Ethene Optimized Geometries

Ethene cas(6,6)/6-31G*
$E(S_0)$=-78.10667; $E(S_1)$=-77.74784

1	6	0.019024	0.000000	-0.013422
2	1	0.056026	0.000000	1.061590
3	1	0.979523	0.000000	-0.543834
4	6	-1.155795	0.000000	-0.686778
5	1	-1.190021	0.000000	-1.761769
6	1	-2.100208	0.000000	-0.172276

Ethene S_1 SOSP cas(6,6)/6-31G* (planar) (Figure 5a)
$E(S_1)$=-77.77594

1	6	0.110382	-0.000001	0.041014
2	1	0.106074	0.000000	1.109360
3	1	1.040689	0.000001	-0.528746
4	6	-1.249983	-0.000001	-0.740512
5	1	-1.233881	0.000000	-1.808381
6	1	-2.164733	0.000001	-0.189226

Ethene Z/V CI cas(6,6)/6-31G* (Figure 5d)
$E(S_2)$=-77.84686; $E(S_1)$=-77.84722

1	6	.167227	.307339	.123837
2	1	-.030667	-.187963	1.062268
3	1	1.031599	-.149072	-.408036
4	6	-.532984	1.398917	-.370324
5	1	-1.351925	1.324546	-1.090457
6	1	-.295559	2.437215	-.123007

Ethene Type I CI cas(6,6)/6-31G* (Figure S1a)
$E(S_1)$=-77.90344; $E(S_0)$=-77.90391

1	6	0.084475	0.086277	0.128568
2	1	0.289011	-0.025475	1.188243
3	1	0.929973	-0.070625	-0.534575
4	6	-1.297234	0.186346	-0.292807
5	1	-1.539187	0.601821	-1.261899
6	1	-0.919461	-0.916614	-0.691884

Ethene Type I/ Type I CI TS cas(6,6)/6-31G* (Figure S1b)
$E(S_1)$=-77.87281; $E(S_0)$=-77.87286

1	6	-0.022217	-0.029768	-0.058874
2	6	-0.069588	0.274459	1.297495
3	1	0.907580	-0.294387	-0.568751
4	1	-0.922284	-0.113594	-0.673159
5	1	-0.082971	0.690215	2.260609
6	1	-0.175416	-0.929535	1.074672

Ethene Type II CI cas(6,6)/6-31G* (Figure S1c)
$E(S_1)$=-77.91722; $E(S_0)$=-77.91752

1	6	-0.092019	-0.273574	-0.013215
2	1	0.047897	-0.074506	1.043925
3	1	0.807083	0.051210	-0.544841
4	6	-1.255788	0.439646	-0.596733
5	1	-1.798229	1.096133	-1.224996
6	1	-0.161365	-1.377181	-0.128494

Ethene Type I/ Type II CI TS cas(6,6)/6-31G* (Figure S1d)
$E(S_1)$=-77.88488; $E(S_0)$=-77.88491

1	6	0.037343	0.108185	0.133338
2	1	0.277425	-0.065440	1.168203
3	1	0.856612	0.028814	-0.563901
4	6	-1.280924	0.436996	-0.236876
5	1	-1.485634	0.697508	-1.268387
6	1	-0.857246	-1.344333	-0.696730

Ethylidene cas(6,6)/6-31G*
$E(S_0)$=-77.97828

1	6	-0.111777	-0.150055	0.007647
2	1	0.117213	-0.188884	1.065190
3	1	0.739740	0.208313	-0.563767
4	6	-1.464534	0.469659	-0.292049
5	1	-1.429126	0.728715	-1.360178
6	1	-0.303938	-1.206019	-0.321199

Ethylidene S_1 cas(6,6)/6-31G*
$E(S_1)$=-77.92111; $E(S_0)$=-77.93795

1	6	-.108275	-.257123	-.009763
2	1	.042772	-.095677	1.053222
3	1	.750981	.150453	-.544644
4	6	-1.365194	.381177	-.505105
5	1	-1.664826	1.042544	-1.286475
6	1	-.107881	-1.359645	-.171591

Cyclohexene H-Shift Optimized Geometries

Cyclohexene cas(6,6)/6-31G*
$E(S_0)$=-233.09367; $E(S_1)$=232.74767

1	6	-1.278531	-0.343454	-0.717036
2	6	-1.235205	-0.155127	0.780081
3	6	-0.102601	0.159473	1.458545
4	6	1.237236	0.341879	0.787410
5	1	2.010924	-0.144183	1.376569
6	1	1.492398	1.400860	0.774287
7	1	-0.146888	0.295650	2.526539
8	1	-2.171934	-0.288319	1.339920
9	1	-2.164342	0.140024	-1.121319
10	1	-1.385679	-1.403342	-0.944471
11	6	-0.021840	0.210818	-1.395635
12	6	1.239704	-0.212410	-0.640910
13	1	0.021882	-0.123700	-2.428109
14	1	-0.075300	1.297299	-1.419331
15	1	1.285640	-1.298889	-0.605016
16	1	2.128832	0.121883	-1.167754

