Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Fusing Cubanes to 1,5-Hexadiene

Jason G. Harrison and Dean J. Tantillo*

Department of Chemistry, University of California, Davis, One Shields Avenue, Davis, California 95616

Supporting Information

Full authorship of *Gaussian 09*:

Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Energies computed using ub3lyp/6-31G(d)

A

Energy: -435447.2784214

C	1.25312	-1.25268	-0.35850
C	1.63796	-0.80065	1.04556
C	1.63764	0.79879	1.04663
C	1.25283	1.25305	-0.35686
C	3.14816	0.77499	0.62507
C	3.14847	-0.77567	0.62396
C	2.63033	0.82554	-0.85344
H	3.91114	1.44031	1.03258
C	2.63055	-0.82415	-0.85458
H	3.91178	-1.44119	1.03057
H	3.15078	1.29772	-1.69056
H	3.15090	-1.29466	-1.69269
C	-1.71887	-0.78614	1.12065
C	-1.17456	-0.81721	-0.35571
C	-1.71896	0.78466	1.12163
C	-3.18648	-0.78430	0.56427
C	-2.64131	-0.78647	-0.90796
C	-1.17464	0.81779	-0.35465
C	-3.18651	0.78343	0.56522
H	-3.99423	-1.41861	0.93396
C	-2.64138	0.78757	-0.90702
H	-3.02069	-1.41572	-1.71650
H	-3.99484	1.41678	0.93527
H	-3.02090	1.41783	-1.71470
C	0.05780	-1.39502	-0.95048
C	0.05771	1.39652	-0.94867
H	0.02559	1.59324	-2.02246
H	0.02569	-1.58992	-2.02460
H	-1.36095	-1.42072	1.93296
H	1.25288	-1.30430	1.93441
H	-1.36094	1.41800	1.93485
H	1.25257	1.30101	1.93628

TS A to A

Energy: -435434.0744305

C	1.21300	-1.07891	-0.35788
C	1.67709	-0.78346	1.08723
C	1.67708	0.78344	1.08724
C	1.21300	1.07891	-0.35788
C	3.16960	0.77845	0.59228
C	3.16961	-0.77846	0.59228
C	2.63555	0.79211	-0.88784

H	3.95366	1.43206	0.97805
C	2.63555	-0.79210	-0.88784
H	3.95367	-1.43206	0.97804
H	3.09337	1.35208	-1.70920
H	3.09337	-1.35206	-1.70921
C	-1.67630	-0.78352	1.08665
C	-1.21362	-1.08096	-0.35810
C	-1.67630	0.78351	1.08666
C	-3.16926	-0.77844	0.59292
C	-2.63586	-0.79228	-0.88742
C	-1.21362	1.08096	-0.35809
C	-3.16926	0.77844	0.59292
H	-3.95309	-1.43202	0.97918
C	-2.63586	0.79229	-0.88742
H	-3.09430	-1.35159	-1.70888
H	-3.95310	1.43201	0.97919
H	-3.09430	1.35160	-1.70887
C	-0.00037	-1.41995	-0.93620
C	-0.00037	1.41996	-0.93619
H	-0.00006	1.59217	-2.01508
H	-0.00006	-1.59215	-2.01509
H	-1.31623	-1.35901	1.94277
H	1.31764	-1.35953	1.94321
H	-1.31623	1.35900	1.94278
H	1.31763	1.35952	1.94321

TS A to J

Energy: -435422.3937271

C	1.30549	-1.31405	-0.34104
C	1.68426	-1.15179	0.99515
C	1.68438	1.15179	0.99514
C	1.30566	1.31412	-0.34107
C	3.13209	0.77983	0.66206
C	3.13199	-0.77996	0.66205
C	2.65422	0.81075	-0.82956
H	3.98227	1.36194	1.03011
C	2.65412	-0.81080	-0.82958
H	3.98203	-1.36233	1.03002
H	3.20899	1.28898	-1.63963
H	3.20883	-1.28909	-1.63967
C	-1.74309	-0.79079	1.13443
C	-1.22168	-0.77704	-0.34963
C	-1.74293	0.79029	1.13475
C	-3.21117	-0.78301	0.57463
C	-2.68859	-0.79042	-0.90734
C	-1.22156	0.77715	-0.34933

C	-3.21103	0.78293	0.57495
H	-4.01828	-1.41553	0.94855
C	-2.68849	0.79092	-0.90699
H	-3.07423	-1.43738	-1.69879
H	-4.01796	1.41552	0.94914
H	-3.07420	1.43820	-1.69814
C	0.09614	-1.10853	-1.01220
C	0.09622	1.10864	-1.01201
H	0.06112	1.30311	-2.08314
H	0.06124	-1.30311	-2.08332
H	-1.39176	-1.43623	1.94143
H	1.18360	-1.35042	1.93742
H	-1.39171	1.43534	1.94212
H	1.18389	1.35084	1.93741

