0	-0.26375	-1.26751	-1.09133
11	1	0	-1.23396	-1.00089	1.79944
12	1	0	0.304735	-1.73024	1.318765
13	1	0	1.188165	0.312887	0.399437
14	1	0	0.530279	0.734906	1.98988
15	1	0	-0.36494	2.470798	0.439325
16	1	0	-2.28848	1.913178	-0.86543
17	17	0	2.589887	-0.0159	-0.4325

Table S-1-14: Optimized parameters of Transition State TS10.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.323332	1.201586	-0.10823
2	6	0	1.839678	1.33736	-0.09656
3	6	0	2.501045	0.0379	0.373746
4	6	0	-0.20473	0.026741	-0.00492
5	6	0	1.881796	-1.18251	-0.31316
6	6	0	0.393104	-1.32741	0.078363
7	1	0	2.177591	1.603241	-1.10683
8	1	0	2.11802	2.168274	0.561548
9	1	0	3.578461	0.077154	0.180353
10	1	0	2.366417	-0.05799	1.458647
11	1	0	1.948111	-1.06179	-1.4009
12	1	0	2.418648	-2.09897	-0.04496
13	1	0	0.287753	-1.72414	1.094878
14	1	0	-0.11827	-2.01841	-0.60004
15	1	0	-1.75527	0.027902	0.02367
16	1	0	-0.28413	2.10019	-0.19833
17	17	0	-3.12604	0.024853	0.026852

Table S-1-15: Optimized parameters of product P1a.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.652227	0.118694	0.898843
2	6	0	-0.12677	1.362099	0.58701
3	6	0	-1.17381	1.123005	-0.49621
4	6	0	0.159619	-1.12802	0.646419
5	6	0	-1.98633	-0.13152	-0.18593
6	6	0	-1.08504	-1.36569	-0.14326
7	1	0	-0.61363	1.68063	1.516195
8	1	0	0.560711	2.158262	0.303342
9	1	0	-1.82779	1.992537	-0.5769
10	1	0	-0.66611	1.00285	-1.45457
11	1	0	-2.4779	-0.01178	0.783535
12	1	0	-2.77421	-0.27615	-0.92638
13	1	0	-0.78467	-1.65097	-1.15732
14	1	0	-1.61557	-2.22644	0.270254
15	1	0	0.730913	-1.98711	0.973955
16	1	0	1.504197	0.213731	1.559928
17	17	0	1.72498	-0.04512	-0.53725

Table S-1-16: Optimized parameters of product P2a.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.19132	-0.95501	0.888679
2	6	0	1.009499	-1.43429	0.144453
3	6	0	1.567973	-0.36172	-0.78748
4	6	0	-0.64392	0.340066	0.818972
5	6	0	1.636981	0.971426	-0.04913
6	6	0	0.232571	1.458345	0.311389
7	1	0	1.770088	-1.73969	0.873229
8	1	0	0.743155	-2.33854	-0.40879
9	1	0	2.552787	-0.65967	-1.14921
10	1	0	0.912404	-0.26399	-1.65417
11	1	0	2.225237	0.84112	0.863775
12	1	0	2.145339	1.727136	-0.64895
13	1	0	-0.24526	1.928684	-0.54724
14	1	0	0.284273	2.218841	1.094763
15	1	0	-1.47471	0.618656	1.45363
16	1	0	-0.78072	-1.6818	1.432905
17	17	0	-1.75314	-0.04492	-0.54537

Table S-1-17: Optimized parameters of product P1.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.045724	-1.0849	0.048795
2	6	0	1.427369	0.382781	0.112932
3	6	0	0.260627	1.271558	-0.31825
4	6	0	-0.19731	-1.4096	-0.0709
5	6	0	-1.04947	0.829239	0.331225
6	6	0	-1.431	-0.59361	-0.12487
7	1	0	1.740066	0.621685	1.13368
8	1	0	2.294573	0.556526	-0.52768
9	1	0	0.474508	2.312262	-0.06932
10	1	0	0.154431	1.216324	-1.40454
11	1	0	-0.93535	0.829614	1.4173
12	1	0	-1.85964	1.518263	0.086246
13	1	0	-1.83409	-0.58683	-1.14013
14	1	0	-2.20165	-1.01124	0.525276
15	1	0	1.831462	-1.82944	0.105555

Table S-1-18: Optimized parameters of product P2.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.193106	-0.8775	-0.0405
2	6	0	-0.14359	-1.49523	-0.02188
3	6	0	-1.28509	-0.56411	0.320628
4	6	0	1.366675	0.426475	0.048852
5	6	0	-1.07252	0.791185	-0.35851
6	6	0	0.237303	1.413114	0.118977
7	1	0	-0.32839	-2.19907	-0.83483
8	1	0	-2.23938	-1.00746	0.03748
9	1	0	-1.30667	-0.41257	1.402803
10	1	0	-1.02977	0.653509	-1.44137
11	1	0	-1.91316	1.453843	-0.14698
12	1	0	0.132482	1.768182	1.149953
13	1	0	0.486936	2.29174	-0.47981
14	1	0	2.375189	0.824627	0.044075
15	1	0	2.047407	-1.53637	-0.13668

Table S-1-19: Optimized parameters of product P3.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.46453	0.173592	-0.10735
2	6	0	-0.59753	1.363523	-0.15989
3	6	0	0.838588	1.130698	0.256854
4	6	0	-0.97728	-1.04315	0.052269
5	6	0	1.346144	-0.18316	-0.32784
6	6	0	0.487478	-1.34963	0.154521
7	1	0	-1.05161	2.258028	0.267749
8	1	0	1.461524	1.969113	-0.05656
9	1	0	0.875787	1.090394	1.351211
10	1	0	1.292734	-0.12158	-1.41672
11	1	0	2.391409	-0.34538	-0.06183
12	1	0	0.722561	-1.59581	1.196292
13	1	0	0.707227	-2.25122	-0.42199
14	1	0	-1.66381	-1.87917	0.128463
15	1	0	-2.53306	0.324369	-0.19797

Table S-1-20: Optimized parameters of product P4.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.061877	0.952961	-0.05437
2	6	0	1.439577	-0.50986	-0.11511
3	6	0	0.262874	-1.33334	0.336267
4	6	0	-0.18668	1.385785	0.052705
5	6	0	-1.03081	-0.95243	-0.32002
6	6	0	-1.38618	0.481245	0.111874
7	1	0	1.723701	-0.78047	-1.13648
8	1	0	2.31076	-0.69937	0.513759
9	1	0	0.203064	-1.51209	1.409025
10	1	0	-0.90167	-0.97574	-1.40391
11	1	0	-1.8335	-1.64308	-0.06203
12	1	0	-1.79353	0.476933	1.127427
13	1	0	-2.17915	0.86734	-0.53319
14	1	0	-0.37037	2.452854	0.109368
15	1	0	1.876718	1.667467	-0.09209

Table S-1-21: Optimized parameters of product P5.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.87866	1.142115	0.07288
2	6	0	-1.49592	-0.22686	0.011339
3	6	0	-0.4915	-1.30374	-0.29941
4	6	0	0.430028	1.363697	-0.00996
5	6	0	0.887867	-1.08762	0.257041
6	6	0	1.452454	0.271818	-0.15746
7	1	0	-1.96822	-0.46765	0.972657
8	1	0	-2.30398	-0.2441	-0.72477
9	1	0	-0.87378	-2.32173	-0.25137
10	1	0	0.802479	-1.11962	1.351146
11	1	0	1.557205	-1.89684	-0.03619
12	1	0	1.794526	0.229026	-1.19515
13	1	0	2.331368	0.501208	0.448477
14	1	0	0.79386	2.384672	0.009244
15	1	0	-1.55916	1.978646	0.179345

Table S-1-22: Optimized parameters of product P6.

Center Number	Atomic Number	Atomic Number	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.430029	1.363697	-0.00996
2	6	0	1.452454	0.271817	-0.15746
3	6	0	0.887867	-1.08762	0.25704
4	6	0	-0.87866	1.142116	0.072879
5	6	0	-0.4915	-1.30374	-0.29941
6	6	0	-1.49592	-0.22686	0.011338
7	1	0	1.794527	0.229026	-1.19515
8	1	0	2.331368	0.501207	0.448478
9	1	0	1.557205	-1.89684	-0.03619
10	1	0	0.802482	-1.11963	1.351145
11	1	0	-0.87379	-2.32173	-0.25137
12	1	0	-1.96822	-0.46765	0.972656
13	1	0	-2.30398	-0.2441	-0.72478
14	1	0	-1.55916	1.978646	0.179346
15	1	0	0.793861	2.384671	0.009246

Table S-1-23: Optimized parameters of product P7.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.18666	1.385786	0.052714
2	6	0	-1.38618	0.481263	0.111839
3	6	0	-1.03083	-0.95243	-0.31999
4	6	0	1.06189	0.952954	-0.05435
5	6	0	0.262873	-1.33334	0.336282
6	6	0	1.439571	-0.50987	-0.11514
7	1	0	-1.7936	0.476999	1.127367
8	1	0	-2.1791	0.867354	-0.53328
9	1	0	-1.83351	-1.64307	-0.06193
10	1	0	-0.90172	-0.97582	-1.40388
11	1	0	0.20309	-1.51207	1.409045
12	1	0	1.72364	-0.78047	-1.13652
13	1	0	2.31078	-0.6994	0.513687
14	1	0	1.876738	1.667452	-0.09204
15	1	0	-0.37034	2.452855	0.109412