Cyclohexene cas(8,8)/6-31G*
$E(S_0)$=-233.11463

1	6	.001903	-.000282	.011094
2	6	.072228	-.003346	1.518646
3	6	1.240864	-.001918	2.208830
4	6	2.594958	-.010068	1.542539
5	1	3.253450	-.704222	2.058687
6	1	3.054408	.972048	1.646847
7	1	1.210472	.013203	3.308253
8	1	-.875919	-.012640	2.076164
9	1	-.765975	.694872	-.319154
10	1	-.314185	-.982822	-.336977
11	6	1.349110	.367019	-.619555
12	6	2.495852	-.384029	.060018
13	1	1.331783	.152950	-1.684298
14	1	1.514174	1.437560	-.517002
15	1	2.323581	-1.454557	-.030193
16	1	3.437225	-.174640	-.439736

Cyclohexene S_1 SOSP cas(8,8)/6-31G* (Figure 5b)
$E(S_1)$=-232.80140

1	6	.010966	.059446	.022531
2	6	-.008435	.118689	1.494149
3	6	1.300961	-.122433	2.268132
4	6	2.580416	-.069974	1.540442
5	1	3.361257	-.634834	2.046773
6	1	2.933295	.984474	1.556252
7	1	1.283446	.083869	3.348990
8	1	-.946874	-.083937	2.032127
9	1	-.807859	.624641	-.419325
10	1	-.176136	-.995779	-.274289
11	6	1.367311	.413475	-.594872
12	6	2.465301	-.430302	.056123
13	1	1.333289	.242919	-1.666137
14	1	1.583179	1.468821	-.440883
15	1	2.223474	-1.485519	-.053870
16	1	3.420338	-.264429	-.431977

Cyclohexene Type I CI cas(6,6)/6-31G* (Figure 1a)
$E(S_1)$=-232.88539; $E(S_0)$=-232.88545

1	6	0.132205	0.337181	0.242507
2	6	-0.444438	-0.668859	1.253775
3	6	2.564785	-0.293561	0.731705
4	6	1.467581	-0.141047	-0.343321
5	1	-0.586657	0.504040	-0.553430
6	1	0.278350	1.303009	0.724208
7	1	1.310756	-1.103047	-0.825376
8	1	1.798321	0.543499	-1.119152
9	6	0.628374	-1.229068	2.154111
10	1	0.338807	-1.901114	2.958326
11	6	2.006894	-0.762528	2.083536
12	1	1.366376	0.245170	2.342143
13	1	-0.895824	-1.507943	0.720857
14	1	3.310178	-1.011064	0.396878
15	1	-1.247306	-0.213703	1.831953
16	1	3.092111	0.642050	0.883486

Cyclohexene Type III CI cas(6,6)/6-31G* (Figure 1b)
$E(S_1)$=-232.87831; $E(S_0)$=-232.87848

1	6	0.028638	-0.020432	-0.086561
2	6	0.073952	0.086157	1.441576
3	6	2.550051	-0.120155	-0.254642
4	6	1.225566	-0.823663	-0.607077
5	1	-0.903747	-0.482396	-0.395627
6	1	0.045328	0.978127	-0.519354
7	1	1.210366	-1.814745	-0.158227
8	1	1.155105	-0.966560	-1.681295
9	6	1.440155	0.559996	1.931297
10	1	1.558942	0.692781	2.993268
11	6	2.581932	0.401152	1.146253
12	1	1.254150	2.261244	1.712978
13	1	-0.122970	-0.891312	1.879713
14	1	3.395424	-0.781394	-0.417900
15	1	-0.705675	0.746897	1.805452
16	1	2.706933	0.725428	-0.925218

Cyclohexene Type II CI cas(6,6)/6-31G* (Figure 1c)
$E(S_1)$=-232.87933; $E(S_0)$=-232.87936

1	6	0.219737	0.385122	0.206270
2	6	-0.363179	-0.569396	1.272786
3	6	2.672125	-0.376866	0.604679
4	6	1.499030	-0.186769	-0.440520
5	1	-0.525771	0.556895	-0.564610
6	1	0.437712	1.353363	0.656647
7	1	1.272437	-1.163282	-0.864791
8	1	1.841715	0.452521	-1.251476
9	6	0.618525	-0.822589	2.493116
10	1	0.412562	-1.798707	2.927842
11	6	1.884726	-0.658023	1.782248
12	1	0.412449	-0.075371	3.299814
13	1	-0.561745	-1.532162	0.804450
14	1	3.335835	-1.167382	0.259184
15	1	-1.311344	-0.187744	1.646679
16	1	3.275700	0.533410	0.649887

Cyclohexene H-shift Carbene Product cas(6,6)/6-31G*
$E(S_0)$=-232.96939

1	6	0.178286	0.368371	0.164137
2	6	-0.363531	-0.574560	1.237105
3	6	2.526966	-0.444663	0.657527
4	6	1.468239	-0.197640	-0.426574
5	1	-0.562015	0.517296	-0.616629
6	1	0.373734	1.347220	0.600291
7	1	1.246299	-1.135153	-0.932782
8	1	1.871732	0.469387	-1.183219
9	6	0.680109	-0.851600	2.324674
10	1	0.338861	-1.601187	3.031052
11	6	2.134919	-1.123200	1.942160
12	1	0.841344	0.069869	2.945204
13	1	-0.652744	-1.514615	0.771495
14	1	3.403619	-0.933214	0.242174
15	1	-1.263927	-0.168768	1.689667
16	1	2.898620	0.515474	1.035923

