The smallest hyperbolic paraboloid hydrocarbon: A high-level ab initio perspective

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S U P P O R T I N G I N F O R M A T I O N

(Tables S1 and S2, total x pages)

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Table S1. CCSD(T) energies relative to isomer **1** (in kJ mol^{-1}) obtained from G4(MP2) theory for the fourteen $C_{13}H_8$ isomers shown in Schemes 1 and 2 and transition structures in Fig 1.

	ΔE_e	ΔH_0	ΔH_{298}
1	0.0	0.0	0.0
2	23.2	16.0	25.4
3	33.4	22.8	31.9
5	37.3	26.1	35.8
4	37.4	26.4	36.0
6	60.5	41.9	52.3
7	60.6	42.4	52.6
8	62.9	44.2	54.5
10	58.3	49.1	57.4
9	66.8	47.7	58.5
11	291.6	273.0	287.0
12	293.6	274.4	288.7
13	364.1	360.4	361.8
14	511.4	485.5	500.9
1-TS[a]	261.6	246.4	248.1
1-TS[b]	76.9	70.7	69.9

[a]Transition structure of **1** for skeletal inversion (see Figure 1b). [a]Transition structure of **1** for π-bond shift (see Figure 1c).

Table S2. B3LYP/6-31G(2df,p) optimized structures (Cartesian coordinates in Å)

1

C	0.000000	0.000000	0.000000
C	1.041606	1.023788	0.554287
C	-1.041606	1.023788	-0.554287
C	-1.041606	-1.023788	0.554287
C	1.041606	-1.023788	-0.554287
C	-0.648396	-2.303202	0.314702
C	2.421173	0.550781	0.384153
C	-2.421173	-0.550781	0.384153
C	0.648396	2.303202	0.314702
C	2.421173	-0.550781	-0.384153
C	-2.421173	0.550781	-0.384153
C	-0.648396	2.303202	-0.314702
C	0.648396	-2.303202	-0.314702
H	-1.283116	3.171408	-0.448390
H	1.283116	3.171408	0.448390
H	3.289262	1.111118	0.708482
H	3.289262	-1.111118	-0.708482
H	1.283116	-3.171408	-0.448390
H	-1.283116	-3.171408	0.448390
H	-3.289262	-1.111118	0.708482
H	-3.289262	1.111118	-0.708482

2

C	2.916156	-1.211981	-0.000024
C	4.304611	-1.206731	0.000485
C	5.003837	-0.000484	0.000741
C	4.305199	1.206106	0.000478
C	2.916747	1.212036	-0.000019
C	2.201122	0.000202	-0.000278
H	4.843957	-2.147995	0.000693
H	4.845005	2.147106	0.000692
C	0.784686	0.000559	-0.000693
C	-0.432839	0.000708	-0.000946
H	2.367924	-2.146950	-0.000202
H	2.368971	2.147273	-0.000205
C	-1.780401	0.000371	-0.001052
C	-3.001248	0.000123	-0.000940
C	-4.351595	-0.000021	-0.000504
C	-5.564874	-0.000170	0.000175
H	6.088528	-0.000749	0.001144
C	-7.015064	-0.000320	0.001393
H	-7.410151	-0.002607	1.023762
H	-7.411214	0.885912	-0.507439

H	-7.411036	-0.884380	-0.511339

3

C	-1.993691	-1.520380	0.000011
C	-3.379678	-1.582082	-0.000010
C	-4.121513	-0.403126	-0.000041
C	-3.472109	0.829460	-0.000053
C	-2.081927	0.922194	-0.000032
C	-1.331810	-0.279234	0.000001
H	-3.878236	-2.545110	-0.000003
C	0.083741	-0.241865	0.000029
C	1.301260	-0.206626	0.000073
H	-1.400775	-2.427856	0.000034
C	2.647927	-0.170048	0.000091
C	3.867611	-0.135801	0.000113
C	5.218791	-0.097080	0.000009
C	6.428525	-0.062092	-0.000111
H	7.489839	-0.031515	-0.000190
H	-5.205708	-0.441094	-0.000058
H	-4.057185	1.743968	-0.000082
C	-1.390606	2.259629	-0.000024
H	-0.745577	2.373895	0.877962
H	-0.745135	2.373685	-0.877709
H	-2.116346	3.076336	-0.000296