Table S-1-24: Optimized parameters of product P8.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.366669	0.42649	0.048857
2	6	0	0.237285	1.413117	0.118967
3	6	0	-1.07253	0.791168	-0.35851
4	6	0	1.193116	-0.87749	-0.0405
5	6	0	-1.28507	-0.56413	0.32064
6	6	0	-0.14357	-1.49523	-0.0219
7	1	0	0.132463	1.768203	1.149937
8	1	0	0.486909	2.291737	-0.47984
9	1	0	-1.91318	1.453816	-0.14698
10	1	0	-1.0298	0.653486	-1.44137
11	1	0	-1.30663	-0.41258	1.402815
12	1	0	-2.23937	-1.00748	0.037519
13	1	0	-0.32837	-2.19905	-0.83487
14	1	0	2.047426	-1.53635	-0.13667
15	1	0	2.375178	0.824655	0.044092

Table S-1-25: Optimized parameters of product P9.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.97719	-1.04323	0.052272
2	6	0	0.487594	-1.34959	0.154506
3	6	0	1.346165	-0.18304	-0.32783
4	6	0	-1.46455	0.173466	-0.10734
5	6	0	0.838486	1.130769	0.256867
6	6	0	-0.59765	1.363467	-0.15991
7	1	0	0.722704	-1.59578	1.196269
8	1	0	0.707416	-2.25115	-0.42203
9	1	0	2.391441	-0.34517	-0.06181
10	1	0	1.292765	-0.12145	-1.41672
11	1	0	0.875666	1.090456	1.351222
12	1	0	1.461352	1.969242	-0.05652
13	1	0	-1.0518	2.257955	0.267686
14	1	0	-2.53309	0.324153	-0.19795
15	1	0	-1.66365	-1.87931	0.128482

Table S-1-26: Optimized parameters of product P10.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.045724	-1.0849	0.048795
2	6	0	1.427369	0.382781	0.112932
3	6	0	0.260627	1.271558	-0.31825
4	6	0	-0.19731	-1.4096	-0.0709
5	6	0	-1.04947	0.829239	0.331225
6	6	0	-1.431	-0.59361	-0.12487
7	1	0	1.740066	0.621685	1.13368
8	1	0	2.294573	0.556526	-0.52768
9	1	0	0.474508	2.312262	-0.06932
10	1	0	0.154431	1.216324	-1.40454
11	1	0	-0.93535	0.829614	1.4173
12	1	0	-1.85964	1.518263	0.086246
13	1	0	-1.83409	-0.58683	-1.14013
14	1	0	-2.20165	-1.01124	0.525276
15	1	0	1.831462	-1.82944	0.105555

Table S-2: Vibrational frequencies for the reactant, pre-reactive complexes, transition states and products for the reaction of Cl atom with cyclohexene at MP2/6-31G(d,p) level of theory.

Table S-2-1: Normal mode frequencies of R1, RC1a, TS1a, TS2a, TS1 and TS2 (cm^{-1}).

R1	RC1a	TS1a	TS2a	TS1	TS2
171.0	91.7	-325.3	-365.0	-193.6	-1209.2
284.2	155.6	108.3	86.6	59.3	63.7
405.9	176.0	155.3	144.5	60.3	89.0
457.6	265.3	236.6	258.2	197.5	181.1
503.5	316.7	293.6	288.0	290.7	277.2
661.0	456.5	363.0	341.3	399.7	353.9
744.3	490.8	461.1	458.6	453.9	447.0
844.8	649.1	505.6	499.6	478.4	508.4
861.2	681.1	680.5	703.0	627.8	547.8
921.3	766.8	798.1	775.3	685.5	699.5
942.4	839.4	833.9	831.1	788.4	780.4
960.1	860.4	860.0	853.4	815.4	855.6
993.1	920.4	919.4	915.0	855.4	877.7
1042.8	939.5	942.5	933.3	873.8	934.0
1084.9	955.6	957.7	950.0	935.4	953.7
1114.3	1039.4	1010.3	1022.9	939.9	979.8
1125.6	1066.7	1045.5	1047.4	980.5	1014.9
1186.3	1084.0	1078.9	1089.3	1016.2	1029.0
1188.1	1114.8	1110.3	1103.5	1062.1	1095.0
1281.5	1181.4	1120.9	1119.6	1115.6	1107.9
1303.1	1193.0	1185.8	1185.4	1132.7	1137.7
1327.5	1229.1	1194.7	1197.5	1197.7	1155.4
1383.5	1284.5	1281.0	1271.6	1201.8	1196.8
1416.5	1319.9	1301.9	1301.6	1287.3	1228.4
1420.2	1331.3	1332.1	1329.9	1301.7	1262.3
1425.2	1388.0	1386.6	1382.7	1323.3	1300.8
1457.2	1418.0	1419.2	1415.8	1365.5	1319.9
1529.4	1422.4	1424.8	1422.7	1387.6	1374.6
1537.5	1426.9	1431.0	1427.1	1406.7	1405.7
1543.3	1478.6	1472.6	1468.1	1422.0	1419.1
1554.3	1516.6	1511.9	1507.4	1525.3	1432.5
1739.0	1522.7	1519.5	1523.2	1531.8	1469.4
3100.1	1544.3	1543.1	1545.5	1538.4	1527.0
3100.4	1551.6	1551.1	1553.2	1548.9	1541.1
3118.3	1704.2	1644.0	1608.4	1589.6	1547.5
3119.4	3099.5	3103.0	3094.2	2081.9	1877.3
3152.7	3118.2	3109.6	3119.0	3118.5	3108.7

3153.0	3120.5	3121.8	3133.0	3127.1	3128.3
3177.1	3134.6	3138.9	3140.3	3129.9	3131.4
3183.2	3167.0	3165.8	3157.4	3134.1	3166.2
3229.0	3168.9	3185.7	3183.8	3173.3	3175.1
3252.1	3184.3	3194.1	3201.2	3183.8	3190.8
	3196.6	3202.5	3204.7	3188.7	3202.2
	3251.4	3269.6	3271.2	3198.0	3250.5
	3272.5	3285.9	3286.4	3262.6	3276.5

Table S-2-2: Normal mode frequencies of TS3, TS4, TS5, TS6 and TS7 (cm^{-1}).

TS3	TS4	TS5	TS6	TS7
-788.6	-771.6	-896.4	-896.4	-771.5
69.8	70.5	67.0	67.0	70.5
90.0	80.6	99.0	99.0	80.6
203.2	149.3	184.0	184.0	149.3
295.2	267.1	243.9	243.9	267.1
411.4	402.7	404.2	404.2	402.7
454.6	424.0	488.7	488.7	424.0
508.4	489.2	502.0	502.0	489.2
550.2	575.2	531.5	531.5	575.2
701.7	678.6	675.3	675.3	678.6
780.2	768.2	759.9	759.9	768.2
860.4	857.7	840.3	840.3	857.7
869.9	877.2	874.9	874.9	877.2
927.0	898.1	922.7	922.7	898.1
966.3	933.1	940.6	940.6	933.1
980.1	968.9	975.2	975.2	968.9
1045.1	981.9	997.2	997.2	981.9
1050.1	1017.1	1030.5	1030.5	1017.1
1091.5	1057.1	1042.7	1042.7	1057.1
1116.9	1078.2	1066.7	1066.7	1078.2
1131.3	1113.2	1087.5	1087.5	1113.2
1162.9	1156.7	1138.9	1138.9	1156.7
1200.9	1161.4	1152.9	1152.9	1161.4
1219.6	1188.9	1198.7	1198.7	1188.9
1306.3	1236.7	1226.5	1226.5	1236.7
1309.7	1285.6	1288.5	1288.5	1285.6
1344.5	1320.2	1320.5	1320.5	1320.2
1386.0	1353.2	1383.4	1383.4	1353.2
1413.1	1389.6	1386.9	1386.9	1389.6
1425.7	1407.3	1417.6	1417.6	1407.3
1434.0	1434.2	1435.0	1435.0	1434.2
1473.5	1449.1	1461.2	1461.2	1449.1
1520.8	1530.3	1509.4	1509.4	1530.3
1531.8	1535.6	1519.1	1519.1	1535.6
1548.4	1550.4	1539.3	1539.3	1550.4
1871.3	2734.1	2804.5	2804.5	2734.1
3103.2	3114.4	3082.0	3082.0	3114.4
3105.2	3122.1	3107.6	3107.6	3122.1
3136.0	3138.0	3124.0	3124.0	3138.0
3162.6	3165.7	3154.9	3154.9	3165.7

3182.3	3180.9	3174.2	3174.2	3180.9
3186.4	3199.3	3184.9	3184.9	3199.3
3197.7	3212.4	3208.1	3208.1	3212.4
3249.4	3238.4	3243.2	3243.2	3238.4
3277.2	3314.6	3324.3	3324.3	3314.6

Table S-2-3: Normal mode frequencies of Transition States TS8, TS9,TS10 and products P1a and P2a (cm^{-1}).