Cyclohexene C-Shift Optimized Geometries

Cyclohexene cas(6,6)/6-31G*
$E(S_0)$=-233.09274; $E(S_1)$=232.74544

1	6	-1.281168	-.344951	-.729834
2	6	-1.239003	-.156121	.795091
3	6	-.101761	.158693	1.464970
4	6	1.234963	.342892	.787972
5	1	2.011748	-.139997	1.375806
6	1	1.487323	1.402536	.772426
7	1	-.139664	.294984	2.533247
8	1	-2.159417	-.287952	1.339883
9	1	-2.167482	.142098	-1.127144
10	1	-1.387826	-1.405331	-.951598
11	6	-.021558	.211157	-1.398481
12	6	1.236907	-.213542	-.639349
13	1	.027544	-.121635	-2.431403
14	1	-.074725	1.297645	-1.421071
15	1	1.280638	-1.300049	-.601711
16	1	2.127775	.118032	-1.165035

Cyclohexene cas(8,8)/6-31G*
$E(S_0)$=-233.11281

1	6	-1.280256	-.346348	-.728974
2	6	-1.245412	-.155440	.796896
3	6	-.112667	.159680	1.473585
4	6	1.248870	.344660	.782272
5	1	2.019596	-.141290	1.374274
6	1	1.495399	1.404863	.767969
7	1	-.150098	.296533	2.541641
8	1	-2.169194	-.287373	1.335521
9	1	-2.167315	.136406	-1.129869
10	1	-1.382028	-1.407576	-.949015
11	6	-.021483	.212890	-1.396016
12	6	1.239517	-.214670	-.642341
13	1	.025758	-.115442	-2.430481
14	1	-.075094	1.299444	-1.413948
15	1	1.280390	-1.301249	-.603815
16	1	2.128309	.113371	-1.173930

Cyclohexene S_1 SOSP cas(8,8)/6-31G* (Figure 5b)
$E(S_1)$=-232.79714

1	6	.014553	.063801	.015606
2	6	-.016822	.145399	1.516385
3	6	1.285525	-.146464	2.286529
4	6	2.584804	-.074042	1.533948
5	1	3.368242	-.633214	2.038381
6	1	2.903764	.989564	1.564392
7	1	1.288213	.050138	3.343899
8	1	-.944565	-.046720	2.025471
9	1	-.803466	.623337	-.430148
10	1	-.170043	-1.000642	-.242793
11	6	1.369742	.411283	-.600543
12	6	2.468695	-.429924	.051771
13	1	1.335854	.235909	-1.671315
14	1	1.585865	1.467308	-.451589
15	1	2.230226	-1.485808	-.059243
16	1	3.423343	-.260797	-.436587

Cyclohexene Z/V CI cas(8,8)/6-31G* (Figure 5e)
$E(S_2)$=-232.85546; $E(S_1)$=-232.85554

1	6	-.021686	.039045	.065997
2	6	-.052630	.110869	1.606853
3	6	1.427973	.091859	2.113596
4	6	2.256203	1.066377	1.549393
5	6	2.318944	1.051896	-.013885
6	6	.872648	1.118423	-.546039
7	1	1.754264	-.870681	2.487399
8	1	-.544261	1.028622	1.918669
9	1	-.597098	-.728755	2.025627
10	1	.332961	-.942752	-.237055
11	1	-1.035609	.141169	-.315248
12	1	2.493563	2.024192	1.994335
13	1	2.902744	1.895744	-.366314
14	1	2.793383	.138143	-.362279
15	1	.458857	2.099797	-.328510
16	1	.887756	1.014171	-1.628841

Trans-Cyclohexene cas(6,6)/6-31G*
$E(S_0)$=-232.99410

1	1	-1.122730	1.086013	-1.095565
2	6	-1.055564	.903334	-.031490
3	6	.151807	1.246045	.570120
4	6	-1.463973	-.523749	.382146
5	1	.250891	.970982	1.611702
6	6	1.320614	.843827	-.291726
7	1	-2.268835	-.903871	-.236532
8	1	-.341456	-2.309989	-.265684
9	1	1.410861	1.437394	-1.195686
10	6	-.126243	-1.342373	.178815
11	1	.645785	-.652745	-1.721366
12	1	.290800	-1.545577	1.161182
13	6	.975029	-.651137	-.686058
14	1	1.867262	-1.269707	-.649066
15	1	2.263467	.908729	.240009
16	1	-1.776655	-.591165	1.418498

Cyclohexene Type III CI (H's cis) cas(6,6)/6-31G* (Figure 3a)
$E(S_1)$=-232.89040; $E(S_0)$=-232.89044

1	6	-0.039030	0.027345	-0.003432
2	6	-0.011382	-0.061841	1.525215
3	6	1.408266	-0.232405	2.004091
4	6	2.620258	2.091306	1.181621
5	6	2.218559	1.090770	0.273618
6	6	0.888790	1.172671	-0.439984
7	1	1.684402	0.165683	2.965863
8	1	-0.423698	0.850650	1.948262
9	1	-0.636938	-0.882894	1.872759
10	1	0.303260	-0.913353	-0.429795
11	1	-1.048856	0.191688	-0.368747
12	1	2.892952	0.311971	-0.052084
13	1	0.428439	2.123535	-0.192953
14	1	1.040016	1.153099	-1.515728
15	1	1.927038	-1.135400	1.723777
16	1	3.636700	2.050107	1.559800