J

Energy: -435435.6854682

C	1.33940	-1.27173	-0.37566
C	1.69074	-1.41616	0.92533
C	1.69003	1.41671	0.92426
C	1.33887	1.27119	-0.37666
C	3.06770	0.81981	0.73144
C	3.06813	-0.81869	0.73206
C	2.71681	0.78382	-0.78855
H	3.97439	1.27439	1.14046
C	2.71703	-0.78419	-0.78801
H	3.97496	-1.27260	1.14152
H	3.29768	1.31338	-1.54699
H	3.29819	-1.31382	-1.54618
C	-1.72578	-0.79170	1.14034
C	-1.25028	-0.77519	-0.35526
C	-1.72607	0.79414	1.13867
C	-3.20530	-0.78191	0.60691
C	-2.72140	-0.79381	-0.88928
C	-1.25058	0.77468	-0.35683
C	-3.20560	0.78262	0.60528
H	-4.00331	-1.41504	0.99920
C	-2.72170	0.79162	-0.89094
H	-3.12949	-1.44841	-1.66367
H	-4.00382	1.41629	0.99625
H	-3.13013	1.44446	-1.66665
C	0.10366	-0.83331	-1.08883
C	0.10359	0.83187	-1.09002
H	0.03184	1.24418	-2.10359
H	0.03111	-1.24677	-2.10188
H	-1.36883	-1.44077	1.94265

H	1.11117	-1.62070	1.82255
H	-1.36942	1.44505	1.93963
H	1.11028	1.62176	1.82126

TS J to K

Energy: -435413.9360365

C	1.30853	1.08475	0.35592
C	1.71850	1.63169	-0.87856
C	1.71918	-1.63153	-0.87895
C	1.30890	-1.08497	0.35550
C	3.04850	-1.26817	-0.69376
C	3.04795	1.26873	-0.69357
C	2.76372	-0.76843	0.71839
H	3.96445	-1.42522	-1.24912
C	2.76351	0.76869	0.71851
H	3.96370	1.42598	-1.24921
H	3.22551	-1.28843	1.56288
H	3.22524	1.28858	1.56311
C	-1.69420	0.79434	-1.13865
C	-1.26342	0.77368	0.37134
C	-1.69384	-0.79278	-1.13969
C	-3.18808	0.78241	-0.64516
C	-2.74685	0.79160	0.86424
C	-1.26311	-0.77391	0.37034
C	-3.18774	-0.78216	-0.64620
H	-3.97552	1.41584	-1.05809
C	-2.74652	-0.79314	0.86318
H	-3.17639	1.44666	1.62665
H	-3.97491	-1.41537	-1.05998
H	-3.17576	-1.44938	1.62474
C	0.06702	0.79802	1.15941
C	0.06718	-0.79881	1.15870
H	0.01569	-1.34762	2.11090
H	0.01606	1.34607	2.11207
H	-1.31625	1.44237	-1.93252
H	1.17370	2.04865	-1.72135
H	-1.31555	-1.43958	-1.93441
H	1.17465	-2.04872	-1.72179

K

Energy: -435413.9360365

C	1.30853	1.08475	0.35592
C	1.71850	1.63169	-0.87856
C	1.71918	-1.63153	-0.87895
C	1.30890	-1.08497	0.35550
C	3.04850	-1.26817	-0.69376

C	3.04795	1.26873	-0.69357
C	2.76372	-0.76843	0.71839
H	3.96445	-1.42522	-1.24912
C	2.76351	0.76869	0.71851
H	3.96370	1.42598	-1.24921
H	3.22551	-1.28843	1.56288
H	3.22524	1.28858	1.56311
C	-1.69420	0.79434	-1.13865
C	-1.26342	0.77368	0.37134
C	-1.69384	-0.79278	-1.13969
C	-3.18808	0.78241	-0.64516
C	-2.74685	0.79160	0.86424
C	-1.26311	-0.77391	0.37034
C	-3.18774	-0.78216	-0.64620
H	-3.97552	1.41584	-1.05809
C	-2.74652	-0.79314	0.86318
H	-3.17639	1.44666	1.62665
H	-3.97491	-1.41537	-1.05998
H	-3.17576	-1.44938	1.62474
C	0.06702	0.79802	1.15941
C	0.06718	-0.79881	1.15870
H	0.01569	-1.34762	2.11090
H	0.01606	1.34607	2.11207
H	-1.31625	1.44237	-1.93252
H	1.17370	2.04865	-1.72135
H	-1.31555	-1.43958	-1.93441
H	1.17465	-2.04872	-1.72179

TS K to L

Energy: -435389.2944060

C	-1.35716	0.77868	-0.35606
C	-1.73180	1.21124	1.04932
C	-1.73503	-1.20831	1.05316
C	-1.35802	-0.78074	-0.35305
C	-3.00740	-1.59920	0.60457
C	-3.00383	1.60339	0.60096
C	-2.75564	-1.23218	-0.71879
H	-3.90441	-1.92820	1.12226
C	-2.75406	1.23231	-0.72162
H	-3.89942	1.93640	1.11852
H	-3.27697	-1.35353	-1.66000
H	-3.27689	1.35041	-1.66241
C	1.69663	0.79873	1.12462
C	1.26359	0.77373	-0.38746
C	1.69631	-0.79152	1.12984
C	3.18948	0.78398	0.62960

C	2.74789	0.78816	-0.87916
C	1.26321	-0.77707	-0.38260
C	3.18910	-0.78028	0.63466
H	3.97710	1.41827	1.04092
C	2.74770	-0.79445	-0.87398
H	3.17655	1.44197	-1.64297
H	3.97631	-1.41246	1.05002
H	3.17703	-1.45338	-1.63303
C	-0.05458	0.80268	-1.18917
C	-0.05480	-0.80956	-1.18479
H	-0.07203	-1.43185	-2.08557
H	-0.07235	1.41959	-2.09361
H	1.32293	1.45285	1.91578
H	-1.16834	1.36378	1.95971
H	1.32355	-1.44039	1.92582
H	-1.17256	-1.36082	1.96421