TS8	TS9	TS10	P1a	P2a
-1209.2	-788.6	-193.6	116.6	80.1
63.7	69.8	59.3	172.3	121.9
89.0	90.0	60.3	281.9	287.0
181.1	203.2	197.5	310.0	301.2
277.2	295.2	290.7	381.7	327.6
353.9	411.4	399.7	461.7	454.9
447.0	454.6	453.9	471.3	500.5
508.4	508.4	478.4	555.5	548.7
547.8	550.1	627.8	645.8	618.8
699.5	701.7	685.5	696.0	716.9
780.4	780.2	788.4	841.6	828.3
855.6	860.4	815.4	844.3	848.9
877.7	869.9	855.4	909.9	908.4
934.0	927.0	873.8	916.5	917.3
953.7	966.3	935.4	934.5	920.7
979.8	980.1	939.9	1044.1	1018.6
1014.9	1045.1	980.5	1078.5	1085.9
1029.0	1050.1	1016.2	1100.0	1094.5
1095.0	1091.5	1062.1	1111.6	1111.9
1107.9	1116.9	1115.6	1159.1	1179.3
1137.7	1131.3	1132.7	1187.4	1189.4
1155.4	1162.9	1197.7	1225.9	1232.7
1196.8	1200.9	1201.8	1289.3	1285.7
1228.4	1219.6	1287.3	1311.3	1305.7
1262.3	1306.3	1301.7	1332.6	1335.3
1300.8	1309.7	1323.3	1381.9	1371.9
1319.9	1344.5	1365.5	1398.5	1384.9
1374.6	1386.0	1387.6	1410.4	1411.8
1405.7	1413.1	1406.7	1428.4	1422.9
1419.1	1425.7	1422.0	1435.7	1430.7
1432.5	1434.0	1525.3	1452.1	1455.1
1469.4	1473.5	1531.8	1522.4	1520.5
1527.0	1520.8	1538.4	1528.1	1534.1
1541.1	1531.8	1548.9	1542.6	1550.1
1547.5	1548.4	1589.7	1552.2	1557.4
1877.3	1871.3	2081.9	3065.1	3085.2
3108.7	3103.2	3118.5	3115.5	3120.4
3128.3	3105.2	3127.1	3119.2	3124.8
3131.4	3136.0	3129.9	3130.0	3137.4

3166.2	3162.6	3134.1	3168.7	3140.9
3175.1	3182.3	3173.3	3178.3	3180.3
3190.8	3186.4	3183.8	3186.9	3198.0
3202.2	3197.7	3188.7	3192.3	3200.8
3250.5	3249.4	3198.0	3193.1	3207.4
3276.5	3277.2	3262.6	3278.9	3280.6

Table S-2-4: Normal mode frequencies of products P1, P2, P3, P4 and P5 (cm^{-1}).

P1	P2	P3	P4	P5
187.4	186.6	186.8	146.0	145.6
292.5	274.0	274.2	237.3	236.9
428.4	442.0	442.1	402.1	402.4
461.4	517.0	517.1	413.4	413.1
497.0	519.0	519.0	505.1	505.0
697.3	633.6	633.6	556.8	556.6
813.1	717.5	717.7	699.1	699.0
854.3	748.7	748.7	777.7	777.5
866.2	872.2	872.1	872.0	872.0
931.9	886.2	886.2	924.0	923.9
946.7	921.1	921.0	952.0	952.0
980.1	996.6	996.6	980.6	980.5
1024.0	1001.7	1001.7	1011.4	1011.2
1066.1	1041.8	1041.8	1060.4	1060.1
1114.5	1084.7	1084.5	1077.0	1076.6
1133.6	1102.4	1102.4	1085.2	1085.1
1193.5	1174.7	1174.6	1150.8	1151.2
1203.4	1186.6	1186.6	1203.8	1203.8
1291.9	1187.5	1187.4	1221.6	1221.6
1307.8	1245.2	1245.0	1239.3	1239.1
1326.1	1307.8	1307.8	1316.2	1316.1
1374.9	1383.6	1383.6	1381.4	1381.5
1391.1	1391.7	1391.6	1389.6	1389.5
1414.5	1416.0	1415.9	1417.3	1417.4
1420.9	1435.1	1435.0	1440.4	1440.6
1528.2	1466.1	1466.0	1464.2	1464.2
1536.0	1528.0	1528.0	1520.3	1520.4
1539.8	1533.2	1533.2	1527.4	1527.5
1552.0	1546.3	1546.3	1540.2	1540.2
2009.4	1584.1	1584.0	2741.5	2737.0
3110.1	3083.1	3083.1	3057.0	3057.2
3121.9	3083.5	3083.5	3080.0	3080.3
3124.1	3128.1	3128.1	3112.7	3112.8
3127.2	3156.9	3157.1	3132.9	3132.4
3163.0	3159.0	3159.1	3163.9	3163.8
3174.8	3189.3	3189.3	3173.9	3173.6
3181.4	3254.2	3254.3	3234.4	3234.5
3190.9	3281.0	3280.8	3280.3	3279.5
3252.9	3290.2	3290.0	3304.3	3303.7

Table S-2-5: Normal mode frequencies of products P6, P7, P8, P9 and P10 (cm^{-1}).

P6	P7	P8	P9	P10
145.6	146.0	186.6	186.8	187.4
236.9	237.3	274.0	274.2	292.5
402.4	402.1	442.0	442.1	428.4
413.1	413.4	517.0	517.1	461.4
505.0	505.1	519.0	519.0	497.0
556.6	556.8	633.6	633.6	697.3
699.0	699.1	717.5	717.7	813.1
777.5	777.7	748.7	748.7	854.3
872.0	872.0	872.2	872.1	866.2
923.9	924.0	886.2	886.2	931.9
952.0	952.0	921.1	921.0	946.7
980.5	980.6	996.6	996.6	980.1
1011.2	1011.4	1001.7	1001.7	1024.0
1060.1	1060.4	1041.8	1041.8	1066.1
1076.6	1077.0	1084.7	1084.5	1114.5
1085.1	1085.2	1102.4	1102.4	1133.6
1151.2	1150.8	1174.7	1174.6	1193.5
1203.8	1203.8	1186.6	1186.6	1203.4
1221.6	1221.6	1187.5	1187.4	1291.9
1239.1	1239.3	1245.2	1245.0	1307.8
1316.1	1316.2	1307.8	1307.8	1326.1
1381.5	1381.4	1383.6	1383.6	1374.9
1389.5	1389.6	1391.7	1391.6	1391.1
1417.4	1417.3	1416.0	1415.9	1414.5
1440.6	1440.4	1435.1	1435.0	1420.9
1464.2	1464.2	1466.1	1466.0	1528.2
1520.4	1520.3	1528.0	1528.0	1536.0
1527.5	1527.4	1533.2	1533.2	1539.8
1540.2	1540.2	1546.3	1546.3	1552.0
2737.1	2741.5	1584.1	1584.0	2009.4
3057.2	3057.0	3083.1	3083.1	3110.1
3080.3	3080.0	3083.5	3083.5	3121.9
3112.8	3112.7	3128.1	3128.1	3124.1
3132.4	3132.9	3156.9	3157.1	3127.2
3163.8	3163.9	3159.0	3159.1	3163.0
3173.6	3173.9	3189.3	3189.3	3174.8
3234.5	3234.4	3254.2	3254.3	3181.4
3279.5	3280.3	3281.0	3280.8	3190.9
3303.7	3304.3	3290.2	3290.0	3252.9

Table S-3: Optimized geometries of the reactant, transition states and products for the reaction of Cl atoms with cycloheptene at MP2/6-31G(d,p) level of theory.

Table S-3-1: Optimized parameters of cycloheptene.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.20793	0.885657	0.541986
2	6	0	-0.07361	1.600305	-0.15233
3	6	0	-1.65679	-0.40376	-0.1689
4	6	0	1.176336	1.119222	-0.29868
5	6	0	-0.48695	-1.32546	-0.5584
6	6	0	1.707496	-0.22734	0.130615
7	6	0	0.661538	-1.30789	0.461305
8	1	0	-0.90984	0.643485	1.568074
9	1	0	-2.06576	1.560811	0.628836
10	1	0	-2.33945	-0.94043	0.502397
11	1	0	-2.23193	-0.14883	-1.06721
12	1	0	-0.08881	-1.01987	-1.53321
13	1	0	-0.87012	-2.34433	-0.68549
14	1	0	1.173021	-2.27723	0.463278
15	1	0	0.266688	-1.17037	1.473921
16	1	0	2.3989	-0.09556	0.97547
17	1	0	2.325051	-0.60302	-0.6974
18	1	0	1.898508	1.758977	-0.80742
19	1	0	-0.27679	2.591946	-0.55486

Table S-3-2: Optimized parameters of Transition State TS1a.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.106372	-1.12505	1.266028
2	6	0	-0.66209	0.1742	1.204128
3	6	0	0.645104	-1.71229	-0.0547
4	6	0	-0.20965	1.371511	0.691688
5	6	0	1.329823	-0.70972	-1.00781
6	6	0	1.043823	1.645073	-0.08078
7	6	0	2.012703	0.473539	-0.30023
8	1	0	0.944676	-0.95523	1.967482
9	1	0	-0.53985	-1.87857	1.742966
10	1	0	1.360759	-2.50583	0.223213
11	1	0	-0.18848	-2.19608	-0.5855
12	1	0	0.578267	-0.30967	-1.70733
13	1	0	2.06931	-1.25808	-1.61478
14	1	0	2.844144	0.850345	-0.91913
15	1	0	2.462223	0.158429	0.657453
16	1	0	1.55364	2.490052	0.421014
17	1	0	0.726438	2.041693	-1.06514
18	1	0	-0.86169	2.237173	0.850813
19	1	0	-1.55781	0.237161	1.82978
20	17	0	-2.05813	0.022648	-0.7124