4

C	-1.635325	-1.618236	0.001149
C	-3.020946	-1.714136	0.000767
C	-3.807350	-0.566138	-0.000793
C	-3.223764	0.707252	-0.001632
C	-1.835319	0.799090	-0.002072
C	-1.025645	-0.352503	-0.000368
H	-3.491566	-2.691635	0.000972
C	0.385693	-0.232974	-0.000692
C	1.598283	-0.124863	-0.000651
H	-1.016418	-2.507616	0.001852
C	2.940490	-0.007448	-0.000403
C	4.155863	0.099265	-0.000054
C	5.502489	0.217571	0.000418
C	6.708064	0.323458	0.000754
H	7.765736	0.416319	0.001165
H	-4.889698	-0.655980	-0.001834
C	-4.085738	1.946088	0.001894
H	-3.480511	2.853926	-0.058168
H	-4.781407	1.947886	-0.844219
H	-4.689836	2.005878	0.914262

H	-1.357082	1.772668	-0.003946

5

C	-1.619238	1.208563	-0.005016
C	-3.005994	1.199999	-0.008640
C	-3.726013	0.000072	-0.007152
C	-3.006124	-1.199940	-0.008648
C	-1.619373	-1.208657	-0.005025
C	-0.899641	-0.000085	-0.002340
H	-3.543167	2.143708	-0.014422
H	-3.543401	-2.143591	-0.014438
C	-5.233142	0.000140	0.019914
C	0.515553	-0.000165	-0.001906
C	1.733142	-0.000186	-0.000904
H	-1.076508	2.146842	-0.008293
H	-1.076746	-2.146994	-0.008309
C	3.080338	-0.000059	0.000360
C	4.300483	0.000022	0.001596
C	5.652264	0.000111	0.002963
C	6.862527	0.000141	0.004218
H	7.924240	-0.000144	0.005280
H	-5.642085	0.886648	-0.473088
H	-5.642182	-0.885786	-0.474060
H	-5.608843	-0.000418	1.050812

6

C	1.779232	-0.852871	0.000000
C	0.835952	-1.861702	0.000000
C	-0.538602	-1.564815	0.000000
C	-0.968546	-0.223204	0.000000
C	0.000000	0.801565	0.000000
C	1.382083	0.491405	0.000000
C	-0.420373	2.161673	0.000000
C	-0.795673	3.306118	0.000000
H	-1.111883	4.319784	0.000000
C	2.366613	1.516869	0.000000
C	3.224406	2.362192	0.000000
H	3.970340	3.117836	0.000000
C	-2.430664	0.134827	0.000000
H	-2.681740	0.740342	0.877202
H	-2.681740	0.740342	-0.877202
H	-3.055594	-0.758185	0.000000
H	2.836760	-1.087931	0.000000
H	1.146294	-2.899932	0.000000
C	-1.467853	-2.646235	0.000000
C	-2.221600	-3.586266	0.000000

H	-2.892288	-4.409591	0.000000

7

C	0.800366	-1.262750	0.000000
C	-0.516696	-1.730863	0.000000
C	-1.568735	-0.800472	0.000000
C	-1.333229	0.568518	0.000000
C	0.000000	1.035720	0.000000
C	1.071688	0.108018	0.000000
C	0.259981	2.432973	0.000000
C	0.452073	3.622432	0.000000
H	0.638801	4.667746	0.000000
C	2.424354	0.551957	0.000000
C	3.576801	0.899992	0.000000
H	4.589487	1.219137	0.000000
H	-2.589475	-1.166256	0.000000
C	-2.480985	1.544272	0.000000
H	-2.443126	2.198294	0.877441
H	-2.443126	2.198294	-0.877441
H	-3.439871	1.021097	0.000000
H	1.623618	-1.965751	0.000000
C	-0.787492	-3.128752	0.000000
C	-1.017581	-4.310904	0.000000
H	-1.219568	-5.353390	0.000000

