

Low energy dissociation processes of ionized cyclohexene: a theoretical insight.

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SUPPORTING INFORMATION

B3LYP/6-31G(d) geometry (cartesian coordinates) of the different minima and transition states investigated and listed in Table 2.

Minima

1

C	-0.001035	0.000043	-0.000061
C	-0.002229	1.414457	0.000295
C	0.001230	2.191124	1.244749
C	-0.238034	1.373724	2.523451
C	0.522647	0.040522	2.478256
C	0.133221	-0.776314	1.237256
H	-0.130838	-0.523743	-0.946616
H	0.021213	1.938446	-0.954730
H	1.003873	2.681544	1.260063
H	-0.671608	3.058089	1.139903
H	0.069076	1.961089	3.392674
H	-1.314750	1.191690	2.633127
H	1.604736	0.222502	2.459883
H	0.320074	-0.546396	3.377876
H	0.783336	-1.648176	1.057994
H	-0.864992	-1.258471	1.368597

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C	0.001221	-0.000372	-0.000231
C	0.001617	1.550824	-0.000256
C	-0.001548	1.959028	1.488615
C	-0.318256	0.732682	2.236004
C	-0.324853	-0.383925	1.380135
C	-0.797926	-0.713981	-1.122537
H	1.051854	-0.363861	-0.128138
H	0.845752	1.969637	-0.552520
H	-0.910741	1.912058	-0.489997
H	-0.684305	2.785312	1.751060
H	0.980877	2.339152	1.839887
H	-0.508553	0.689910	3.305734
H	-0.515860	-1.404127	1.705543
H	-1.855904	-0.441876	-1.059990
H	-0.704814	-1.800673	-1.048073
H	-0.410369	-0.399282	-2.094320

6(chair)

C	-1.141020	-0.393341	-0.667399
C	-1.195317	-0.477211	0.783383
C	0.386147	-0.685264	1.285129
C	1.141064	0.393263	0.667367
C	1.195305	0.477256	-0.783406
C	-0.386205	0.685295	-1.285084
H	0.373113	-0.666748	2.375912
H	-1.534040	0.447837	1.259287
H	-1.760340	-1.326354	1.170735
H	-1.439535	-1.252235	-1.266879
H	1.439887	1.252031	1.266878
H	1.760415	1.326400	-1.170609
H	1.533914	-0.447745	-1.259517
H	-0.677763	1.678078	-0.929687
H	-0.373019	0.666895	-2.375874
H	0.677529	-1.678147	0.929817

6(planar)

C	-1.299615	0.042428	-0.774119
C	-1.248154	-0.000612	0.690816
C	-0.034122	-0.043099	1.512342
C	1.292878	-0.196152	0.761721
C	1.248151	0.000581	-0.690841
C	0.040882	0.196829	-1.499926
H	-2.200733	-0.001137	1.217998
H	-0.148367	-0.820964	2.285359
H	-0.016945	0.887512	2.112290
H	1.705620	-1.208379	0.938469
H	0.109628	1.209398	-1.942931
H	0.091926	-0.454134	-2.388363
H	-2.016008	0.819756	-1.087541
H	-1.798184	-0.888476	-1.107533
H	2.072218	0.455459	1.190336
H	2.200719	0.001113	-1.218040

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C	0.002109	-0.019113	0.010984
C	0.025232	1.524191	0.012258
C	-0.079935	2.117497	1.357288
C	-0.611589	1.346265	2.478839
C	-1.196783	0.029774	2.235838
C	-1.105376	-0.607384	0.909882
H	0.276170	3.125872	1.552437
H	-1.156976	1.950392	3.220312
H	0.318435	1.093745	3.062336
H	-1.662168	-0.486285	3.071785
H	-1.015979	-1.697089	1.006816
H	-2.097226	-0.460899	0.433705
H	0.974045	-0.389491	0.355143
H	-0.126468	-0.381396	-1.011456
H	0.898158	1.919925	-0.522201
H	-0.841930	1.914591	-0.560110