Cyclohexene Type III CI (H's trans) cas(6,6)/6-31G* (Figure 3b)
$E(S_1)$=-232.88988; $E(S_0)$=-232.88999

1	6	-0.088552	0.112382	-0.028764
2	6	0.012427	-0.272988	1.449949
3	6	1.445311	-0.210135	1.912264
4	6	2.697051	2.083782	1.267142
5	6	2.051028	1.344576	0.256370
6	6	0.627965	1.449876	-0.229066
7	1	1.661881	0.164246	2.898976
8	1	-0.595850	0.408762	2.038430
9	1	-0.394247	-1.271383	1.607680
10	1	0.391541	-0.649381	-0.639944
11	1	-1.124111	0.169932	-0.350841
12	1	2.102872	2.821815	1.800045
13	1	2.677135	0.685327	-0.329450
14	1	0.102611	2.234256	0.308632
15	1	0.627376	1.725307	-1.281139
16	1	2.120268	-0.979785	1.572119

Cyclohexene Type II CI cas(6,6)/6-31G* (Figure 3c)
$E(S_1)$=-232.88832; $E(S_0)$=-232.88835

1	1	-2.985869	.075755	1.474888
2	6	-2.114101	.030306	.874230
3	6	-.669685	-.000274	.543916
4	6	-.136803	-1.196846	-.253339
5	1	-.153869	.022637	1.512234
6	6	-.096891	1.179099	-.328120
7	1	-.693955	-1.304915	-1.175828
8	1	1.698015	-1.287240	-1.437219
9	1	-.683822	1.258955	-1.234205
10	6	1.320118	-.814385	-.538461
11	1	1.657465	1.080506	-1.608816
12	1	1.953687	-1.142892	.278889
13	6	1.333822	.733878	-.634484
14	1	2.022422	1.153589	.090549
15	1	-.154563	2.131849	.185216
16	1	-.226214	-2.128996	.294690

Cyclohexene C-shift Carbene Product (cis) cas(6,6)/6-31G*
$E(S_0)$=-232.95221

1	1	0.079978	-0.898872	0.135350
2	6	-0.024674	-0.156685	0.940332
3	6	1.387792	0.227601	1.300831
4	6	1.574048	1.482863	2.163477
5	1	2.098741	0.199920	0.480005
6	6	1.722941	-1.008579	2.297332
7	1	0.620163	1.756953	2.603351
8	1	2.563576	1.747381	4.107509
9	1	0.891528	-1.699151	2.407697
10	6	2.557130	1.067408	3.262123
11	1	1.205261	-0.274441	4.262241
12	1	3.569851	1.030742	2.866248
13	6	2.087537	-0.341098	3.632867
14	1	2.832243	-0.912190	4.177434
15	1	2.550398	-1.565762	1.877277
16	1	1.922898	2.329665	1.581211

Cyclohexene C-shift Carbene Product (trans) cas(6,6)/6-31G*
$E(S_0)$=-232.95086

1	1	-2.357519	0.021671	-0.409377
2	6	-2.114543	-0.129435	0.654230
3	6	-0.650845	0.217177	0.767314
4	6	-0.031359	-1.201392	0.283890
5	1	-0.364336	0.373640	1.800474
6	6	0.009904	1.261566	-0.149808
7	1	-0.789486	-1.906034	-0.046411
8	1	0.449752	-0.908506	-1.806846
9	1	-0.609438	1.438763	-1.025916
10	6	0.947539	-0.834103	-0.844001
11	1	1.780888	1.106807	-1.441814
12	1	1.799350	-1.505418	-0.870555
13	6	1.334364	0.622137	-0.579921
14	1	2.054586	0.675064	0.233234
15	1	0.142144	2.214777	0.350873
16	1	0.468761	-1.655688	1.128770

Norbornene H-shift Optimized Geometries

Norbornene cas(6,6)/6-31G*
$E(S_0)$=-270.93672; $E(S_1)$=-270.60785

1	1	1.138843	1.343106	1.908026
2	6	0.540847	0.679525	1.273710
3	6	0.541545	-0.680828	1.274717
4	6	-0.325744	1.123427	0.104480
5	1	1.126996	-1.334893	1.894253
6	6	-0.324852	-1.124196	0.104985
7	1	-2.004609	-0.001301	-0.785388
8	1	-0.693166	2.140835	0.147384
9	1	1.462685	1.197158	-1.182452
10	1	-0.691688	-2.141791	0.148101
11	6	0.462971	0.778432	-1.190015
12	6	-1.377076	-0.000746	0.101724
13	1	1.462393	-1.198270	-1.183660
14	1	-0.047290	1.169397	-2.064592
15	1	-2.003597	-0.000909	0.986204
16	6	0.462871	-0.779137	-1.190163
17	1	-0.048592	-1.169809	-2.064197