Table S-3-3: Optimized parameters of Transition State TS2a.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.909711	-1.40425	0.861957
2	6	0	-0.35557	-0.73043	1.31396
3	6	0	1.233721	-1.26867	-0.64363
4	6	0	-0.72452	0.580241	1.059441
5	6	0	1.389563	0.181646	-1.17816
6	6	0	0.153912	1.675422	0.507764
7	6	0	1.50777	1.264731	-0.09405
8	1	0	1.750351	-1.0099	1.461995
9	1	0	0.838596	-2.4755	1.107295
10	1	0	2.170499	-1.8272	-0.81013
11	1	0	0.443509	-1.78335	-1.21087
12	1	0	0.528064	0.427308	-1.81808
13	1	0	2.285532	0.223363	-1.81951
14	1	0	1.951661	2.171967	-0.538
15	1	0	2.203407	0.949812	0.702249
16	1	0	0.315652	2.384425	1.343106
17	1	0	-0.43772	2.224113	-0.24367
18	1	0	-1.63586	0.928943	1.555811
19	1	0	-1.08154	-1.3343	1.86657
20	17	0	-2.00116	-0.15717	-0.73885

Table S-3-4: Optimized parameters of Transition State TS1.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.51152	-1.47592	-0.51577
2	6	0	-0.03094	-1.21566	-0.25561
3	6	0	-2.45147	-0.78246	0.486256
4	6	0	0.480043	-0.03129	-0.27494
5	6	0	-2.10526	0.688758	0.793813
6	6	0	0.027076	1.37115	-0.42579
7	6	0	-1.51665	1.468942	-0.39185
8	1	0	-1.75102	-1.15064	-1.53269
9	1	0	-1.6905	-2.5553	-0.48908
10	1	0	-3.46764	-0.84159	0.076812
11	1	0	-2.45931	-1.34479	1.426972
12	1	0	-1.38681	0.728695	1.620724
13	1	0	-3.01369	1.18456	1.152903
14	1	0	-1.77284	2.531255	-0.3101
15	1	0	-1.93549	1.114677	-1.33989
16	1	0	0.437447	1.802195	-1.34637
17	1	0	0.434041	1.955611	0.409323
18	1	0	1.976335	-0.06649	-0.03686
19	1	0	0.613357	-2.07305	-0.06332
20	17	0	3.33344	-0.0839	0.231465

Table S-3-5: Optimized parameters of Transition State TS2.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.4425	0.402347	-0.03414
2	6	0	-1.4204	1.468398	-0.34377
3	6	0	-2.09199	-0.98983	-0.58955
4	6	0	-0.17871	1.501848	0.089702
5	6	0	-0.65161	-1.43184	-0.27889
6	6	0	0.483864	0.475058	0.940068
7	6	0	-0.12329	-0.91164	1.064745
8	1	0	-2.56225	0.332589	1.052528
9	1	0	-3.41668	0.708868	-0.42719
10	1	0	-2.80307	-1.70504	-0.15788
11	1	0	-2.24818	-1.0039	-1.67422
12	1	0	0.022275	-1.08142	-1.06768
13	1	0	-0.60359	-2.52573	-0.2973
14	1	0	0.650804	-1.58328	1.45275
15	1	0	-0.92088	-0.8963	1.821427
16	1	0	0.882324	0.880964	1.877807
17	1	0	1.545581	0.271822	0.342671
18	1	0	0.44504	2.352689	-0.18041
19	1	0	-1.75296	2.305613	-0.95643
20	17	0	2.900552	-0.06723	-0.40442

Table S-3-6: Optimized parameters of Transition State TS3.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.821933	0.927439	-0.88887
2	6	0	1.104484	1.599185	0.257213
3	6	0	2.581974	-0.34814	-0.48306
4	6	0	0.071189	1.073977	0.944001
5	6	0	1.7432	-1.3118	0.37577
6	6	0	-0.55673	-0.28875	0.775632
7	6	0	0.25748	-1.33066	-0.01333
8	1	0	1.098764	0.678869	-1.67348
9	1	0	2.527031	1.632609	-1.34144
10	1	0	2.902111	-0.85795	-1.40081
11	1	0	3.493761	-0.0766	0.062509
12	1	0	1.820876	-1.02409	1.430918
13	1	0	2.172315	-2.31707	0.296038
14	1	0	-0.17053	-2.31733	0.197651
15	1	0	0.146653	-1.1755	-1.09215
16	1	0	-1.64174	-0.169	0.301811
17	1	0	-0.71835	-0.68278	1.770288
18	1	0	-0.36015	1.685091	1.735459
19	1	0	1.438521	2.595804	0.543288
20	17	0	-3.2265	0.005904	-0.39025

Table S-3-7: Optimized parameters of Transition State TS4.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.326521	0.916307	-1.00965
2	6	0	1.017218	1.585804	0.29686
3	6	0	2.242404	-0.30658	-0.82838
4	6	0	0.210531	1.067224	1.193855
5	6	0	1.736262	-1.26143	0.259021
6	6	0	-0.47039	-0.24699	1.064197
7	6	0	0.207855	-1.37927	0.279775
8	1	0	0.389763	0.589534	-1.46422
9	1	0	1.779992	1.621678	-1.70601
10	1	0	2.296149	-0.83025	-1.786
11	1	0	3.25704	0.017267	-0.58739
12	1	0	2.077967	-0.92429	1.238148
13	1	0	2.175439	-2.24816	0.099448
14	1	0	-0.08601	-2.32241	0.742396
15	1	0	-0.17095	-1.42221	-0.7438
16	1	0	-1.50273	-0.04048	0.510705
17	1	0	-0.81681	-0.58986	2.039581
18	1	0	0.009204	1.616972	2.106088
19	1	0	1.491849	2.537171	0.509561
20	17	0	-2.85431	-0.01502	-0.49956

Table S-3-8: Optimized parameters of Transition State TS5.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.11155	1.105607	-0.87246
2	6	0	0.860709	1.530744	0.542519
3	6	0	2.161838	-0.01802	-0.94519
4	6	0	0.168342	0.789557	1.380847
5	6	0	1.881001	-1.1369	0.060279
6	6	0	-0.43203	-0.52201	1.009981
7	6	0	0.391629	-1.4886	0.134633
8	1	0	0.173636	0.740295	-1.29747
9	1	0	1.424352	1.952284	-1.48341
10	1	0	2.153312	-0.4242	-1.95963
11	1	0	3.161225	0.388217	-0.77507
12	1	0	2.235531	-0.85005	1.050216
13	1	0	2.445139	-2.02587	-0.22882
14	1	0	0.26968	-2.49478	0.537667
15	1	0	-0.0186	-1.51998	-0.87688
16	1	0	-1.40893	-0.25984	0.410151
17	1	0	-0.84094	-1.02133	1.888143
18	1	0	-0.00656	1.137403	2.391944
19	1	0	1.283822	2.467615	0.886837
20	17	0	-2.80764	0.020468	-0.49455

Table S-3-9: Optimized parameters of Transition State TS6.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.50399	1.572676	0.307588
2	6	0	-2.51426	0.660765	-0.35329
3	6	0	-0.03515	1.304451	-0.06942
4	6	0	-2.51418	-0.66097	-0.35326
5	6	0	0.484796	0.000086	0.494452
6	6	0	-1.5038	-1.57273	0.307657
7	6	0	-0.03499	-1.30432	-0.06945
8	1	0	-1.73327	2.597828	0.036355
9	1	0	-1.61055	1.519056	1.390416
10	1	0	0.067507	1.304859	-1.14998
11	1	0	0.574812	2.116756	0.313122
12	1	0	0.554631	0.000095	1.576832
13	1	0	1.76376	0.000179	0.193431
14	1	0	0.575102	-2.11657	0.313019
15	1	0	0.067593	-1.30465	-1.15001
16	1	0	-1.73294	-2.59793	0.036504
17	1	0	-1.61037	-1.51904	1.39048
18	1	0	-3.32306	-1.15566	-0.86608
19	1	0	-3.32322	1.155326	-0.86611
20	17	0	3.262321	-1E-06	-0.16492

Table S-3-10: Optimized parameters of Transition State TS7.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.50399	1.572676	0.307588
2	6	0	-2.51426	0.660765	-0.35329
3	6	0	-0.03515	1.304451	-0.06942
4	6	0	-2.51418	-0.66097	-0.35326
5	6	0	0.484796	0.000086	0.494452
6	6	0	-1.5038	-1.57273	0.307657
7	6	0	-0.03499	-1.30432	-0.06945
8	1	0	-1.73327	2.597828	0.036355
9	1	0	-1.61055	1.519056	1.390416
10	1	0	0.067507	1.304859	-1.14998
11	1	0	0.574812	2.116756	0.313122
12	1	0	0.554631	0.000095	1.576832
13	1	0	1.76376	0.000179	0.193431
14	1	0	0.575102	-2.11657	0.313019
15	1	0	0.067593	-1.30465	-1.15001
16	1	0	-1.73294	-2.59793	0.036504
17	1	0	-1.61037	-1.51904	1.39048
18	1	0	-3.32306	-1.15566	-0.86608
19	1	0	-3.32322	1.155326	-0.86611
20	17	0	3.262321	-1E-06	-0.16492