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C	-0.019656	0.010254	0.083050
C	1.449636	0.060636	0.312041
C	2.199153	1.317167	0.055256
C	1.468443	2.125871	-1.043570
C	0.904121	1.103452	-2.058447
C	0.444998	-0.104717	-1.325698
H	1.961120	-0.844733	0.631941
H	0.475992	-1.089031	-1.788138
H	1.645512	0.818571	-2.815221
H	0.663475	2.728447	-0.611307
H	3.233985	1.081935	-0.222852
H	-0.535202	0.949965	0.304969
H	-0.517741	-0.873154	0.477762
H	0.049387	1.516813	-2.622713
H	2.151932	2.823715	-1.532817
H	2.268655	1.883393	1.001016

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C	-0.960017	0.627929	-1.090928
C	-0.956817	0.817688	0.562615
C	0.445613	0.670407	1.176920
C	1.363373	-0.278978	0.363016
C	0.516210	-1.367954	-0.372817
C	-0.642494	-0.724301	-0.932946
H	0.219609	-2.213791	0.264973
H	1.920982	0.286405	-0.389644
H	0.326793	0.294116	2.197494
H	-0.164411	1.271644	-1.489118
H	-1.941103	0.865940	-1.507219
H	1.082916	-1.817308	-1.209585
H	2.098627	-0.778204	0.999431
H	0.926773	1.649810	1.251113
H	-1.373848	1.828533	0.634395
H	-1.691547	0.144109	1.012998

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C	-1.473986	-0.041669	0.060888
C	-1.154223	0.856782	1.050466
C	1.099149	-0.880531	1.088427
C	1.469582	0.038598	0.136140
C	0.726899	0.327102	-1.127430
C	-0.668348	-0.300882	-1.170081
H	-2.371669	-0.646114	0.191558
H	-0.402037	1.629178	0.921019
H	0.354504	-1.649013	0.903752
H	2.360503	0.637687	0.324881
H	1.334866	-0.013187	-1.981103
H	-1.232528	0.060453	-2.044913
H	0.678134	1.418237	-1.251372
H	-0.612933	-1.388734	-1.317516
H	-1.717784	0.884056	1.979251
H	1.614498	-0.928962	2.043976

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C	-1.347915	-0.243078	-0.739531
C	-1.245915	-0.440939	0.710685
C	-0.077443	0.188607	1.280442
C	0.910367	0.479222	0.028985
C	-0.132287	0.615538	-1.139311
H	-2.321775	0.180882	-1.036249
H	0.288654	0.326959	-2.104599
H	-0.417639	1.669585	-1.210928
H	-1.358120	-1.244829	-1.209363
C	1.866206	-0.614498	-0.061537
H	1.542555	-1.634581	-0.259063
H	2.927941	-0.458851	0.104756
H	-0.346816	1.215503	1.594586
H	0.336494	-0.304146	2.168395
H	-1.919941	-1.082773	1.275049
H	1.430564	1.423136	0.199016

12

C	0.221305	-0.243384	-0.433963
C	0.232004	0.070878	1.033307
C	1.632882	0.114249	1.536735
C	2.507608	0.014077	0.357232
C	1.689851	0.008525	-0.868850
H	-0.487286	0.367548	-1.003590
H	1.901561	-0.714595	2.228933
H	-0.640597	0.126080	1.670291
H	1.916699	1.003725	2.134771
H	2.096300	-0.618939	-1.671779
H	1.811334	1.048756	-1.246497
H	-0.061754	-1.292431	-0.621427
C	3.968146	-0.074323	0.392561
H	4.404792	0.251279	1.339761
H	4.222289	-1.143635	0.256434
H	4.430466	0.437072	-0.460604