Norbornene cas(8,8)/6-31G*
$E(S_0)$=-270.95744

1	1	1.137812	1.343313	1.909027
2	6	.540864	.679175	1.273484
3	6	.543916	-.681290	1.271183
4	6	-.327905	1.122963	.105962
5	1	1.143706	-1.344939	1.904546
6	6	-.322928	-1.124960	.102228
7	1	-2.006727	-.003164	-.782606
8	1	-.697326	2.139542	.151124
9	1	1.457573	1.202741	-1.184642
10	1	-.687853	-2.143298	.144135
11	6	.458845	.781670	-1.190622
12	6	-1.377213	-.003301	.103086
13	1	1.462826	-1.192695	-1.188725
14	1	-.054266	1.172782	-2.063460
15	1	-2.001821	-.006159	.988914
16	6	.462280	-.775969	-1.193225
17	1	-.049242	-1.166409	-2.067288

Norbornene S_1 SOSP cas(8,8)/6-31G* (Figure 5c)
$E(S_1)$=-270.65578

1	1	1.081347	1.424445	1.966162
2	6	.532476	.777595	1.281078
3	6	.531244	-.777260	1.281812
4	6	-.288045	1.141102	.114746
5	1	1.080832	-1.424351	1.966091
6	6	-.289692	-1.140543	.115865
7	1	-1.952609	.000924	-.785943
8	1	-.649673	2.162308	.127109
9	1	1.455326	1.195179	-1.238259
10	1	-.652734	-2.161238	.128928
11	6	.456705	.777545	-1.212918
12	6	-1.353383	.001119	.119775
13	1	1.453796	-1.198049	-1.237006
14	1	-.092007	1.177646	-2.062053
15	1	-1.993311	.002023	.990716
16	6	.455730	-.779060	-1.212137
17	1	-.093460	-1.179384	-2.060845

Norbornene Type I CI (exo) cas(6,6)/6-31G* (Figure 2a)
$E(S_1)$=-270.71249; $E(S_0)$=-270.71267

1	6	.006985	-.087627	.080925
2	6	.012536	.037950	1.648966
3	6	2.247169	-.004847	1.086795
4	6	1.525978	-.172477	-.291655
5	1	-.548978	-.954263	-.264532
6	1	-.458183	.790186	-.358184
7	1	1.786907	-1.118771	-.755559
8	1	1.803567	.621527	-.978175
9	6	1.247464	.962167	1.797351
10	1	1.518571	1.174258	2.829007
11	1	1.091781	1.906107	1.290668
12	6	.490219	-1.365663	2.028939
13	1	-.143063	-2.229907	1.917437
14	6	1.934782	-1.352953	1.873027
15	1	1.786487	-.629003	2.791437
16	1	-.919575	.382864	2.078835
17	1	3.291814	.274659	1.063254

Norbornene Type III CI (exo) cas(6,6)/6-31G* (Figure 2b)
$E(S_1)$=-270.72452; $E(S_0)$=-270.72458

1	6	-.007872	.083503	-.072454
2	6	.060526	-.178999	1.455351
3	6	2.239790	-.056491	.870863
4	6	1.493572	.156337	-.480811
5	1	-.547523	-.694517	-.600111
6	1	-.514441	1.021520	-.269884
7	1	1.762340	-.593663	-1.214577
8	1	1.743233	1.125063	-.897800
9	6	1.284455	.673129	1.841112
10	1	1.566497	.570568	2.882155
11	1	1.164319	1.726273	1.606458
12	6	.647299	-1.581923	1.628900
13	1	.069691	-2.482920	1.702412
14	6	1.988705	-1.508659	1.211988
15	1	1.032953	-1.714358	3.477253
16	1	-.862379	.009805	1.987298
17	1	3.273962	.255565	.861092

Norbornene Type II CI cas(6,6)/6-31G* (Figure 2c)
$E(S_1)$=-270.69525; $E(S_0)$=-270.69532

1	6	.053539	-.063614	-.007838
2	6	.156421	-.140724	1.549472
3	6	2.308591	-.015626	.803183
4	6	1.508683	.250879	-.505634
5	1	-.292647	-1.010445	-.409440
6	1	-.655847	.690431	-.320692
7	1	1.799330	-.414564	-1.305870
8	1	1.598310	1.269378	-.865748
9	6	1.414083	.751234	1.839547
10	1	1.793154	.648919	2.850339
11	1	1.245634	1.796889	1.607119
12	6	.603307	-1.698526	1.970954
13	1	-.088655	-2.388678	1.487050
14	6	1.773996	-1.277401	1.320663
15	1	.560944	-1.890242	3.076680
16	1	-.748748	.122682	2.090043
17	1	3.365031	.179639	.809414

Norbornene Type I CI (endo) cas(6,6)/6-31G* (Figure 2d)
$E(S_1)$=-270.69039; $E(S_0)$=-270.69053

1	6	.040364	-.035759	-.065722
2	6	-.004799	-.000786	1.495881
3	6	2.236647	-.024368	.961887
4	6	1.566243	.074590	-.432035
5	1	-.427893	-.931358	-.461475
6	1	-.514651	.805312	-.460669
7	1	1.875081	-.717511	-1.105152
8	1	1.786641	1.019867	-.914757
9	6	1.254130	.885782	1.787951
10	1	1.509257	.915837	2.843595
11	1	1.173588	1.903290	1.407833
12	6	.475224	-1.330584	2.125300
13	1	.040355	-1.811095	2.978883
14	6	1.864307	-1.409679	1.645405
15	1	1.173160	-1.516460	.720180
16	1	-.948119	.361514	1.886045
17	1	3.289083	.229180	.995905