8

C	1.408552	0.467556	0.000000
C	1.963181	-0.817437	0.000000
C	1.151114	-1.942515	0.000000
C	-0.238859	-1.836585	0.000000
C	-0.816760	-0.549431	0.000000
C	0.000000	0.607256	0.000000
H	3.042022	-0.919401	0.000000
C	2.261993	1.605829	0.000000
C	-2.234035	-0.418266	0.000000
C	3.013629	2.546416	0.000000
H	3.663163	3.386265	0.000000
C	-3.436196	-0.343362	0.000000
H	-4.494587	-0.257823	0.000000
C	-0.589850	1.899645	0.000000
C	-1.085424	2.996717	0.000000
H	-1.522440	3.964264	0.000000
H	1.605171	-2.928181	0.000000
C	-1.108181	-3.065466	0.000000
H	-1.763644	-3.086799	0.877112
H	-1.763644	-3.086799	-0.877112

H	-0.501020	-3.973667	0.000000

9

C	-0.002128	-0.008506	1.217593
C	-0.005068	-1.408433	1.196037
C	-0.003144	-2.124172	0.000000
C	-0.005068	-1.408433	-1.196037
C	-0.002128	-0.008506	-1.217593
C	0.000426	0.713682	-0.000000
H	-0.010508	-1.936727	2.143306
H	-0.010508	-1.936727	-2.143306
C	-0.005068	0.669900	2.469094
C	0.024478	-3.632341	0.000000
C	-0.005068	0.669900	-2.469094
C	-0.007041	1.212276	3.543932
H	-0.008684	1.705555	4.484161
C	-0.007041	1.212276	-3.543932
H	-0.008684	1.705555	-4.484161
C	0.001148	2.133377	-0.000000
C	0.002290	3.337310	-0.000000
H	0.003510	4.398938	-0.000000
H	1.055317	-4.006935	0.000000
H	-0.469980	-4.039822	0.886112
H	-0.469980	-4.039822	-0.886112

10

C	4.236041	0.023815	-0.540329
C	3.223433	-0.919193	-0.387874
C	1.978069	-0.549134	0.123475
C	1.759418	0.783525	0.474366
C	2.770907	1.728237	0.320757
C	4.012361	1.351899	-0.185559
H	3.402039	-1.952618	-0.671132
H	0.790865	1.082384	0.860788
C	0.908106	-1.617463	0.327003
H	1.071293	-2.431625	-0.390834
H	1.035774	-2.073798	1.320380
H	2.585610	2.761522	0.595230
H	4.798760	2.089130	-0.307479
H	5.197504	-0.279214	-0.941726
C	-0.463551	-1.149195	0.208463
C	-1.610670	-0.764614	0.118691
C	-2.888846	-0.337425	0.017563
C	-4.041310	0.048310	-0.071080
C	-5.320929	0.476466	-0.169859
C	-6.465134	0.859513	-0.257303

H	-7.469220	1.195779	-0.335108

11

C	-5.209379	-0.924003	-0.000249
H	-5.521161	-1.966742	-0.000801
C	-6.152479	0.036153	0.000436
C	-3.819491	-0.699245	-0.000314
C	-2.607062	-0.559366	-0.000400
C	-1.274830	-0.394979	-0.000485
C	-0.058203	-0.246121	-0.000553
C	1.269623	-0.085049	-0.000630
C	2.486322	0.061818	-0.000667
C	3.819223	0.223200	-0.000722
C	5.031813	0.353517	-0.000712
C	6.424592	0.564394	-0.000897
H	6.747135	1.604707	-0.004181
C	7.345667	-0.409877	0.002622
H	7.066838	-1.457210	0.005947
H	8.403372	-0.173889	0.002233
H	-7.191345	-0.285936	0.000399
C	-5.909214	1.509325	0.001243
H	-4.842854	1.744758	0.001302
H	-6.370791	1.978343	-0.876768
H	-6.370681	1.977365	0.879832

12

C	-5.062330	0.533918	-0.002162
H	-5.439065	1.556686	-0.007333
C	-5.936723	-0.487483	0.003526
H	-5.548595	-1.503496	0.008676
C	-3.663318	0.385143	-0.001949
C	-2.445901	0.304477	-0.001997
C	-1.108019	0.196523	-0.001921
C	0.113668	0.097352	-0.001822
C	1.446742	-0.012162	-0.001694
C	2.668080	-0.113688	-0.001562
C	4.005946	-0.226910	-0.001402
C	5.222356	-0.314895	-0.001133
C	-7.422218	-0.331954	0.003346
H	-7.721285	0.719669	-0.001963
H	-7.866866	-0.822132	-0.871980
H	-7.866131	-0.813038	0.884074
C	6.621551	-0.477830	-0.001232
H	6.979381	-1.506545	-0.008011
C	7.509078	0.527082	0.006286
H	7.194914	1.564343	0.013159