L

Energy: -435389.2944060

C	-1.35716	0.77868	-0.35606
C	-1.73180	1.21124	1.04932
C	-1.73503	-1.20831	1.05316
C	-1.35802	-0.78074	-0.35305
C	-3.00740	-1.59920	0.60457
C	-3.00383	1.60339	0.60096
C	-2.75564	-1.23218	-0.71879
H	-3.90441	-1.92820	1.12226
C	-2.75406	1.23231	-0.72162
H	-3.89942	1.93640	1.11852
H	-3.27697	-1.35353	-1.66000
H	-3.27689	1.35041	-1.66241
C	1.69663	0.79873	1.12462
C	1.26359	0.77373	-0.38746
C	1.69631	-0.79152	1.12984
C	3.18948	0.78398	0.62960
C	2.74789	0.78816	-0.87916
C	1.26321	-0.77707	-0.38260
C	3.18910	-0.78028	0.63466
H	3.97710	1.41827	1.04092
C	2.74770	-0.79445	-0.87398
H	3.17655	1.44197	-1.64297
H	3.97631	-1.41246	1.05002
H	3.17703	-1.45338	-1.63303
C	-0.05458	0.80268	-1.18917
C	-0.05480	-0.80956	-1.18479
H	-0.07203	-1.43185	-2.08557

H	-0.07235	1.41959	-2.09361
H	1.32293	1.45285	1.91578
H	-1.16834	1.36378	1.95971
H	1.32355	-1.44039	1.92582
H	-1.17256	-1.36082	1.96421

TS L to M

Energy: -435409.6099529

C	-1.35868	1.05534	-0.42748
C	-1.76265	0.77225	1.02805
C	-1.76312	-0.77171	1.02859
C	-1.35921	-1.05603	-0.42677
C	-3.12061	-1.29466	0.57606
C	-3.11986	1.29573	0.57524
C	-2.63284	-1.62277	-0.67779
H	-4.06729	-1.42454	1.08491
C	-2.63193	1.62281	-0.67881
H	-4.06628	1.42691	1.08422
H	-3.09600	-2.02902	-1.57427
H	-3.09482	2.02874	-1.57557
C	1.69296	0.79565	1.13763
C	1.27663	0.77726	-0.37615
C	1.69256	-0.79314	1.13932
C	3.19134	0.78248	0.65908
C	2.76792	0.79043	-0.85503
C	1.27628	-0.77785	-0.37456
C	3.19096	-0.78170	0.66076
H	3.97454	1.41549	1.08069
C	2.76757	-0.79272	-0.85332
H	3.20725	1.44451	-1.61264
H	3.97382	-1.41420	1.08377
H	3.20664	-1.44862	-1.60951
C	-0.06216	0.78404	-1.17020
C	-0.06226	-0.78566	-1.16913
H	-0.02788	-1.30567	-2.13353
H	-0.02857	1.30279	-2.13530
H	1.30874	1.44835	1.92486
H	-1.24749	1.29069	1.84031
H	1.30810	-1.44399	1.92797
H	-1.24823	-1.28987	1.84119

M

Energy: -435435.3690353

C	-1.32517	1.27599	-0.33682
C	-1.71538	0.78533	1.04566
C	-1.71536	-0.78539	1.04562

C	-1.32516	-1.27596	-0.33686
C	-3.18755	-0.81670	0.52896
C	-3.18757	0.81665	0.52900
C	-2.61254	-1.41471	-0.73917
H	-4.01798	-1.27263	1.07555
C	-2.61256	1.41479	-0.73910
H	-4.01802	1.27252	1.07562
H	-3.05367	-1.61011	-1.71555
H	-3.05369	1.61025	-1.71546
C	1.73184	0.79347	1.13662
C	1.26339	0.77394	-0.36072
C	1.73178	-0.79338	1.13666
C	3.21322	0.78226	0.60761
C	2.73695	0.79283	-0.89123
C	1.26337	-0.77393	-0.36069
C	3.21317	-0.78228	0.60769
H	4.01018	1.41494	1.00292
C	2.73695	-0.79290	-0.89117
H	3.14961	1.44659	-1.66383
H	4.01010	-1.41496	1.00305
H	3.14960	-1.44672	-1.66372
C	-0.10540	0.83141	-1.07310
C	-0.10540	-0.83140	-1.07310
H	-0.06403	-1.24453	-2.08672
H	-0.06402	1.24451	-2.08674
H	1.37111	1.44622	1.93462
H	-1.39087	1.31167	1.94527
H	1.37099	-1.44607	1.93469
H	-1.39083	-1.31177	1.94519

TS J to M

Energy: -435422.3935953

C	-1.30567	1.31432	-0.34102
C	-1.68394	1.15105	0.99544
C	-1.68358	-1.15149	0.99474
C	-1.30524	-1.31391	-0.34174
C	-3.13174	-0.78029	0.66217
C	-3.13192	0.77960	0.66255
C	-2.65403	-0.81075	-0.82968
H	-3.98127	-1.36329	1.03028
C	-2.65431	0.81070	-0.82915
H	-3.98170	1.36232	1.03056
H	-3.20886	-1.28834	-1.64010
H	-3.20922	1.28920	-1.63899
C	1.74280	0.78997	1.13498
C	1.22142	0.77741	-0.34919