Norbornene Type III CI (endo) cas(6,6)/6-31G* (Figure 2e)
$E(S_1)$=-270.71901; $E(S_0)$=-270.71907

1	6	-.000742	.066302	-.026067
2	6	-.008661	-.005411	1.517550
3	6	2.198033	.008231	1.040857
4	6	1.517296	-.006972	-.364267
5	1	-.575942	-.726337	-.486827
6	1	-.425956	1.009607	-.351325
7	1	1.775191	-.900334	-.921395
8	1	1.834939	.846215	-.952887
9	6	1.211837	.887524	1.840765
10	1	1.443040	.928166	2.899059
11	1	1.121373	1.899173	1.458507
12	6	.556494	-1.363769	1.953348
13	1	.079986	-2.022697	2.653206
14	6	1.926464	-1.361141	1.632040
15	1	-.006032	-2.647691	.686269
16	1	-.950309	.265324	1.977630
17	1	3.235872	.307750	1.025389

Norbornene H-shift Carbene Product cas(6,6)/6-31G*
$E(S_0)$=-270.83266

1	6	-0.023543	0.054839	0.020825
2	6	0.081696	-0.145683	1.541595
3	6	2.256110	-0.014701	0.934023
4	6	1.464995	0.043696	-0.419084
5	1	-0.605480	-0.723366	-0.461207
6	1	-0.492687	1.004316	-0.213760
7	1	1.703683	-0.794028	-1.066309
8	1	1.742214	0.944151	-0.953442
9	6	1.295263	0.725465	1.882506
10	1	1.591037	0.663295	2.925613
11	1	1.169043	1.771999	1.622510
12	6	0.683643	-1.538679	1.769457
13	1	0.117218	-2.380020	1.384931
14	6	2.132935	-1.483706	1.224344
15	1	0.842337	-1.731888	2.857765
16	1	-0.831012	0.055331	2.088716
17	1	3.267672	0.359209	0.850759

Norbornene C-shift Optimized Geometries

Norbornene cas(6,6)/6-31G*
$E(S_0)$=-270.93683

1	1	1.137429	1.326934	1.913762
2	6	0.551475	0.679076	1.287935
3	6	0.544138	-0.680848	1.275483
4	6	-0.332965	1.128675	0.092980
5	1	1.125737	-1.340511	1.892838
6	6	-0.323639	-1.120845	0.106085
7	1	-2.008019	-0.005952	-0.782685
8	1	-0.699028	2.146106	0.139411
9	1	1.460661	1.200075	-1.183913
10	1	-0.690644	-2.138474	0.149640
11	6	0.461603	0.779967	-1.193690
12	6	-1.377413	0.000929	0.102370
13	1	1.463621	-1.195364	-1.181564
14	1	-0.045305	1.167116	-2.072012
15	1	-2.001469	0.002685	0.988483
16	6	0.463437	-0.777821	-1.189414
17	1	-0.047080	-1.171746	-2.062590

Norbornene cas(8,8)/6-31G*
$E(S_0)$=-270.95797

1	1	1.134357	1.335052	1.913079
2	6	.554731	.679732	1.289211
3	6	.554690	-.679759	1.289229
4	6	-.332049	1.125752	.093138
5	1	1.134337	-1.335101	1.913052
6	6	-.332071	-1.125743	.093134
7	1	-2.012345	.000020	-.781051
8	1	-.697845	2.143413	.140690
9	1	1.461109	1.197787	-1.183892
10	1	-.697881	-2.143400	.140668
11	6	.461362	.779137	-1.194158
12	6	-1.378444	.000013	.101887
13	1	1.461166	-1.197734	-1.183782
14	1	-.044879	1.169161	-2.071735
15	1	-2.000323	.000018	.989500
16	6	.461400	-.779131	-1.194132
17	1	-.044778	-1.169216	-2.071719

Norbornene S_1 SOSP cas(8,8)/6-31G* (Figure 5c)

$E(S_1)$=-270.65417

1	1	1.060581	1.416250	1.981485
2	6	.552575	.777306	1.291813
3	6	.551805	-.777139	1.292591
4	6	-.289866	1.140351	.099886
5	1	1.050504	-1.415968	1.989056
6	6	-.290357	-1.140066	.100066
7	1	-1.957723	.000569	-.772443
8	1	-.650516	2.161205	.124306
9	1	1.453476	1.196059	-1.245759
10	1	-.651612	-2.160693	.125388
11	6	.455036	.777848	-1.221300
12	6	-1.346723	.000538	.126180
13	1	1.452516	-1.197774	-1.245587
14	1	-.091415	1.175650	-2.072918
15	1	-1.977637	.000774	1.003877
16	6	.454449	-.778675	-1.221081
17	1	-.092553	-1.176233	-2.072439

Norbornene Z/V CI cas(8,8)/6-31G* (Figure 5f)