Table S-3-11: Optimized parameters of Transition State TS8.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.02798	1.290443	0.241392
2	6	0	-1.45028	1.631036	-0.15785
3	6	0	0.47076	0.046381	-0.47026
4	6	0	-2.49001	0.818123	-0.06314
5	6	0	-0.02224	-1.30223	0.011229
6	6	0	-2.47093	-0.60073	0.465197
7	6	0	-1.51303	-1.55365	-0.26381
8	1	0	0.620953	2.123875	-0.00068
9	1	0	0.040117	1.143458	1.316774
10	1	0	0.490289	0.149409	-1.54852
11	1	0	1.759753	0.021821	-0.2195
12	1	0	0.163527	-1.38643	1.07916
13	1	0	0.559494	-2.08127	-0.47131
14	1	0	-1.73427	-2.57052	0.049542
15	1	0	-1.70282	-1.5088	-1.33332
16	1	0	-3.47485	-1.00638	0.39514
17	1	0	-2.22451	-0.59239	1.526595
18	1	0	-3.44861	1.194465	-0.38139
19	1	0	-1.6091	2.620493	-0.55335
20	17	0	3.269549	-0.00494	0.092017

Table S-3-12: Optimized parameters of Transition State TS9.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.02798	1.290443	0.241392
2	6	0	-1.45028	1.631036	-0.15785
3	6	0	0.47076	0.046381	-0.47026
4	6	0	-2.49001	0.818123	-0.06314
5	6	0	-0.02224	-1.30223	0.011229
6	6	0	-2.47093	-0.60073	0.465197
7	6	0	-1.51303	-1.55365	-0.26381
8	1	0	0.620953	2.123875	-0.00068
9	1	0	0.040117	1.143458	1.316774
10	1	0	0.490289	0.149409	-1.54852
11	1	0	1.759753	0.021821	-0.2195
12	1	0	0.163527	-1.38643	1.07916
13	1	0	0.559494	-2.08127	-0.47131
14	1	0	-1.73427	-2.57052	0.049542
15	1	0	-1.70282	-1.5088	-1.33332
16	1	0	-3.47485	-1.00638	0.39514
17	1	0	-2.22451	-0.59239	1.526595
18	1	0	-3.44861	1.194465	-0.38139
19	1	0	-1.6091	2.620493	-0.55335
20	17	0	3.269549	-0.00494	0.092017

Table S-3-13: Optimized parameters of Transition State TS10.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.57738	-0.03038	0.7081
2	6	0	0.063484	1.269124	0.269541
3	6	0	0.011795	-1.40856	0.30857
4	6	0	1.312849	1.609803	-0.10475
5	6	0	1.281523	-1.38924	-0.54117
6	6	0	2.558088	0.783901	-0.26099
7	6	0	2.440472	-0.6751	0.165925
8	1	0	-0.66461	0.015183	1.803082
9	1	0	-1.69904	0.015856	0.304077
10	1	0	0.235629	-1.97634	1.21949
11	1	0	-0.76072	-1.97725	-0.2215
12	1	0	1.086272	-0.90732	-1.50782
13	1	0	1.554646	-2.42883	-0.75783
14	1	0	3.390137	-1.17781	-0.05053
15	1	0	2.296282	-0.73089	1.253422
16	1	0	3.369159	1.276326	0.293042
17	1	0	2.858333	0.818962	-1.31922
18	1	0	1.448623	2.665368	-0.34622
19	1	0	-0.64001	2.102664	0.303513
20	17	0	-3.23645	0.079223	-0.2497

Table S-3-14: Optimized parameters of Transition State TS11.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.2257	0.017665	-0.63816
2	6	0	-1.65651	1.380946	-0.30518
3	6	0	-1.12984	-1.01603	-0.94095
4	6	0	-0.43225	1.6121	0.272041
5	6	0	-0.54107	-1.65226	0.324416
6	6	0	0.418969	0.628977	1.013365
7	6	0	-0.30065	-0.6482	1.455274
8	1	0	-2.87078	-0.33854	0.171068
9	1	0	-2.86987	0.14203	-1.51469
10	1	0	-1.54356	-1.80516	-1.57907
11	1	0	-0.33658	-0.53208	-1.52346
12	1	0	0.400492	-2.15468	0.068316
13	1	0	-1.22475	-2.42881	0.688925
14	1	0	0.291395	-1.13102	2.240681
15	1	0	-1.25135	-0.35923	1.914329
16	1	0	0.814595	1.150378	1.893982
17	1	0	1.368359	0.365383	0.343759
18	1	0	-0.07998	2.641301	0.25802
19	1	0	-2.07845	2.219338	-0.85309
20	17	0	2.622515	0.017173	-0.5408

Table S-3-15: Optimized parameters of Transition State TS12.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.028246	-1.36039	0.269678
2	6	0	0.483846	0.039674	0.103293
3	6	0	-1.3799	-1.61374	-0.29123
4	6	0	0.046195	1.254207	0.059304
5	6	0	-2.46163	-0.6731	0.248258
6	6	0	-1.40191	1.696202	0.171797
7	6	0	-2.44841	0.72766	-0.37937
8	1	0	0.740154	-2.03433	-0.22035
9	1	0	0.054102	-1.60015	1.341011
10	1	0	-1.34842	-1.53659	-1.38475
11	1	0	-1.63994	-2.65147	-0.04873
12	1	0	-2.37861	-0.59529	1.341863
13	1	0	-3.4373	-1.128	0.041405
14	1	0	-3.4313	1.191007	-0.23072
15	1	0	-2.30723	0.627965	-1.46332
16	1	0	-1.49964	2.656266	-0.3477
17	1	0	-1.60761	1.897256	1.232429
18	1	0	0.781043	2.055886	-0.03081
19	1	0	1.951037	0.04323	0.013436
20	17	0	3.348532	0.038304	-0.07848

Table S-3-16: Optimized parameters of Product P1a.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.19259	-1.12627	1.124979
2	6	0	-0.94599	0.154116	0.893125
3	6	0	0.624687	-1.69909	-0.03939
4	6	0	-0.41242	1.345899	0.504587
5	6	0	1.471852	-0.68981	-0.82533
6	6	0	0.968516	1.644157	0.026487
7	6	0	1.974586	0.494273	0.002239
8	1	0	0.46473	-0.94749	1.981473
9	1	0	-0.90451	-1.88555	1.449358
10	1	0	1.272666	-2.47071	0.383768
11	1	0	-0.05677	-2.19782	-0.72715
12	1	0	0.881271	-0.30213	-1.65625
13	1	0	2.317632	-1.22041	-1.26655
14	1	0	2.899048	0.882794	-0.42934
15	1	0	2.223714	0.182664	1.01911
16	1	0	1.347195	2.476258	0.631037
17	1	0	0.86989	2.049093	-0.98725
18	1	0	-1.08439	2.196276	0.515935
19	1	0	-1.94005	0.201244	1.319631
20	17	0	-1.71896	0.01742	-0.7267

Table S-3-17: Optimized parameters of Product P2a.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.882118	-1.42707	0.756144
2	6	0	-0.53094	-0.99127	0.978976
3	6	0	1.48848	-1.03339	-0.60013
4	6	0	-1.02803	0.274356	0.809813
5	6	0	1.513797	0.477045	-0.91997
6	6	0	-0.23198	1.534648	0.622887
7	6	0	1.250847	1.394994	0.273166
8	1	0	1.502194	-1.02976	1.565291
9	1	0	0.928721	-2.51228	0.850653
10	1	0	2.506686	-1.42836	-0.60875
11	1	0	0.939008	-1.55788	-1.38097
12	1	0	0.771569	0.695157	-1.6869
13	1	0	2.487125	0.724735	-1.34742
14	1	0	1.620769	2.396439	0.043266
15	1	0	1.817304	1.063951	1.14588
16	1	0	-0.33666	2.101781	1.554887
17	1	0	-0.73321	2.127323	-0.14405
18	1	0	-2.04706	0.435505	1.139348
19	1	0	-1.24696	-1.75303	1.260693
20	17	0	-1.66325	-0.15526	-0.81866

Table S-3-18: Optimized parameters of Product P1.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.47684	0.451618	0.484526
2	6	0	-0.63586	1.512925	-0.20897
3	6	0	-1.35829	-0.94886	-0.13363
4	6	0	0.646402	1.430577	-0.30577
5	6	0	0.071734	-1.39435	-0.48283
6	6	0	1.723902	0.473523	0.028288
7	6	0	1.153415	-0.88805	0.477473
8	1	0	-1.1913	0.415271	1.536435
9	1	0	-2.52211	0.761969	0.467375
10	1	0	-1.79763	-1.65599	0.574523
11	1	0	-1.96899	-0.9988	-1.03722
12	1	0	0.322437	-1.05281	-1.48924
13	1	0	0.088172	-2.48499	-0.52035
14	1	0	1.986856	-1.59225	0.514002
15	1	0	0.764808	-0.8127	1.494361
16	1	0	2.384075	0.898707	0.787798
17	1	0	2.334566	0.318835	-0.86549
18	1	0	-1.14768	2.378401	-0.6167