C	1.74266	-0.79110	1.13414
C	3.21088	0.78258	0.57525
C	2.68842	0.79109	-0.90673
C	1.22139	-0.77668	-0.34988
C	3.21082	-0.78340	0.57450
H	4.01782	1.41505	0.94961
C	2.68832	-0.79020	-0.90751
H	3.07447	1.43865	-1.69749
H	4.01779	-1.41626	0.94816
H	3.07381	-1.43703	-1.69914
C	-0.09627	1.10923	-1.01197
C	-0.09624	-1.10812	-1.01258
H	-0.06116	-1.30218	-2.08377
H	-0.06089	1.30402	-2.08301
H	1.39190	1.43486	1.94262
H	-1.18332	1.35087	1.93752
H	1.39105	-1.43661	1.94097
H	-1.18300	-1.35135	1.93682

TS A to M

Energy: -435424.8484606

C	1.30039	1.31346	-0.34810
C	2.62127	1.23814	-0.77724
C	2.62105	-1.23799	-0.77764
C	1.30017	-1.31330	-0.34855
C	3.16168	-0.78339	0.57939
C	3.16182	0.78297	0.57964
C	1.66225	-0.79894	1.03263
H	3.94553	-1.33985	1.10350
C	1.66238	0.79861	1.03288
H	3.94573	1.33908	1.10402
H	1.31333	-1.29350	1.94094
H	1.31355	1.29297	1.94133
C	0.08830	1.13085	-1.03177
C	0.08815	-1.13010	-1.03225
H	3.10172	1.41418	-1.73586
H	3.10152	-1.41375	-1.73631
C	-1.21734	-0.77032	-0.35748
C	-1.72210	-0.79114	1.13591
C	-1.21733	0.77018	-0.35712
C	-1.72209	0.79067	1.13623
H	-1.36360	-1.43860	1.93816
H	-1.36316	1.43780	1.93854
C	-2.69069	-0.79039	-0.89889
C	-3.19519	-0.78303	0.58906
C	-2.69061	0.79075	-0.89860

C	-3.19519	0.78296	0.58936
H	-3.99853	-1.41506	0.97199
H	-3.08418	1.44016	-1.68406
H	-3.99860	1.41474	0.97256
H	0.03506	-1.43358	-2.07799
H	0.03480	1.43503	-2.07727
H	-3.08467	-1.43954	-1.68436

TS A to P

Energy: -435422.6638718

C	1.27867	-1.33305	-0.33555
C	1.68957	-1.15630	1.00838
C	1.68957	1.15630	1.00838
C	1.27867	1.33305	-0.33555
C	3.12368	0.77754	0.63829
C	3.12368	-0.77754	0.63829
C	2.62223	0.81092	-0.84727
H	3.97943	1.36193	0.98994
C	2.62223	-0.81092	-0.84727
H	3.97943	-1.36193	0.98994
H	3.16952	1.28987	-1.66226
H	3.16952	-1.28987	-1.66226
C	-1.72472	-0.78690	1.12633
C	-1.19131	-0.80019	-0.35434
C	-1.72472	0.78690	1.12633
C	-3.19419	-0.78373	0.57336
C	-2.66106	-0.78774	-0.90358
C	-1.19131	0.80019	-0.35434
C	-3.19419	0.78373	0.57336
H	-4.00080	-1.41733	0.94670
C	-2.66106	0.78774	-0.90358
H	-3.04278	-1.42455	-1.70491
H	-4.00080	1.41733	0.94670
H	-3.04278	1.42455	-1.70491
C	0.05644	-1.33519	-0.97347
C	0.05644	1.33519	-0.97347
H	0.04251	1.43697	-2.05869
H	0.04251	-1.43697	-2.05869
H	-1.36404	-1.42305	1.93639
H	1.22036	-1.38427	1.95987
H	-1.36404	1.42305	1.93639
H	1.22036	1.38427	1.95987

P

Energy: -435502.8203318

C	1.23599	-1.48287	-0.29349

C	1.63758	-0.79525	1.00716
C	1.63736	0.79461	1.00726
C	1.23595	1.48252	-0.29340
C	3.09504	0.80188	0.44477
C	3.09513	-0.80189	0.44431
C	2.51222	1.50399	-0.75896
H	3.92790	1.25411	0.99185
C	2.51204	-1.50328	-0.75975
H	3.92821	-1.25440	0.99080
H	2.94101	1.79314	-1.71661
H	2.94055	-1.79139	-1.71784
C	-1.58032	-0.80443	1.03932
C	-1.21387	-1.29105	-0.34747
C	-1.58033	0.80478	1.03904
C	-3.09159	-0.77411	0.61442
C	-2.55514	-0.82577	-0.85856
C	-1.21391	1.29101	-0.34792
C	-3.09159	0.77437	0.61417
H	-3.85383	-1.44522	1.01271
C	-2.55519	0.82563	-0.85881
H	-3.06528	-1.28403	-1.70890
H	-3.85385	1.44557	1.01228
H	-3.06544	1.28355	-1.70926
C	-0.05571	-1.65304	-0.92817
C	-0.05554	1.65275	-0.92842
H	-0.05411	1.92255	-1.98520
H	-0.05460	-1.92293	-1.98492
H	-1.19415	-1.28738	1.93809
H	1.39478	-1.26591	1.96321
H	-1.19414	1.28807	1.93762
H	1.39421	1.26525	1.96322