$E(S_2)$=-270.67669; $E(S_1)$=-270.67753

1	1	-.261600	.480932	-.085824
2	6	-.094977	.180281	.932567
3	6	1.178570	.033916	1.489834
4	6	-.715319	-1.364474	1.135667
5	1	1.341039	.107791	2.557201
6	6	1.575996	-1.495989	1.073297
7	1	.320114	-3.167501	1.849856
8	1	-1.726629	-1.425110	1.501406
9	1	-.931965	-1.364347	-1.054621
10	1	2.583952	-1.771712	1.337626
11	6	-.432515	-1.918687	-.269878
12	6	.409257	-2.085069	1.926307
13	1	1.460367	-1.107086	-1.082222
14	1	-.774475	-2.949498	-.328373
15	1	.474886	-1.822656	2.972756
16	6	1.127525	-1.839616	-.359220
17	1	1.544888	-2.797424	-.651186

Norbornene Type III CI (H's cis) cas(6,6)/6-31G* (Figure 4a)

$E(S_1)$=-270.73598; $E(S_0)$=-270.73602

1	1	-.174226	-.988136	.396385
2	6	.122266	-.640237	1.382542
3	6	1.266375	.218188	1.404072
4	6	.538588	2.199705	1.836400
5	1	1.847603	.402319	.512591
6	6	1.876996	.733686	2.702612
7	1	2.227956	2.902701	3.062491
8	1	.131589	2.865223	1.085999
9	1	-1.194208	1.279437	2.786255
10	1	2.770790	.215711	3.031853
11	6	-.260882	1.762357	3.048561
12	6	1.997103	2.194015	2.267865
13	1	.292508	-.190895	3.905836
14	1	-.498479	2.613344	3.683382
15	1	2.700546	2.339933	1.455298
16	6	.736602	.782161	3.740173
17	1	1.087869	1.161326	4.692022

Norbornene Type I CI (H's trans) cas(6,6)/6-31G* (Figure 4b)
$E(S_1)$=-270.71932; $E(S_0)$=-270.71937

1	1	1.859223	.799722	.696524
2	6	1.075696	.673516	1.423454
3	6	.394500	-.591775	1.345037
4	6	-.445020	1.063315	.176547
5	1	-.258626	-.754658	2.199650
6	6	-.191025	-1.162456	.074904
7	1	-2.011245	-.159041	-.766884
8	1	-.825178	2.048004	.431097
9	1	1.279434	1.449626	-1.158413
10	1	-.420542	-2.220506	.098249
11	6	.364064	.869902	-1.115171
12	6	-1.378601	-.167990	.120732
13	1	1.660250	-.928254	-1.068812
14	1	-.247344	1.171963	-1.965223
15	1	-2.011890	-.295065	.991997
16	6	.607472	-.674571	-1.143314
17	1	.231372	-1.121729	-2.057256

Norbornene Type III CI (H's trans) cas(6,6)/6-31G* (Figure 4c)
$E(S_1)$=-270.73359; $E(S_0)$=-270.73363

1	6	.033273	.078648	-.023570
2	6	-.009565	.032449	1.508610
3	6	1.478229	-.026535	1.873663
4	6	1.639793	-1.302099	1.062601
5	6	1.143439	-.966285	-.330129
6	6	-.309997	-1.386629	1.957103
7	6	-1.004251	-2.484750	1.360727
8	1	-1.367211	-2.353592	.343684
9	1	-.043071	-1.561451	2.990695
10	1	2.081609	.807604	1.518987
11	1	2.411943	-2.039649	1.234911
12	1	.780799	-1.829657	-.875118
13	1	-.622302	.795369	1.975368
14	1	-.917282	-.165610	-.482653
15	1	1.946711	-.528871	-.921856
16	1	1.650096	-.155440	2.935852
17	1	.312004	1.071120	-.362965

Norbornene Type II CI cas(6,6)/6-31G* (Figure 4d)
$E(S_1)$=-270.71889; $E(S_0)$=-270.71954

1	1	.529059	.183915	.188694
2	6	.075866	.051349	1.137588
3	6	-.002504	-.109720	2.582842
4	6	.203293	-1.562467	3.314528
5	1	-.873958	.371603	3.005196
6	6	1.300320	.180757	3.419113
7	1	1.407489	-1.234745	5.180182
8	1	-.611891	-2.263225	3.396681
9	1	1.338569	-2.357793	1.630264
10	1	1.594009	1.202014	3.630333
11	6	1.499850	-2.045090	2.655276
12	6	.709921	-.745294	4.507356
13	1	2.685991	-.380286	1.811849
14	1	1.937463	-2.881413	3.186870
15	1	-.085680	-.282428	5.078092
16	6	2.346301	-.744488	2.775133
17	1	3.216909	-.873365	3.410467