H	8.574175	0.327076	0.005681

13

C	0.515895	-0.667916	-0.318415
C	1.931930	-0.827376	0.242491
C	1.931906	0.827323	0.242498
C	0.515899	0.667922	-0.318431
C	2.074820	-0.000026	1.505377
H	3.045080	-0.000047	1.996670
H	1.230845	-0.000041	2.190348
C	3.157209	-0.667660	-0.650227
C	3.157173	0.667703	-0.650211
C	-3.371611	-0.689018	0.036865
C	-2.161613	-1.444522	-0.057263
C	-1.020997	-0.716268	-0.198137
C	-1.020950	0.716247	-0.198140
C	-2.161557	1.444527	-0.057241
C	-3.371571	0.689050	0.036903
H	-4.314698	-1.220627	0.111253
H	-2.178068	-2.527465	-0.005350
H	-2.177960	2.527467	-0.005250
H	-4.314633	1.220698	0.111355
H	3.825173	-1.423596	-1.047712
H	3.825062	1.423693	-1.047725

14

C	3.704565	-0.294662	-0.095331
C	2.380580	-0.214654	-0.100514
C	1.130958	-0.139237	-0.105754
C	-0.158893	-0.061124	-0.111706
C	-1.437231	0.016240	-0.117683
C	-2.697209	0.092412	-0.123321
C	-4.007749	0.174099	-0.129997
C	-5.241640	0.236858	-0.128040
C	-6.630966	0.379051	-0.142578
H	-7.007114	1.238594	-0.698206
C	-7.504678	-0.410683	0.510021
H	-8.563119	-0.180618	0.509346
H	-7.177494	-1.266928	1.087674
C	6.374762	-0.446283	-0.083213
C	7.087496	0.830898	0.401139
H	6.792643	1.074666	1.424914
H	6.713073	-0.704641	-1.096932
H	6.670466	-1.301641	0.541232
H	8.172202	0.690659	0.376684
H	6.833744	1.681493	-0.236484

C	4.927604	-0.368179	-0.091063

TS for planarization

C	0.000000	0.000000	0.000000
C	0.000000	1.135560	1.147900
C	0.000000	1.135560	-1.147900
C	-0.000000	-1.135560	-1.147900
C	-0.000000	-1.135560	1.147900
C	0.000000	-2.416882	-0.706120
C	0.000000	0.662528	2.520985
C	-0.000000	-0.662528	-2.520985
C	0.000000	2.416882	0.706120
C	-0.000000	-0.662528	2.520985
C	0.000000	0.662528	-2.520985
C	0.000000	2.416882	-0.706120
C	-0.000000	-2.416882	0.706120
H	0.000000	3.266878	-1.374750
H	-0.000000	3.266878	1.374750
H	0.000000	1.354629	3.351885
H	-0.000000	-1.354629	3.351885
H	-0.000000	-3.266878	1.374750
H	-0.000000	-3.266878	-1.374750
H	-0.000000	-1.354629	-3.351885
H	0.000000	1.354629	-3.351885

TS for π-bond shift

C	0.000000	0.000000	0.238873
C	0.000000	1.471056	0.762428
C	-1.392663	0.000000	-0.436982
C	-0.000000	-1.471056	0.762428
C	1.392663	-0.000000	-0.436982
C	1.176452	-2.122761	0.291611
C	1.176452	2.122761	0.291611
C	-1.176452	-2.122761	0.291611
C	-1.176452	2.122761	0.291611
C	1.981319	1.276735	-0.454857
C	-1.981319	-1.276735	-0.454857
C	-1.981319	1.276735	-0.454857
C	1.981319	-1.276735	-0.454857
H	-2.983952	1.486918	-0.803551
H	-1.361908	3.181202	0.448383
H	1.361908	3.181202	0.448383
H	2.983952	1.486918	-0.803551
H	2.983952	-1.486918	-0.803551
H	1.361908	-3.181202	0.448383
H	-1.361908	-3.181202	0.448383

H	-2.983952	-1.486918	-0.803551