TS P to P

Energy: -435488.4002634

C	1.24501	-1.40054	-0.31940
C	1.62690	-0.79832	1.02267
C	1.62667	0.79834	1.02261
C	1.24463	1.40036	-0.31951
C	3.11153	0.77972	0.51925
C	3.11172	-0.77928	0.51934
C	2.53948	1.30051	-0.79612
H	3.90704	1.32757	1.03464
C	2.53983	-1.30039	-0.79597
H	3.90736	-1.32688	1.03481
H	2.99035	1.50702	-1.76326
H	2.99112	-1.50665	-1.76296

C	-1.62669	-0.79841	1.02257
C	-1.24463	-1.40039	-0.31958
C	-1.62690	0.79820	1.02269
C	-3.11151	-0.77974	0.51918
C	-2.53946	-1.30065	-0.79614
C	-1.24501	1.40052	-0.31936
C	-3.11172	0.77931	0.51932
H	-3.90710	-1.32747	1.03458
C	-2.53986	1.30064	-0.79589
H	-2.99058	-1.50718	-1.76316
H	-3.90740	1.32666	1.03498
H	-2.99113	1.50723	-1.76283
C	0.00023	-1.61609	-0.93384
C	-0.00019	1.61616	-0.93375
H	-0.00022	1.95426	-1.97039
H	0.00028	-1.95406	-1.97052
H	-1.32489	-1.27698	1.95629
H	1.32526	-1.27686	1.95647
H	-1.32522	1.27675	1.95646
H	1.32483	1.27681	1.95637

B

Energy: -435423.9615695

C	1.30685	-1.13754	-0.43522
C	2.39295	-1.25046	0.60329
C	2.26965	0.21016	1.27067
C	1.30678	1.13755	0.43509
C	3.47049	0.68698	0.36178
C	3.47051	-0.68698	-0.36164
C	2.39302	1.25046	-0.60323
H	4.33397	1.24177	0.73186
C	2.26979	-0.21018	-1.27065
H	4.33403	-1.24182	-0.73161
H	2.50693	2.10051	-1.28157
H	2.25565	-0.27229	-2.36121
C	-2.37568	-1.08955	0.79617
C	-1.25218	-0.76908	-0.25067
C	-2.36794	0.39140	1.31095
C	-3.47954	-0.74225	-0.25397
C	-2.36819	-0.39139	-1.31094
C	-1.25216	0.76913	0.25048
C	-3.47953	0.74216	0.25421
H	-4.36819	-1.34383	-0.45332
C	-2.37588	1.08956	-0.79612
H	-2.37085	-0.69734	-2.35895
H	-4.36816	1.34369	0.45378

H	-2.36503	1.97751	-1.43337
C	0.03616	-1.49675	-0.16253
C	0.03617	1.49681	0.16224
H	-2.36454	-1.97752	1.43338
H	2.50679	-2.10050	1.28166
H	-2.37047	0.69740	2.35894
H	2.25537	0.27229	2.36123
H	0.00345	2.24084	-0.64136
H	0.00343	-2.24083	0.64104

TS B to *ent*-B

Energy: -435410.2213059

C	-1.28136	-0.92518	0.37831
C	-2.38975	-1.19328	-0.65426
C	-2.33963	0.22712	-1.31748
C	-1.28136	0.92518	-0.37831
C	-3.48647	0.70195	-0.34211
C	-3.48647	-0.70195	0.34211
C	-2.38976	1.19328	0.65426
H	-4.36364	1.27483	-0.64681
C	-2.33963	-0.22712	1.31748
H	-4.36364	-1.27483	0.64681
H	-2.43251	2.11108	1.24690
H	-2.33725	-0.37287	2.40074
C	2.38978	-1.19350	-0.65396
C	1.28143	-0.92526	0.37852
C	2.33956	0.22667	-1.31747
C	3.48647	-0.70181	0.34232
C	2.33956	-0.22667	1.31747
C	1.28143	0.92526	-0.37852
C	3.48647	0.70181	-0.34232
H	4.36355	-1.27461	0.64746
C	2.38978	1.19350	0.65396
H	2.33718	-0.37211	2.40078
H	4.36355	1.27461	-0.64746
H	2.43274	2.11140	1.24644
C	-0.00003	-1.45904	0.21411
C	-0.00003	1.45904	-0.21411
H	2.43274	-2.11140	-1.24644
H	-2.43250	-2.11108	-1.24690
H	2.33718	0.37211	-2.40078
H	-2.33725	0.37287	-2.40074
H	0.00003	2.16498	0.62462
H	0.00003	-2.16498	-0.62462

TS B to N

Energy: -435382.9854628

C	-1.42507	1.28994	-0.28626
C	-2.41170	1.33740	0.71415
C	-2.37373	-0.90446	1.25412
C	-1.42462	-1.29133	0.28914
C	-3.51372	-0.75113	0.22626
C	-3.52222	0.76245	-0.14968
C	-2.40761	-1.01890	-0.83407
H	-4.43275	-1.34282	0.28031
C	-2.38680	0.55086	-1.21968
H	-4.44601	1.31232	-0.35486
H	-2.51629	-1.71195	-1.67219
H	-2.49480	0.79460	-2.27816
C	2.46701	1.08373	0.82426
C	1.35590	0.74530	-0.22216
C	2.45232	-0.41547	1.32184
C	3.54902	0.74118	-0.24920
C	2.44347	0.40908	-1.32571
C	1.35969	-0.75223	0.22833
C	3.55180	-0.74610	0.23834
H	4.43567	1.34536	-0.44806
C	2.46338	-1.09065	-0.82846
H	2.46330	0.75159	-2.36175
H	4.44071	-1.34877	0.43131
H	2.46700	-1.98058	-1.46201
C	-0.08808	1.09921	0.09380
C	-0.09067	-1.06092	-0.07641
H	2.47327	1.97493	1.45644
H	-2.40614	1.75147	1.71904
H	2.47947	-0.75726	2.35796
H	-2.36815	-0.88894	2.34032
H	-0.05177	-1.13496	-1.17201
H	-0.03373	1.30720	1.17189