Norbornene C-shift Carbene Product (cis) cas(6,6)/6-31G*
$E(S_0)$=-270.77659

1	1	-0.102927	0.999418	0.623619
2	6	-0.128918	-0.067209	0.892530
3	6	0.025584	-0.074193	2.396854
4	6	0.426676	-1.343754	3.182095
5	1	-0.874007	0.399991	2.795409
6	6	1.321716	0.509669	3.133673
7	1	1.675188	-0.745929	4.973871
8	1	-0.280782	-2.141584	3.365158
9	1	1.615449	-2.140963	1.527175
10	1	1.481105	1.573694	3.247699
11	6	1.759437	-1.726823	2.517681
12	6	0.892922	-0.395256	4.307839
13	1	2.684542	0.005542	1.481448
14	1	2.318128	-2.446114	3.106497
15	1	0.073511	0.017033	4.885239
16	6	2.439972	-0.323581	2.486338
17	1	3.352401	-0.290237	3.071998

Norbornene C-shift Carbene Product (trans) cas(6,6)/6-31G*
$E(S_0)$=-270.77497

1	1	-0.135261	0.282544	0.119765
2	6	0.025021	-0.229700	1.077327
3	6	1.448652	0.023017	1.497871
4	6	2.486224	-1.071216	0.905546
5	1	1.529615	-0.002827	2.578436
6	6	2.497421	0.984928	0.867014
7	1	4.498601	-0.067401	0.747781
8	1	2.485877	-2.085999	1.275922
9	1	1.490090	-1.277098	-1.047831
10	1	2.552809	2.020884	1.175610
11	6	2.386055	-0.850056	-0.611573
12	6	3.565038	-0.041468	1.301559
13	1	1.515009	1.129621	-1.097086
14	1	3.236879	-1.282943	-1.126578
15	1	3.767612	-0.025296	2.365122
16	6	2.402454	0.707237	-0.640746
17	1	3.260737	1.102935	-1.172413

Figure Caption

Figure S1 – CAS(6,6)/6-31G* optimized structures for the [1,2]-hydrogen shift in ethene. Gradient difference and derivative coupling vectors are shown below each structure. (a) Type I conical intersection, (b) Type I / Type I conical intersection transition structure, (c) Type II conical intersection, and (d) Type I / Type II conical intersection transition structure.

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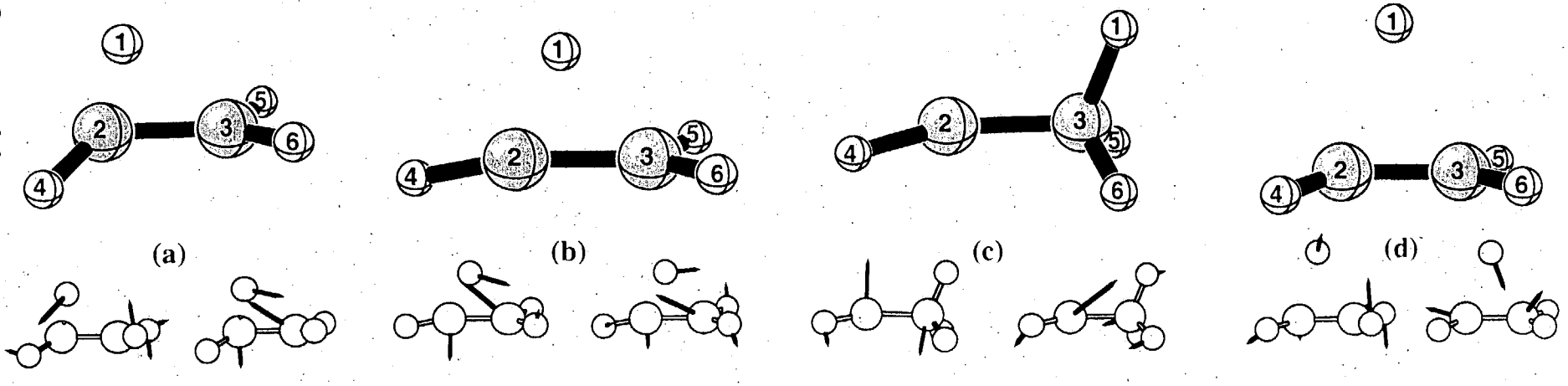
H1-C2=1.232Å
H1-C3=1.639Å
C2-C3=1.448Å
H1-C2-C3=75°
H1-C3-C2=47°°
H4-C2-C3=120°
H1-C2-C3-H4=89°
H1-C2-C3-H5=-110°
H1-C2-C3-H6=58°
H4-C2-C3-H6=-31°

H1-C2=1.229Å
H1-C3=1.455Å
C2-C3=1.391Å
H1-C2-C3=67°
H1-C3-C2=51°
H4-C2-C3=169°
H1-C2-C3-H4=180°
H1-C2-C3-H5=-87°
H1-C2-C3-H6=87°
H4-C2-C3-H6=--93°

H1-C2=2.172Å
H1-C3=1.112Å
C2-C3=1.484Å
H1-C2-C3=28°
H1-C3-C2=113°
H4-C2-C3=159°°
H1-C2-C3-H4=119°,
H1-C2-C3-H5=-122°
H1-C2-C3-H6=118°
H4-C2-C3-H6=-1°

H1-C2=1.889Å
H1-C3=1.897Å
C2-C3=1.408Å
H1-C2-C3=69°
H1-C3-C2=68°
H4-C2-C3=119°
H1-C2-C3-H4=80°
H1-C2-C3-H5= -105°
H1-C2-C3-H6=76°
H4-C2-C3-H6=-5°



Type I

Type II

Figure S1