13

C	-0.950393	0.636574	-1.264118
C	-0.952525	0.371615	0.559980
C	0.327150	0.665914	1.236532
C	1.429801	0.006893	0.375101
C	0.703543	-1.122878	-0.394097
C	-0.742734	-0.629800	-0.571042
H	-1.926282	0.673109	0.937467
H	-1.559667	-1.346451	-0.687154
H	0.672458	-2.044766	0.195131
H	1.864141	0.742395	-0.310198
H	0.248258	0.177319	2.228801
H	-0.124699	1.297406	-1.515508
H	-1.941446	0.930310	-1.599365
H	1.166006	-1.354031	-1.357579
H	2.250850	-0.377065	0.983348
H	0.461328	1.731862	1.470918

14

C	-0.396965	0.369173	-0.187729
C	1.119645	0.377227	0.117707
C	1.519040	1.791906	0.107158
C	0.395825	2.654667	0.029365
C	-0.844403	1.835871	0.012391
H	-0.948017	-0.325851	0.448188
H	1.740269	-0.231397	-0.559585
H	1.357129	-0.043276	1.117354
H	2.546438	2.143662	0.168253
H	-1.575782	2.206612	-0.720483
H	-1.348754	1.983671	0.987755
H	-0.566677	0.062738	-1.224944
C	0.445186	4.126220	-0.033176
H	1.398363	4.537274	0.308708
H	0.311201	4.432663	-1.086799
H	-0.389568	4.581771	0.512329

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C	-0.669800	-0.313910	-0.390516
C	-0.579677	-0.065905	1.065100
C	0.593145	0.072161	-1.057259
C	-1.803076	-0.844895	-1.051314
H	-1.505232	0.314919	1.515591
H	0.897499	-0.599702	-1.870010
H	-2.668159	-1.190754	-0.490362
H	-1.835885	-0.919604	-2.135746
C	0.707381	0.764935	1.260467
C	1.601964	0.317242	0.086004
H	1.163219	0.598363	2.238167
H	2.361681	1.053405	-0.182948
H	2.117379	-0.620964	0.322396
H	0.465887	1.831501	1.183821
H	-0.448373	-1.079609	1.508437
H	0.352357	1.034673	-1.564233

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C	-1.281344	-0.137048	-0.776587
C	-1.387903	-0.133377	0.787436
C	-0.036765	0.170921	1.185214
C	0.912379	0.489294	0.172246
C	-0.013285	0.713859	-1.071899
H	-2.183400	0.271514	-1.235750
H	-1.852175	-0.990446	1.290633
H	-1.954770	0.753776	1.151324
H	0.491573	0.424904	-1.997282
H	-0.259829	1.778186	-1.135643
H	-1.164320	-1.168534	-1.120259
C	1.724175	-0.897128	0.109978
H	2.335975	-1.026847	1.003062
H	1.080255	-1.767329	-0.034209
H	2.364439	-0.785675	-0.770732
H	1.638706	1.271319	0.410521

C5H7+

C	-0.102688	-2.490781	0.098451
C	0.020506	-0.959815	0.082912
C	-0.009882	-0.585566	1.510588
C	-0.134474	-1.694902	2.341074
C	-0.190554	-2.826285	1.533307
H	0.749885	-3.010189	-0.367870
H	-0.790316	-0.454203	-0.465811
H	0.944183	-0.592416	-0.392536
H	0.058248	0.442301	1.860732
H	-0.178679	-1.680482	3.423605
H	-0.287813	-3.844455	1.904288
H	-0.984625	-2.871635	-0.441321

CH3

C	0.000000	1.565514	-3.173869
H	0.937244	2.075849	-2.991956
H	-0.937244	2.075849	-2.991956
H	0.000000	0.546142	-3.538701

C4H6⁺

C	0.008346	0.000000	-0.011334
C	0.003374	0.000000	1.378336
C	1.200767	0.000000	2.124139
C	1.195800	0.000000	3.513810
H	0.939548	0.000000	-0.573633
H	-0.918698	0.000000	-0.578150
H	-0.948528	0.000000	1.906002
H	2.152667	0.000000	1.596471
H	2.122849	0.000000	4.080619
H	0.264603	0.000000	4.076114