N

Energy: -435405.5595406

C	1.48115	1.28762	0.19426
C	2.45532	1.58005	-0.70449
C	2.35962	-1.25841	-1.15809
C	1.46787	-1.32454	-0.13501
C	3.50649	-0.78297	-0.27446
C	3.53302	0.82617	0.02625
C	2.50753	-0.95072	0.90402
H	4.49503	-1.24915	-0.30362
C	2.46943	0.60590	1.15227
H	4.53518	1.22897	0.20016

H	2.69626	-1.60022	1.76283
H	2.60836	0.97422	2.17067
C	-2.49053	0.97610	-0.97979
C	-1.40670	0.77715	0.12111
C	-2.48630	-0.58241	-1.25333
C	-3.58408	0.78843	0.12621
C	-2.49600	0.59592	1.25279
C	-1.42253	-0.78668	-0.10397
C	-3.59816	-0.75116	-0.14607
H	-4.46649	1.42154	0.23435
C	-2.52847	-0.96237	0.97895
H	-2.52669	1.08951	2.22654
H	-4.49164	-1.36550	-0.27008
H	-2.56799	-1.75295	1.73247
C	0.12157	0.74102	-0.16962
C	0.09864	-0.78577	0.19445
H	-2.49965	1.76740	-1.73358
H	2.39717	1.94057	-1.73134
H	-2.51076	-1.07600	-2.22729
H	2.24308	-1.29257	-2.23983
H	0.06391	-0.83254	1.29513
H	0.09692	0.78669	-1.26919

TS N to N

Energy: -435380.9412278

C	-1.46752	1.30268	-0.27336
C	-2.43299	1.19792	0.77231
C	-2.39342	-0.75045	1.22293
C	-1.46752	-1.30263	0.27327
C	-3.54027	-0.76485	0.18673
C	-3.54030	0.76487	-0.18659
C	-2.43310	-1.19786	-0.77225
H	-4.47362	-1.31546	0.32190
C	-2.39352	0.75042	-1.22285
H	-4.47367	1.31547	-0.32168
H	-2.47345	-1.66972	-1.75033
H	-2.42186	0.78120	-2.30833
C	2.49371	1.08817	0.84316
C	1.39764	0.76058	-0.21332
C	2.47422	-0.42050	1.31997
C	3.57516	0.74525	-0.23605
C	2.47444	0.42051	-1.31993
C	1.39763	-0.76049	0.21316
C	3.57513	-0.74524	0.23627
H	4.46278	1.34899	-0.43278
C	2.49385	-1.08813	-0.84312

H	2.50179	0.78195	-2.35009
H	4.46273	-1.34896	0.43314
H	2.51555	-1.97198	-1.48541
C	-0.11424	0.81075	0.09349
C	-0.11424	-0.81100	-0.09387
H	2.51538	1.97201	1.48547
H	-2.47329	1.67031	1.75014
H	2.50133	-0.78194	2.35013
H	-2.42166	-0.78136	2.30840
H	-0.06496	-0.96655	-1.18347
H	-0.06495	0.96605	1.18314

TS N to O

Energy: -435373.3615898

C	1.54818	0.96424	-0.11160
C	2.58358	1.70862	-0.80839
C	2.51805	-1.61740	-1.00068
C	1.54628	-0.98540	-0.12125
C	3.54928	-1.40083	-0.13498
C	3.52714	1.45306	0.13859
C	2.63880	-0.83421	0.94953
H	4.62659	-1.50893	-0.20851
C	2.55932	0.72090	1.05239
H	4.59883	1.61259	0.19902
H	2.55038	-1.40046	1.88119
H	2.37173	1.13848	2.04530
C	-2.59077	0.82184	-1.10245
C	-1.48273	0.80041	-0.00390
C	-2.57488	-0.75967	-1.14253
C	-3.66108	0.78834	0.04245
C	-2.55139	0.77219	1.16258
C	-1.48569	-0.78847	-0.00039
C	-3.66156	-0.77422	0.00116
H	-4.54979	1.42127	0.07420
C	-2.56819	-0.80779	1.12379
H	-2.56972	1.40241	2.05444
H	-4.54970	-1.40844	-0.01207
H	-2.58727	-1.47725	1.98738
C	0.06738	0.66714	-0.31039
C	0.06793	-0.71950	0.24097
H	-2.62899	1.49058	-1.96605
H	2.62128	2.17995	-1.78781
H	-2.61448	-1.39088	-2.03314
H	2.46158	-1.99523	-2.01817
H	0.08535	-0.66825	1.34132
H	0.00632	0.54859	-1.40646