Table S-3-19: Optimized parameters of Product P2.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.79403	1.21213	0.533629
2	6	0	0.519129	1.501741	-0.14233
3	6	0	-1.65874	0.149029	-0.15817
4	6	0	1.513348	0.656331	-0.31773
5	6	0	-0.90047	-1.13265	-0.52795
6	6	0	1.529301	-0.77245	0.052349
7	6	0	0.244953	-1.48084	0.42691
8	1	0	-0.59399	0.894841	1.559268
9	1	0	-1.36799	2.135599	0.615819
10	1	0	-2.48466	-0.08889	0.516655
11	1	0	-2.10684	0.572738	-1.05885
12	1	0	-0.48021	-1.04005	-1.53032
13	1	0	-1.60853	-1.96165	-0.57135
14	1	0	0.439321	-2.55472	0.405681
15	1	0	-0.01932	-1.24227	1.462809
16	1	0	2.397582	-1.05835	0.650046
17	1	0	2.425945	1.020623	-0.77647
18	1	0	0.677766	2.522352	-0.47353

Table S-3-20: Optimized parameters of Product P3.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.95876	1.085639	0.534788
2	6	0	0.289417	1.56167	-0.14984
3	6	0	-1.64341	-0.08648	-0.18933
4	6	0	1.402744	0.865745	-0.26026
5	6	0	-0.68492	-1.22251	-0.56529
6	6	0	1.618464	-0.51355	0.227072
7	6	0	0.425892	-1.43349	0.473326
8	1	0	-0.70696	0.77971	1.551791
9	1	0	-1.66631	1.909282	0.630891
10	1	0	-2.42434	-0.46982	0.471726
11	1	0	-2.14469	0.279404	-1.08753
12	1	0	-0.22723	-1.01913	-1.53437
13	1	0	-1.25715	-2.14493	-0.68058
14	1	0	0.785184	-2.46247	0.442187
15	1	0	0.026488	-1.28305	1.477567
16	1	0	2.395697	-1.00907	-0.35733
17	1	0	2.253474	1.323291	-0.75212
18	1	0	0.269299	2.55469	-0.58507

Table S-3-21: Optimized parameters of Product P4.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.88803	1.171013	0.502148
2	6	0	0.397631	1.553509	-0.17118
3	6	0	-1.66931	0.026372	-0.15961
4	6	0	1.497504	0.726168	-0.2456
5	6	0	-0.81679	-1.19804	-0.51689
6	6	0	1.552475	-0.60779	0.108701
7	6	0	0.357451	-1.45757	0.441111
8	1	0	-0.66546	0.884266	1.534528
9	1	0	-1.54067	2.042914	0.568969
10	1	0	-2.46849	-0.2685	0.525815
11	1	0	-2.15727	0.396259	-1.06395
12	1	0	-0.40148	-1.07335	-1.51754
13	1	0	-1.46314	-2.0778	-0.55397
14	1	0	0.651809	-2.50602	0.368984
15	1	0	0.031336	-1.31224	1.477349
16	1	0	2.515952	-1.09914	0.066277
17	1	0	2.415466	1.163709	-0.62397
18	1	0	0.496395	2.567887	-0.53459

Table S-3-22: Optimized parameters of Product P5.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.94572	1.129482	0.496131
2	6	0	0.325753	1.564206	-0.16405
3	6	0	-1.66943	-0.04985	-0.16429
4	6	0	1.453703	0.766192	-0.25413
5	6	0	-0.76324	-1.24224	-0.50607
6	6	0	1.581893	-0.52795	0.082788
7	6	0	0.439433	-1.41908	0.448867
8	1	0	-0.72659	0.861318	1.533597
9	1	0	-1.63667	1.971899	0.553305
10	1	0	-2.46528	-0.36867	0.515476
11	1	0	-2.16243	0.289825	-1.07735
12	1	0	-0.36379	-1.11609	-1.51263
13	1	0	-1.37249	-2.14895	-0.52169
14	1	0	0.779239	-2.45526	0.423737
15	1	0	0.105921	-1.24294	1.476413
16	1	0	2.571034	-0.94478	0.121294
17	1	0	2.351466	1.244811	-0.63141
18	1	0	0.385275	2.584241	-0.51631

Table S-3-23: Optimized parameters of Product P6.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.535349	0.369826	0.381387
2	6	0	0.671617	1.47424	-0.16397
3	6	0	1.301409	-0.9912	-0.31231
4	6	0	-0.67161	1.474244	-0.16397
5	6	0	-5E-06	-1.612	0.111007
6	6	0	-1.53535	0.369834	0.381388
7	6	0	-1.30142	-0.99119	-0.31231
8	1	0	2.585534	0.63749	0.258992
9	1	0	1.37021	0.249321	1.457048
10	1	0	1.314864	-0.84831	-1.39412
11	1	0	2.118544	-1.6685	-0.05689
12	1	0	-6E-06	-1.9523	1.148282
13	1	0	-2.11856	-1.66849	-0.05689
14	1	0	-1.31487	-0.8483	-1.39412
15	1	0	-2.58553	0.637506	0.258993
16	1	0	-1.37021	0.24933	1.457049
17	1	0	-1.18082	2.324843	-0.60283
18	1	0	1.180834	2.324836	-0.60283

Table S-3-24: Optimized parameters of Product P7.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.535349	0.369826	0.381387
2	6	0	0.671617	1.47424	-0.16397
3	6	0	1.301409	-0.9912	-0.31231
4	6	0	-0.67161	1.474244	-0.16397
5	6	0	-5E-06	-1.612	0.111007
6	6	0	-1.53535	0.369834	0.381388
7	6	0	-1.30142	-0.99119	-0.31231
8	1	0	2.585534	0.63749	0.258992
9	1	0	1.37021	0.249321	1.457048
10	1	0	1.314864	-0.84831	-1.39412
11	1	0	2.118544	-1.6685	-0.05689
12	1	0	-6E-06	-1.9523	1.148282
13	1	0	-2.11856	-1.66849	-0.05689
14	1	0	-1.31487	-0.8483	-1.39412
15	1	0	-2.58553	0.637506	0.258993
16	1	0	-1.37021	0.24933	1.457049
17	1	0	-1.18082	2.324843	-0.60283
18	1	0	1.180834	2.324836	-0.60283

Table S-3-25: Optimized parameters of Product P8.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.323657	-0.99075	0.338894
2	6	0	1.62819	0.412314	-0.1614
3	6	0	0.082491	-1.5755	-0.27726
4	6	0	0.78101	1.42653	-0.1683
5	6	0	-1.2703	-1.08485	0.149544
6	6	0	-0.64884	1.418079	0.335884
7	6	0	-1.57608	0.360926	-0.28211
8	1	0	2.173315	-1.63266	0.128842
9	1	0	1.216855	-0.96847	1.423582
10	1	0	0.176386	-1.98869	-1.26967
11	1	0	-1.35053	-1.14396	1.235099
12	1	0	-2.03864	-1.73922	-0.25389
13	1	0	-2.59821	0.593685	0.008863
14	1	0	-1.53439	0.434387	-1.36615
15	1	0	-1.0789	2.397492	0.14984
16	1	0	-0.6489	1.295088	1.41919
17	1	0	1.13812	2.370342	-0.54871
18	1	0	2.624084	0.581515	-0.53856

Table S-3-26: Optimized parameters of Product P9.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)	Center Number	
			X	Y	Z
1	6	0	1.275677	-1.02209	0.350411
2	6	0	1.645889	0.354284	-0.17296
3	6	0	0.034316	-1.5688	-0.27794
4	6	0	0.814157	1.412348	-0.17549
5	6	0	-1.29768	-1.04594	0.139461
6	6	0	-0.5988	1.421567	0.353044
7	6	0	-1.55485	0.410084	-0.29171
8	1	0	2.113114	-1.7014	0.18217
9	1	0	1.132443	-0.96141	1.436579
10	1	0	0.126288	-2.00168	-1.26703
11	1	0	-1.37867	-1.08877	1.231953
12	1	0	-2.09225	-1.67961	-0.26191
13	1	0	-2.581	0.674132	-0.01956
14	1	0	-1.4815	0.486986	-1.37927
15	1	0	-1.01048	2.423511	0.218289
16	1	0	-0.58634	1.2429	1.435442
17	1	0	1.195165	2.350282	-0.56622
18	1	0	2.650928	0.486342	-0.55937

Table S-3-27: Optimized parameters of Product P10.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)	Center Number	
			X	Y	Z
1	6	0	-0.11007	1.638151	-0.29698
2	6	0	1.23352	1.165444	0.08289
3	6	0	-1.36173	0.931544	0.190337
4	6	0	1.666729	-0.0811	0.097575
5	6	0	-1.527	-0.52625	-0.22559
6	6	0	0.916708	-1.32589	-0.28185
7	6	0	-0.47696	-1.48184	0.331695
8	1	0	-0.19927	2.718535	-0.1819
9	1	0	-1.36665	1.002506	1.284062
10	1	0	-2.22355	1.499484	-0.16585
11	1	0	-1.53085	-0.58544	-1.31667
12	1	0	-2.51344	-0.85697	0.10807
13	1	0	-0.80895	-2.50586	0.145503
14	1	0	-0.40851	-1.36652	1.416712
15	1	0	1.522197	-2.18925	-0.0025
16	1	0	0.829125	-1.35411	-1.37374
17	1	0	2.703605	-0.22835	0.380703
18	1	0	1.949011	1.945597	0.317181