C2H4

C	0.000000	0.000000	0.001954
C	0.000000	0.000000	1.332946
H	0.923822	0.000000	-0.571867
H	-0.923822	0.000000	-0.571867
H	0.923823	0.000000	1.906767
H	-0.923823	0.000000	1.906767

Transition states

TS1/6

C	-1.102319	0.663597	-0.818846
C	-1.132663	0.026381	0.588341
C	0.049078	0.284237	1.409011
C	1.321300	0.303273	0.619743
C	1.118239	-0.587997	-0.657247
C	-0.332922	-0.584654	-1.045382
H	-2.074262	0.716798	-1.304962
H	0.008173	0.211213	2.489589
H	2.174035	-0.047711	1.207243
H	-0.770246	-1.389856	-1.637667
H	1.567188	1.331805	0.315684
H	-0.549543	1.598821	-0.876957
H	1.682395	-0.173017	-1.503766
H	1.472430	-1.611571	-0.504989
H	-2.128829	-0.127641	1.009407
H	-0.905620	-1.137863	0.232697

TS1/7

C	0.000000	0.000000	0.000000
C	0.000000	1.485743	0.000000
C	0.000000	2.219005	1.243249
C	-0.193555	1.538189	2.500654
C	-0.200054	0.060130	2.564641
C	0.458733	-0.608276	1.339210
H	-0.008353	2.044946	-0.930229
H	-0.169463	3.296325	1.217767
H	1.076478	2.106363	1.736184
H	-0.256830	2.143702	3.402807
H	0.227974	-0.296362	3.507922
H	-1.274785	-0.205618	2.615317
H	1.547359	-0.505466	1.430345
H	0.246400	-1.679647	1.356068
H	0.608272	-0.380627	-0.830108
H	-1.029593	-0.326712	-0.237986

TS5/12

C	-0.398241	0.150995	-0.094784
C	-0.154646	1.635112	-0.060139
C	-0.033146	2.024413	1.443640
C	-0.375282	0.771221	2.190479
C	-0.469690	-0.329698	1.261439
C	-0.576504	-0.657874	-1.323623
H	0.644908	-0.484936	0.802608
H	0.695396	1.938193	-0.681274
H	-1.040731	2.092770	-0.528604
H	-0.695979	2.855197	1.715239
H	0.982769	2.364773	1.696901
H	-0.453490	0.672631	3.265512
H	-0.816903	-1.331077	1.513009
H	-1.549553	-0.378954	-1.758083
H	-0.594947	-1.732431	-1.126637
H	0.179949	-0.424716	-2.080727

TS6/7

C	-1.257874	0.315718	-0.735871
C	-1.067781	0.617279	0.718641
C	0.157477	0.424067	1.373883
C	1.373079	-0.077405	0.664672
C	1.148911	-0.491525	-0.752226
C	-0.227947	-0.690885	-1.296633
H	0.242718	0.733685	2.416011
H	1.858360	-0.859836	1.272845
H	2.082451	0.770030	0.727982
H	2.014199	-0.784133	-1.335748
H	-0.222675	-0.630025	-2.389149
H	-0.587239	-1.710433	-1.064866
H	-1.155402	1.291361	-1.237068
H	-2.287115	-0.009009	-0.919083
H	-1.877029	1.088122	1.278946
H	-0.823473	-0.473239	1.415336