O

Energy: -435373.9241219

C	1.57073	0.86487	-0.14676
C	2.60987	1.66727	-0.83532
C	2.56154	-1.60554	-1.00108
C	1.57525	-0.88120	-0.16320
C	3.55092	-1.45640	-0.09027
C	3.50858	1.52126	0.16236
C	2.64296	-0.82553	0.95764
H	4.62102	-1.64441	-0.11463
C	2.56395	0.74237	1.06007
H	4.56193	1.76792	0.26335
H	2.48077	-1.38541	1.88285
H	2.32073	1.15209	2.04363
C	-2.60795	0.84889	-1.07899
C	-1.49066	0.79835	0.00868
C	-2.59411	-0.73146	-1.15908
C	-3.66805	0.78711	0.07423
C	-2.54791	0.74089	1.18344
C	-1.49475	-0.79206	-0.02634
C	-3.67117	-0.77380	-0.00707
H	-4.55502	1.42066	0.13082
C	-2.56855	-0.83774	1.10504
H	-2.55763	1.34840	2.09102
H	-4.56022	-1.40650	-0.02948
H	-2.58224	-1.52806	1.95207
C	0.04978	0.67316	-0.30716
C	0.06081	-0.72528	0.21569
H	-2.65352	1.53888	-1.92526
H	2.66575	2.10197	-1.83079
H	-2.64302	-1.33919	-2.06536
H	2.53286	-1.98342	-2.01986
H	0.07834	-0.70508	1.31665
H	-0.01719	0.57117	-1.40611

TS O to O

Energy: -435342.0838541

C	-1.58787	0.81168	0.01166
C	-2.67597	1.27223	0.94769
C	-2.54604	-1.18545	1.09239
C	-1.58784	-0.81214	-0.01218
C	-3.49784	-1.58585	0.14250
C	-3.49756	1.58634	-0.14194
C	-2.67658	-1.27249	-0.94768
H	-4.53673	-1.89201	0.22874

C	-2.54632	1.18583	-1.09243
H	-4.53608	1.89391	-0.22762
H	-2.70873	-1.47021	-2.01125
H	-2.46317	1.25080	-2.16952
C	2.59533	0.78555	1.13497
C	1.49987	0.79504	0.02387
C	2.57805	-0.79636	1.13124
C	3.67703	0.78168	0.00031
C	2.57809	0.79645	-1.13111
C	1.49997	-0.79515	-0.02392
C	3.67714	-0.78140	-0.00004
H	4.56515	1.41598	-0.00605
C	2.59563	-0.78549	-1.13487
H	2.60655	1.45065	-2.00517
H	4.56533	-1.41562	0.00646
H	2.62575	-1.42998	-2.01682
C	-0.04968	0.68703	0.28855
C	-0.04961	-0.68747	-0.28926
H	2.62510	1.43005	2.01693
H	-2.70885	1.46715	2.01173
H	2.60664	-1.45056	2.00529
H	-2.46303	-1.24931	2.16955
H	-0.04620	-0.58092	-1.38744
H	-0.04649	0.58004	1.38671

TS B to Q

Energy: -435403.5554159

C	-1.34100	1.23487	-0.39148
C	-2.37059	1.44365	0.57988
C	-2.12934	-0.60289	1.30647
C	-1.30604	-1.30240	0.32085
C	-3.40074	-0.70281	0.42370
C	-3.45321	0.71872	-0.19667
C	-2.42485	-1.19180	-0.68489
H	-4.28207	-1.26384	0.74755
C	-2.31254	0.31979	-1.20999
H	-4.38276	1.20174	-0.51014
H	-2.65163	-1.95276	-1.43568
H	-2.38563	0.49088	-2.28616
C	2.26693	0.96902	0.94566
C	1.23108	0.76927	-0.22509
C	2.25487	-0.56565	1.25852
C	3.46013	0.78087	-0.04572
C	2.44972	0.56383	-1.22906
C	1.23617	-0.80347	0.07211
C	3.45231	-0.75918	0.25787

H	4.34888	1.41330	-0.08515
C	2.44162	-0.97430	-0.91708
H	2.53068	1.00775	-2.22315
H	4.33519	-1.37258	0.44652
H	2.50106	-1.76802	-1.66605
C	-0.02162	1.57523	-0.18104
C	-0.03217	-1.54007	-0.12121
H	2.17924	1.76661	1.68764
H	-2.40391	2.07920	1.46255
H	2.18033	-1.00999	2.25283
H	-2.00978	-0.50710	2.38177
H	-0.02984	-2.09720	-1.06336
H	0.06579	2.41584	0.51397

Q

Energy: -435470.9946316

C	-1.42074	1.42639	-0.26300
C	-2.50834	1.70328	0.50538
C	-2.11012	-1.18445	1.28107
C	-1.23828	-1.48131	0.28461
C	-3.24887	-0.80640	0.33467
C	-3.39868	0.71145	-0.16937
C	-2.22028	-1.07637	-0.79535
H	-4.18508	-1.36800	0.40152
C	-2.21515	0.46627	-1.16926
H	-4.40838	0.97126	-0.50187
H	-2.42881	-1.75202	-1.63082
H	-2.30462	0.71267	-2.22982
C	2.24056	1.05842	0.91161
C	1.19315	1.26083	-0.13773
C	2.24452	-0.54677	1.16967
C	3.34319	0.86500	-0.16413
C	2.14628	0.61125	-1.16902
C	1.35553	-1.29458	0.15306
C	3.44527	-0.64909	0.14292
H	4.15542	1.56877	-0.35092
C	2.35787	-0.98367	-0.91317
H	2.12515	0.92830	-2.21347
H	4.34659	-1.23915	0.31373
H	2.49210	-1.59168	-1.81160
C	-0.05554	1.66994	0.16594
C	0.12740	-1.76740	-0.13402
H	2.31635	1.67834	1.80896
H	-2.61623	2.28136	1.42213
H	2.28016	-0.86913	2.21183
H	-2.02399	-1.16466	2.36496