Table S-3-28: Optimized parameters of Product P11.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)	Center Number	
			X	Y	Z
1	6	0	-1.25415	1.115233	-0.00925
2	6	0	0.008506	1.678297	-0.01056
3	6	0	-1.65201	-0.32117	0.136712
4	6	0	1.265099	1.104068	0.019674
5	6	0	-0.6748	-1.38143	-0.36593
6	6	0	1.647221	-0.33569	-0.14155
7	6	0	0.663618	-1.38569	0.36846
8	1	0	-2.07898	1.818778	-0.02115
9	1	0	-1.84027	-0.51879	1.201025
10	1	0	-2.61643	-0.4634	-0.3578
11	1	0	-0.49966	-1.25049	-1.43746
12	1	0	-1.1551	-2.35553	-0.24404
13	1	0	1.135056	-2.36446	0.251491
14	1	0	0.492176	-1.24617	1.439529
15	1	0	2.616284	-0.49197	0.338898
16	1	0	1.816357	-0.52777	-1.20965
17	1	0	2.099129	1.794309	0.063652
18	1	0	0.010502	2.763805	-0.00989

Table S-3-29: Optimized parameters of Product P12.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)	Center Number	
			X	Y	Z
1	6	0	-1.26356	1.097236	0.053722
2	6	0	-0.00424	1.661547	0.000675
3	6	0	-1.66721	-0.34327	0.09596
4	6	0	1.258422	1.102464	-0.05377
5	6	0	-0.64675	-1.36081	-0.40073
6	6	0	1.668908	-0.33552	-0.09621
7	6	0	0.653339	-1.35776	0.400975
8	1	0	-2.08852	1.796704	0.121631
9	1	0	-1.93609	-0.60135	1.128803
10	1	0	-2.59315	-0.4537	-0.47686
11	1	0	-0.42642	-1.17545	-1.4558
12	1	0	-1.10741	-2.35003	-0.34823
13	1	0	1.118938	-2.34466	0.348771
14	1	0	0.431752	-1.17315	1.455865
15	1	0	2.595631	-0.44221	0.475976
16	1	0	1.938616	-0.59334	-1.12913
17	1	0	2.079	1.806834	-0.12465
18	1	0	-0.00582	2.746927	-0.00011

Table S-4: Vibrational frequencies for the reactant, pre-reactive complexes, transition states and products for the reaction of Cl atoms with cycloheptene at MP2/6-31G(d,p) level of theory.

Table S-4-1: Normal mode frequencies of R1, RC1a, TS1a, TS2a, TS1 and TS2 (cm^{-1}).

R1	RC1a	TS1a	TS2a	TS1	TS2
114.6	104.0	-277.1	-327.5	-231.2	-1036.3
206.0	109.7	112.9	75.1	52.1	61.4
280.6	142.2	127.9	117.3	63.6	84.3
346.9	200.0	164.9	185.5	136.2	146.6
378.5	264.5	239.1	236.2	196.4	194.5
425.0	302.9	281.7	271.6	274.7	277.8
557.6	372.3	326.7	342.5	337.4	353.4
682.1	384.1	379.1	377.8	369.0	377.8
714.8	527.8	391.1	394.0	407.7	419.9
777.7	664.8	571.7	548.4	544.5	521.3
855.7	678.6	689.3	686.1	646.5	575.2
877.0	765.6	753.2	777.5	653.9	697.7
899.9	776.9	780.7	780.8	777.3	766.8
919.0	861.4	866.4	862.9	809.8	791.0
987.3	874.5	874.5	869.2	830.3	878.4
1003.8	896.3	894.7	892.8	870.0	888.4
1028.2	915.1	931.9	904.5	905.6	922.5
1059.5	993.5	997.3	979.8	919.1	944.7
1083.0	1015.7	1005.4	1022.0	928.4	991.2
1121.0	1064.7	1022.4	1030.0	993.5	1018.8
1165.6	1085.9	1064.7	1067.4	1023.1	1054.1
1207.9	1118.0	1090.9	1085.1	1051.7	1078.4
1253.1	1167.4	1126.4	1123.5	1080.3	1105.0
1256.3	1177.5	1180.3	1180.3	1134.7	1124.1
1294.3	1244.2	1210.2	1210.6	1162.0	1152.7
1325.9	1260.4	1263.4	1256.1	1215.3	1172.1
1340.1	1275.3	1272.4	1269.1	1234.9	1220.8
1378.1	1290.4	1289.6	1291.9	1265.0	1260.8
1403.2	1330.9	1329.1	1325.0	1295.6	1270.4
1418.7	1348.9	1349.4	1345.6	1327.8	1288.5
1429.1	1385.4	1388.5	1388.8	1342.8	1315.1
1433.0	1406.1	1408.9	1400.2	1362.2	1339.1
1463.7	1428.1	1428.4	1431.8	1375.5	1385.5
1530.7	1432.7	1437.2	1432.7	1401.0	1399.6
1538.1	1444.1	1447.9	1444.7	1421.0	1411.2
1545.4	1488.9	1482.5	1478.9	1432.9	1434.1
1557.1	1514.8	1504.8	1514.4	1477.9	1437.0
1570.6	1533.4	1528.2	1529.6	1529.9	1476.2
1740.7	1541.0	1540.0	1536.0	1535.9	1524.3
3092.9	1560.3	1557.7	1558.3	1542.0	1541.2

3113.5	1562.6	1559.6	1563.3	1557.0	1557.8
3124.6	1714.6	1673.8	1626.5	1562.9	1560.3
3125.3	3095.2	3092.3	3102.9	2095.0	1898.5
3133.3	3115.9	3113.7	3114.9	3120.3	3105.8
3136.1	3125.3	3126.8	3128.5	3121.4	3122.4
3164.3	3129.0	3127.1	3131.0	3130.8	3133.3
3176.9	3137.6	3135.7	3141.9	3132.4	3140.4
3181.3	3142.4	3138.3	3169.6	3143.4	3165.1
3188.3	3176.3	3179.9	3181.1	3171.9	3172.6
3216.1	3182.8	3184.2	3186.7	3173.1	3175.1
3245.0	3188.5	3191.7	3196.9	3187.5	3189.0
	3202.7	3208.5	3211.7	3191.3	3199.0
	3240.3	3256.5	3261.1	3200.0	3240.4
	3264.0	3274.8	3278.8	3247.3	3264.1

Table S-4-2: Normal mode frequencies of transition states TS3, TS4, TS5, TS6, TS7 and TS8 (cm^{-1}).

TS3	TS4	TS5	TS6	TS7	TS8
-677.9	-931.9	-931.9	-904.1	-904.1	-931.9
28.4	64.2	64.2	59.4	59.4	64.2
80.5	79.9	79.9	80.9	80.9	79.9
155.8	88.2	88.2	145.9	145.9	88.2
221.3	194.5	194.5	201.0	201.0	194.5
283.4	277.2	277.2	261.5	261.5	277.2
349.9	326.5	326.5	304.8	304.8	326.5
357.9	357.3	357.3	356.9	356.9	357.3
437.4	431.1	431.1	443.4	443.4	431.1
565.3	502.4	502.4	489.5	489.5	502.4
613.7	542.6	542.6	552.4	552.4	542.6
714.9	683.0	683.0	664.9	664.9	683.0
776.5	758.6	758.6	725.7	725.7	758.6
798.9	807.1	807.1	797.8	797.8	807.1
870.8	872.7	872.7	862.1	862.1	872.7
889.8	881.4	881.4	883.3	883.3	881.4
917.1	913.6	913.6	920.7	920.7	913.6
956.4	918.9	918.9	931.9	931.9	918.9
993.5	980.3	980.3	965.0	965.0	980.3
1019.5	996.4	996.4	975.8	975.8	996.4
1036.0	1022.1	1022.1	983.3	983.3	1022.1
1079.5	1052.5	1052.5	1041.1	1041.1	1052.5
1112.3	1081.3	1081.3	1054.6	1054.6	1081.3
1125.3	1112.2	1112.2	1105.4	1105.4	1112.2
1155.5	1128.4	1128.4	1106.5	1106.5	1128.4
1183.8	1165.0	1165.0	1161.6	1161.6	1165.0
1233.9	1178.6	1178.6	1184.0	1184.0	1178.6
1250.4	1201.7	1201.7	1201.7	1201.7	1201.7
1274.0	1268.1	1268.1	1259.3	1259.3	1268.1
1313.6	1281.4	1281.4	1284.0	1284.0	1281.4
1333.8	1310.0	1310.0	1296.6	1296.6	1310.0
1352.2	1334.5	1334.5	1323.2	1323.2	1334.5
1375.6	1364.4	1364.4	1358.5	1358.5	1364.4
1395.7	1404.4	1404.4	1381.6	1381.6	1404.4
1408.2	1406.0	1406.0	1382.9	1382.9	1406.0
1427.5	1410.8	1410.8	1416.2	1416.2	1410.8
1442.0	1442.9	1442.9	1455.6	1455.6	1442.9
1480.9	1455.8	1455.8	1463.2	1463.2	1455.8
1537.6	1528.2	1528.2	1531.5	1531.5	1528.2
1541.1	1534.5	1534.5	1535.1	1535.1	1534.5
1554.7	1536.8	1536.8	1541.8	1541.8	1536.8
1567.4	1548.0	1548.0	1545.8	1545.8	1548.0

1903.2	3100.4	3100.4	1731.3	1731.3	3100.4
3122.8	3113.2	3113.2	3107.1	3107.1	3113.2
3135.1	3118.7	3118.7	3111.4	3111.4	3118.7
3137.0	3121.3	3121.3	3132.0	3132.0	3121.3
3143.4	3157.6	3157.6	3132.3	3132.3	3157.6
3167.1	3176.4	3176.4	3170.5	3170.5	3176.4
3176.3	3178.8	3178.8	3180.4	3180.4	3178.8
3192.4	3182.2	3182.2	3180.9	3180.9	3182.2
3195.1	3185.8	3185.8	3195.9	3195.9	3185.8
3200.5	3199.6	3199.6	3200.8	3200.8	3199.6
3244.7	3239.1	3239.1	3236.2	3236.2	3239.1
3268.4	3596.6	3596.6	3258.6	3258.6	3596.6

Table S-4-3: Normal mode frequencies of TS9, TS10, TS11, TS12, P1a and P2a (cm^{-1}).