TS6/10

C	-0.985188	-0.746877	-0.691791
C	-1.159460	-0.839208	0.687160
C	0.976866	-0.772018	0.983361
C	0.972225	0.612857	0.830218
C	0.527527	1.302258	-0.415559
C	-0.335029	0.414894	-1.364585
H	-1.168987	-1.635871	-1.294135
H	-1.375877	0.041456	1.286070
H	1.219327	-1.428110	0.151558
H	1.129284	1.229017	1.714835
H	1.407585	1.663893	-0.970146
H	-1.105489	1.044702	-1.836379
H	-0.008808	2.212860	-0.123471
H	0.259592	0.030463	-2.201583
H	-1.471904	-1.781277	1.132854
H	1.133640	-1.208573	1.967568

TS7/8

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.470987
C	1.425664	0.000000	-0.494876
C	2.463120	0.832021	0.178987
C	1.851458	1.659565	1.332364
C	0.980501	0.775024	2.211936
H	-0.495224	0.976304	-0.247548
H	-0.630534	-0.780482	-0.430734
H	-0.720490	-0.601358	2.027876
H	1.664659	-0.675231	-1.311754
H	2.950253	1.503457	-0.545447
H	3.268302	0.185399	0.569412
H	2.632053	2.112690	1.948538
H	1.248132	2.481840	0.930247
H	1.556741	-0.026791	2.735792
H	0.488514	1.268562	3.068067

TS8/9

C	-0.946563	0.677055	-1.103793
C	-0.988353	0.570558	0.458149
C	0.337123	0.699354	1.192223
C	1.387001	-0.130651	0.398040
C	0.656524	-1.259180	-0.415494
C	-0.676590	-0.696231	-0.756748
H	-1.931279	0.933335	0.874871
H	0.557358	-2.189472	0.152669
H	1.923820	0.513788	-0.302594
H	0.218754	0.339831	2.218868
H	-0.124170	1.254832	-1.524741
H	-1.916943	0.912918	-1.542118
H	1.185280	-1.489441	-1.347545
H	2.128979	-0.580340	1.061535
H	0.625879	1.754031	1.248165
H	-1.282523	-0.614909	0.526626

TS8/13

C	-0.737346	0.712559	-1.333746
C	-0.788753	0.735798	0.453852
C	0.516881	0.701972	1.143477
C	1.369303	-0.361917	0.415351
C	0.338330	-1.329310	-0.213204
C	-0.893683	-0.476898	-0.537493
H	-1.640112	1.323910	0.785046
H	-1.890103	-0.923935	-0.540631
H	0.039232	-2.103985	0.499205
H	1.994563	0.110498	-0.349751
H	0.302726	0.399460	2.187299
H	0.240915	1.073787	-1.642964
H	-1.604056	1.232817	-1.732521
H	0.712641	-1.826752	-1.113592
H	2.047010	-0.880250	1.096354
H	0.968794	1.701229	1.242131

TS9/15

C	-1.109970	0.407005	-1.018091
C	-1.046930	0.858568	0.561204
C	0.268595	0.501988	1.289054
C	1.374487	-0.014505	0.351042
C	0.810872	-1.207954	-0.491657
C	-0.488677	-0.856335	-0.973487
H	0.780596	-2.166508	0.050187
H	1.717883	0.771968	-0.329364
H	0.065657	-0.262147	2.047102
H	-0.476867	1.124850	-1.566850
H	-2.135828	0.434196	-1.393788
H	1.439662	-1.410522	-1.383113
H	2.244925	-0.366265	0.911584
H	0.636752	1.384232	1.822109
H	-1.205435	1.937811	0.483888
H	-1.917609	0.419779	1.049858

TS11/12

C	-1.328905	0.453818	-0.826265
C	-1.317789	0.637160	0.659702
C	0.002809	0.307323	1.265055
C	0.802290	-0.239286	0.077664
C	0.164624	0.311661	-1.216415
H	-1.793435	1.298226	-1.349366
H	0.342383	-0.334130	-2.079397
H	0.584993	1.296942	-1.438514
H	-1.919677	-0.433281	-1.109956
C	1.486622	-1.472856	0.125798
H	1.717974	-1.954737	1.075523
H	1.940677	-1.887231	-0.773574
H	0.483823	1.218199	1.666411
H	-0.045038	-0.394817	2.108102
H	-2.110135	1.119172	1.220825
H	1.940529	0.084743	0.166714