H	0.10373	-2.18521	-1.14585
H	-0.07897	2.13251	1.15798

TS Q to *ent*-Q

Energy: -435452.9174832

C	-1.33220	1.37199	-0.21596
C	-2.35242	1.51383	0.71007
C	-2.17320	-1.07427	1.22012
C	-1.32342	-1.43321	0.18721
C	-3.35182	-0.74707	0.28312
C	-3.38539	0.76748	-0.09371
C	-2.32983	-1.01987	-0.85778
H	-4.28845	-1.30771	0.36986
C	-2.24021	0.54961	-1.15300
H	-4.33930	1.23669	-0.35548
H	-2.54893	-1.64382	-1.72862
H	-2.33778	0.85794	-2.19592
C	2.34949	1.50768	0.71419
C	1.32989	1.37061	-0.21460
C	2.17476	-1.06833	1.21889
C	3.38486	0.76897	-0.09373
C	2.23933	0.55140	-1.15298
C	1.32482	-1.43163	0.18610
C	3.35386	-0.74529	0.28105
H	4.33676	1.24295	-0.35418
C	2.33112	-1.01879	-0.85904
H	2.33574	0.86060	-2.19573
H	4.29009	-1.30641	0.36885
H	2.54946	-1.64193	-1.73060
C	-0.00056	1.71713	0.09137
C	0.00133	-1.66964	-0.23502
H	2.36474	1.94237	1.71163
H	-2.36801	1.95045	1.70672
H	2.06997	-1.03884	2.29945
H	-2.06690	-1.04285	2.30053
H	0.00096	-1.88189	-1.30734
H	-0.00082	2.30900	1.01301

Protonated A

Energy: -435659.8208516

C	1.22949	-1.23064	-0.36399
C	1.60926	-0.78778	1.05688
C	1.60930	0.78718	1.05717
C	1.22984	1.23102	-0.36359
C	3.12250	0.77471	0.62889
C	3.12241	-0.77531	0.62838

C	2.61606	0.80853	-0.86080
H	3.88012	1.44143	1.03651
C	2.61571	-0.80819	-0.86126
H	3.88000	-1.44240	1.03545
H	3.11572	1.30100	-1.69615
H	3.11500	-1.30049	-1.69694
C	-1.65264	-0.79086	1.09122
C	-1.16739	-1.12135	-0.35672
C	-1.65242	0.79047	1.09138
C	-3.14174	-0.77848	0.59045
C	-2.61040	-0.79910	-0.88774
C	-1.16708	1.12117	-0.35660
C	-3.14153	0.77861	0.59071
H	-3.92523	-1.42961	0.97317
C	-2.61037	0.79948	-0.88751
H	-3.06689	-1.35044	-1.70973
H	-3.92484	1.42978	0.97372
H	-3.06700	1.35098	-1.70931
C	0.06209	-1.66065	-0.92833
C	0.06256	1.66117	-0.92785
H	0.04355	1.95362	-1.97676
H	0.04299	-1.95252	-1.97739
H	-1.29906	-1.35277	1.95427
H	1.21467	-1.31464	1.92538
H	-1.29870	1.35200	1.95462
H	1.21471	1.31364	1.92592
H	-0.73879	0.00064	-0.65701

Protonated B

Energy: -435634.4623386

C	-1.23500	-1.06432	0.29932
C	-2.31686	-1.06778	-0.81942
C	-2.30807	0.44390	-1.28629
C	-1.23519	1.06446	-0.29972
C	-3.43513	0.74499	-0.22684
C	-3.43498	-0.74516	0.22734
C	-2.31659	1.06774	0.81942
H	-4.30701	1.36900	-0.41226
C	-2.30749	-0.44394	1.28632
H	-4.30673	-1.36924	0.41311
H	-2.35371	1.87371	1.55289
H	-2.34620	-0.71260	2.34141
C	2.35871	-1.18582	-0.71954
C	1.28442	-1.19161	0.33407
C	2.23129	0.31804	-1.25186
C	3.43425	-0.71456	0.29901

C	2.23147	-0.31807	1.25188
C	1.28415	1.19143	-0.33397
C	3.43408	0.71482	-0.29905
H	4.29204	-1.30297	0.61927
C	2.35846	1.18583	0.71956
H	2.19813	-0.47745	2.33009
H	4.29169	1.30343	-0.61938
H	2.46932	1.97279	1.46782
C	0.04811	-1.74667	0.13091
C	0.04791	1.74671	-0.13115
H	2.46973	-1.97275	-1.46780
H	-2.35425	-1.87371	-1.55293
H	2.19779	0.47747	-2.33006
H	-2.34723	0.71261	-2.34136
H	0.02584	2.41863	0.72964
H	0.02616	-2.41844	-0.72999
H	-0.69681	-0.00026	-0.00044

Select barrier heights in kcal/mol comparing unsubstituted and substituted Fused Cubanes.

	A to A	J to K	K to L	M to L	N to O	O to O
$\Delta G^{\ddagger}_{unsub}$	12.5	30.7	53.7	34.8	70.9	100.2
$\Delta G^{\ddagger}_{sub}$	15.9	30.2	52.0	33.0	68.6	98.5

IRCs and significant structures for transformation from A to P