TS9	TS10	TS11	TS12	P1a	P2a
-931.9	-829.6	-870.6	-324.2	90.6	50.1
64.2	37.7	73.2	45.5	129.3	96.1
79.9	93.3	90.0	70.8	193.4	244.2
88.2	148.7	158.7	128.7	269.4	290.3
194.5	207.7	243.2	189.7	273.9	309.7
277.2	346.1	271.4	301.0	344.6	323.9
326.5	351.6	354.4	333.2	382.3	354.1
357.3	364.4	373.1	357.8	396.5	394.5
431.1	431.2	408.2	404.6	529.3	525.0
502.4	497.7	501.0	498.6	563.0	557.8
542.6	517.7	586.8	626.1	649.8	671.4
683.0	708.7	682.4	667.8	727.8	685.8
758.6	774.3	752.9	777.2	771.1	795.9
807.1	785.8	802.7	816.0	802.7	831.1
872.7	864.0	856.9	843.2	868.1	861.4
881.4	881.5	893.6	858.5	873.9	890.5
913.6	926.4	932.0	896.5	938.0	897.1
918.9	938.2	961.5	920.2	994.3	987.5
980.3	993.0	980.6	935.3	1010.0	1018.4
996.4	996.4	1011.4	991.1	1060.4	1057.0
1022.1	1032.8	1029.6	1002.1	1074.0	1070.4
1052.5	1090.9	1076.2	1063.3	1113.0	1104.6
1081.3	1112.3	1108.6	1105.1	1175.0	1160.2
1112.2	1119.7	1118.1	1144.7	1193.0	1186.9
1128.4	1150.8	1154.1	1156.3	1239.5	1232.4
1165.0	1188.3	1185.0	1196.1	1259.3	1262.9
1178.6	1215.5	1231.5	1224.7	1270.6	1268.8
1201.7	1280.0	1262.8	1283.9	1305.6	1285.0
1268.1	1284.4	1289.2	1289.7	1315.4	1307.7
1281.4	1308.4	1300.0	1301.4	1348.0	1341.3
1310.0	1325.0	1333.7	1328.2	1389.7	1378.9
1334.5	1344.5	1344.4	1359.7	1399.5	1405.6
1364.4	1406.1	1389.2	1402.3	1420.7	1415.0
1404.4	1415.6	1406.2	1412.7	1437.1	1425.2
1406.0	1421.8	1423.9	1425.6	1440.6	1429.0
1410.8	1444.1	1435.4	1434.8	1443.5	1445.9
1442.9	1447.2	1442.4	1437.8	1468.9	1469.0
1455.8	1482.0	1478.9	1523.9	1519.0	1519.2
1528.2	1521.8	1522.9	1527.6	1529.7	1538.9
1534.5	1529.2	1534.0	1532.4	1542.5	1543.1
1536.8	1540.4	1546.2	1541.3	1553.5	1555.0
1548.0	1546.2	1556.2	1545.7	1559.4	1568.9
3100.4	1847.9	1843.5	2112.5	3053.2	3071.2

3113.2	3098.0	3103.0	3108.2	3116.5	3113.1
3118.7	3107.0	3111.2	3112.5	3120.9	3113.9
3121.3	3116.0	3125.7	3116.8	3124.0	3126.4
3157.6	3122.3	3134.9	3118.4	3130.1	3133.4
3176.4	3169.3	3166.1	3121.2	3138.7	3145.3
3178.8	3172.3	3173.9	3167.4	3170.6	3163.4
3182.2	3175.6	3181.6	3168.5	3174.5	3176.7
3185.8	3182.7	3189.7	3170.9	3176.6	3181.4
3199.6	3184.2	3199.7	3176.5	3181.4	3187.8
3239.1	3238.3	3238.8	3184.3	3193.7	3205.9
3596.6	3262.2	3264.3	3226.3	3256.5	3262.0

Table S-4-4: Normal mode frequencies of products P1, P2, P3, P5, P7, P9, P10 and P12 (cm^{-1}).

P1	P2	P3	P5	P7	P9	P10	P12
129.4	137.5	137.5	109.0	109.0	127.9	129.0	93.1
191.7	235.6	235.5	194.6	194.6	219.8	160.7	190.0
274.3	268.6	268.6	292.9	292.9	302.6	315.0	326.0
352.4	351.1	351.0	310.8	310.8	320.0	361.6	345.6
376.4	371.2	371.2	336.3	336.3	398.8	395.7	364.7
433.4	510.5	510.5	447.3	447.3	459.5	440.7	453.1
556.2	558.2	558.2	487.3	487.3	484.3	560.5	505.6
680.5	634.5	634.4	607.6	607.6	576.0	662.6	687.0
773.8	712.6	712.6	666.6	666.6	717.8	719.6	776.4
810.8	742.3	742.3	733.0	733.0	742.3	786.7	803.2
875.7	800.9	800.9	799.1	799.1	807.6	811.9	866.2
893.5	872.5	872.5	867.5	867.5	865.5	871.7	882.3
901.1	883.7	883.6	911.1	911.1	904.2	909.4	900.9
927.6	948.9	948.9	931.7	931.7	939.8	932.6	919.7
996.1	977.6	977.5	964.3	964.3	969.4	947.9	992.1
1024.6	985.3	985.3	983.8	983.8	975.4	998.0	999.4
1053.5	1013.6	1013.6	1030.7	1030.7	1010.0	1009.5	1067.4
1076.0	1056.4	1056.3	1045.4	1045.4	1049.5	1069.9	1098.6
1129.5	1099.0	1099.0	1098.9	1098.9	1094.2	1105.1	1140.0
1162.7	1134.6	1134.5	1103.1	1103.1	1124.2	1135.2	1160.1
1213.5	1199.1	1199.1	1187.1	1187.1	1186.1	1184.9	1193.3
1239.2	1220.4	1220.4	1220.6	1220.6	1209.3	1237.3	1251.0
1266.8	1241.9	1241.9	1226.8	1226.8	1248.6	1275.8	1282.0
1295.8	1269.8	1269.8	1279.2	1279.2	1268.8	1280.7	1299.9
1332.8	1284.5	1284.5	1295.1	1295.1	1298.2	1296.2	1326.0
1344.4	1328.3	1328.2	1323.4	1323.4	1326.3	1332.9	1351.1
1374.5	1379.4	1379.4	1361.5	1361.5	1345.4	1397.4	1394.5
1390.9	1397.9	1397.9	1366.4	1366.4	1383.5	1405.7	1404.2
1405.2	1401.6	1401.6	1385.5	1385.5	1398.5	1432.1	1423.7
1423.1	1432.2	1432.1	1412.0	1412.0	1405.4	1444.3	1431.3
1431.8	1436.5	1436.5	1463.1	1463.1	1444.7	1462.2	1432.9
1527.4	1474.5	1474.5	1470.4	1470.4	1453.1	1489.3	1523.7
1536.6	1529.0	1529.0	1530.5	1530.5	1524.9	1523.8	1530.4
1542.3	1538.8	1538.8	1537.3	1537.3	1531.9	1529.6	1534.5
1556.8	1551.2	1551.2	1540.2	1540.2	1538.4	1546.1	1541.9
1564.2	1556.0	1556.0	1541.9	1541.9	1544.1	1547.7	1546.9
2014.6	1579.0	1579.0	1730.2	1730.2	1983.9	1584.1	2033.8
3113.6	3094.7	3094.8	3106.0	3106.0	3088.5	3071.9	3103.3
3114.3	3110.4	3110.5	3110.2	3110.2	3093.2	3074.2	3104.3
3126.4	3115.2	3115.2	3111.5	3111.5	3093.4	3111.8	3110.8
3128.0	3129.3	3129.4	3112.3	3112.3	3113.5	3114.3	3111.6
3135.5	3163.3	3163.4	3171.0	3171.0	3164.1	3133.5	3116.4
3163.3	3166.9	3166.9	3171.5	3171.5	3170.1	3133.7	3158.7

3165.0	3178.7	3178.7	3173.3	3173.3	3172.3	3170.1	3159.8
3181.0	3192.3	3192.3	3173.7	3173.7	3177.7	3171.5	3162.6
3185.1	3236.6	3236.7	3225.8	3225.8	3230.7	3223.9	3169.6
3192.2	3269.6	3269.6	3249.3	3249.3	3262.6	3249.1	3178.2
3238.2	3280.2	3280.2	3253.2	3253.2	3263.0	3259.6	3213.7