TS11/13

C	-0.928287	0.522080	-1.677533
C	-0.671833	0.740629	0.709582
C	0.665336	0.712589	1.139579
C	1.421091	-0.386980	0.476425
C	0.338169	-1.222882	-0.252221
C	-0.895731	-0.278747	-0.416518
H	-1.356715	1.552528	0.950551
H	-1.841679	-0.809868	-0.283221
H	0.058871	-2.080491	0.369022
H	2.102228	0.127040	-0.224399
H	-0.488380	0.132834	1.777993
H	-0.015889	0.937972	-2.094827
H	-1.868178	0.756565	-2.163921
H	0.686528	-1.611654	-1.210437
H	2.065572	-0.952590	1.156616
H	1.085166	1.427529	1.846739

TS11/15

C	-0.811461	0.638648	-1.409051
C	-0.671820	0.855867	0.468024
C	0.648997	0.707605	1.090883
C	1.379053	-0.484814	0.572763
C	0.311907	-1.348527	-0.149711
C	-0.891623	-0.425959	-0.415410
H	-0.583824	1.754958	-0.314713
H	-1.879198	-0.867803	-0.304308
H	-0.024595	-2.162699	0.496975
H	2.187667	-0.170411	-0.108640
H	0.133312	0.874503	-1.897232
H	-1.717570	1.071521	-1.830362
H	0.684357	-1.801523	-1.072277
H	1.888408	-1.031372	1.377236
H	-1.563858	1.186935	1.004246
H	1.084982	1.488966	1.704077

TS12/14

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.561252
C	1.439334	0.000000	1.955049
C	2.269453	-0.005832	0.764822
C	1.444852	-0.103235	-0.416306
C	1.920764	-0.238355	-1.808888
H	-0.565929	0.824122	2.011847
H	3.335908	-0.229132	0.780068
H	1.830475	0.082563	2.963876
H	2.167903	1.125786	1.081934
H	-0.579740	-0.835069	-0.414751
H	-0.458502	0.907497	-0.420466
H	-0.448417	-0.918604	1.974488
H	3.009939	-0.207231	-1.887926
H	1.570205	-1.190909	-2.236032
H	1.491873	0.547330	-2.447496

TS13/14

C	-0.602400	-0.252941	-0.507391
C	-0.671191	-0.048685	1.017502
C	0.780111	-0.096319	-0.902023
C	-1.649441	-0.875595	-1.283084
H	-1.035051	0.679580	-1.078974
H	-1.599940	0.426982	1.341401
H	1.143387	-0.258249	-1.914426
H	-2.653685	-0.923829	-0.873511
H	-1.498802	-1.143888	-2.325599
C	0.593982	0.778786	1.325745
C	1.609199	0.360013	0.231397
H	0.972046	0.602443	2.334166
H	2.341967	1.126134	-0.050446
H	2.214270	-0.509228	0.558106
H	0.380457	1.849194	1.234076
H	-0.626213	-1.040699	1.482339

TS13/16

C	-0.986047	0.723425	-1.196388
C	-0.922707	0.369150	0.530540
C	0.336095	0.658259	1.285278
C	1.417808	-0.057254	0.406970
C	0.661867	-1.167885	-0.370908
C	-0.778077	-0.645100	-0.499790
H	-1.285450	1.441486	-0.223106
H	-1.584080	-1.346703	-0.708389
H	0.628688	-2.101286	0.199840
H	1.865941	0.669439	-0.277976
H	0.214413	0.151465	2.253228
H	-0.127895	1.230207	-1.634510
H	-1.940821	0.803393	-1.715824
H	1.109434	-1.391940	-1.343022
H	2.222117	-0.454682	1.029818
H	0.524019	1.715052	1.485741