Supporting Information

Title : Conformational Study of 1,2 - Cycloundecadiene by Dynamic NMR Spectroscopy and Computational Methods

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CONFORMATIONS OF 1,2-CYCLOUNDECADIENE FROM MM3 SEARCH.

CONFORMER 1a

STERIC ENERGY= -27.6677 KCAL/MOL

Coordinates :

6	0.50202	1.81036	0.58761
6	-0.73951	1.68138	0.17475
6	-1.98971	1.57858	-0.21808
6	-2.77400	0.28164	-0.14658
6	-2.00476	-0.93389	0.39787
6	-1.00769	-1.53009	-0.61640
6	0.11184	-2.35136	0.05397
6	1.21250	-1.46413	0.66650
6	2.14169	-0.84629	-0.40364
6	2.66548	0.56204	-0.06545
6	1.66843	1.69564	-0.37245
1	0.70889	2.05176	1.64246
1	-2.51341	2.48135	-0.57272
1	-3.66061	0.46146	0.50428
1	-3.17295	0.04316	-1.15829
1	-1.48614	-0.64638	1.33943
1	-2.73180	-1.72948	0.68481
1	-1.56812	-2.18059	-1.32766
1	-0.56138	-0.71965	-1.23284
1	-0.33297	-3.00042	0.84319
1	0.57266	-3.03903	-0.69242
1	0.74789	-0.66722	1.28452
1	1.82887	-2.07034	1.37048
1	3.00942	-1.53194	-0.54851
1	1.62859	-0.80826	-1.38994
1	2.98698	0.60678	1.00001
1	3.58490	0.74165	-0.67214
1	1.28899	1.57969	-1.41275
1	2.21422	2.66707	-0.35356

FREE ENERGY AT 298.16 K = 111.991 KCAL/MOL

FREE ENERGY AT 173.16 K = 123.604 KCAL/MOL

FREE ENERGY AT 106.86 K = 128.720 KCAL/MOL

CONFORMER 1b STERIC ENERGY= -27.2659 KCAL/MOL

6	0.47406	-1.82720	0.53988
6	-0.79396	-1.67541	0.22888
6	-2.06515	-1.54424	-0.07570
6	-2.77323	-0.20128	-0.09060
6	-1.89618	0.99851	-0.49579
6	-0.98500	1.53418	0.62766
6	0.20699	2.36204	0.10351
6	1.30464	1.51166	-0.56720
6	2.12188	0.67319	0.44149
6	2.64157	-0.66689	-0.11034
6	1.53673	-1.65812	-0.52837
1	0.78063	-2.03499	1.57699
1	-2.64264	-2.44084	-0.35418
1	-3.60712	-0.27625	-0.82693
1	-3.24962	-0.01897	0.89829
1	-1.29402	0.71205	-1.38630
1	-2.55523	1.83246	-0.83403
1	-1.59908	2.16898	1.30839
1	-0.61494	0.69722	1.25606
1	-0.17075	3.11956	-0.62179
1	0.65939	2.93602	0.94528
1	0.84450	0.85286	-1.33314
1	2.00152	2.17935	-1.12535
1	2.98632	1.28297	0.79426
1	1.51602	0.47323	1.35187
1	3.31289	-0.47455	-0.97914
1	3.27553	-1.14812	0.67139
1	1.99744	-2.65169	-0.73142
1	1.06933	-1.33352	-1.48422

FREE ENERGY AT 298.16 K = 112.570 KCAL/MOL

FREE ENERGY AT 173.16 K = 124.112 KCAL/MOL

FREE ENERGY AT 106.86 K = 129.193 KCAL/MOL

CONFORMER 1c STERIC ENERGY= -27.0480 KCAL/MOL

0	1		
6	-0.215918	-2.140468	-0.216998
6	0.987045	-1.730436	0.049553
6	2.174669	-1.277627	0.316329
6	2.750124	0.032718	-0.194190
6	1.703739	1.052132	-0.657056
6	0.940741	1.694411	0.513823
6	-0.411278	2.356962	0.171782
6	-1.639409	1.452653	0.379548
6	-1.898083	0.402891	-0.721148
6	-2.453497	-0.933449	-0.212127
6	-1.446984	-1.783019	0.586494
1	-0.366862	-2.753085	-1.093803
1	2.820476	-1.877553	0.938834
1	3.358913	0.467488	0.595628
1	3.436085	-0.187165	-1.009848
1	2.201074	1.834663	-1.224964
1	1.026917	0.566349	-1.347845
1	0.775975	0.951424	1.287816
1	1.595466	2.440498	0.958111
1	-0.534171	3.224972	0.813947
1	-0.397257	2.740865	-0.847031
1	-1.533838	0.966544	1.345473
1	-2.522893	2.080132	0.467381
1	-2.598442	0.818569	-1.441187
1	-0.992353	0.203745	-1.276667
1	-3.329445	-0.757474	0.409109
1	-2.797524	-1.516441	-1.064002
1	-1.944137	-2.697327	0.902661
1	-1.144875	-1.266809	1.490328

FREE ENERGY AT 298.16 K = 112.503 KCAL/MOL

FREE ENERGY AT 173.16 K = 124.118 KCAL/MOL

FREE ENERGY AT 106.86 K = 129.232 KCAL/MOL

CONFORMER 1d STERIC ENERGY= -26.4531 KCAL/MOL

0	1		
6	1.06531	1.95407	-0.16304
6	-0.22340	1.83100	0.06293
6	-1.50454	1.68956	0.31932
6	-2.38709	0.80408	-0.53790

6	-2.64090	-0.61593	0.00549
6	-1.47057	-1.59453	-0.21553
6	-0.32788	-1.47152	0.81192
6	1.02328	-1.98586	0.28117
6	1.67623	-1.10280	-0.81155
6	2.66497	-0.04065	-0.29582
6	2.05834	1.07258	0.57054
1	1.44262	2.71620	-0.86288
1	-1.96428	2.24682	1.15108
1	-3.36280	1.32527	-0.67145
1	-1.94703	0.72615	-1.55786
1	-2.91200	-0.57437	1.08489
1	-3.53430	-1.02843	-0.52123
1	-1.85872	-2.63960	-0.18072
1	-1.08161	-1.45696	-1.24829
1	-0.22427	-0.42193	1.14734
1	-0.60719	-2.04788	1.72472
1	1.73649	-2.10197	1.12935
1	0.86775	-3.01195	-0.12692
1	2.23444	-1.77360	-1.50722
1	0.89571	-0.61187	-1.43297
1	3.46712	-0.55286	0.28536
1	3.17515	0.42871	-1.16970
1	2.87602	1.72328	0.95687
1	1.58575	0.62651	1.47197

FREE ENERGY AT 298.16 K = 113.311 KCAL/MOL

FREE ENERGY AT 173.16 K = 124.955 KCAL/MOL

FREE ENERGY AT 106.86 K = 130.087 KCAL/MOL

CONFORMER 1e STERIC ENERGY= -26.0421 KCAL/MOL

0	1		
6	1.13950	1.74891	0.65426
6	0.00000	1.69171	0.00000
6	-1.13950	1.74891	-0.65426
6	-2.40073	0.98783	-0.30088
6	-2.32304	-0.18198	0.69875
6	-1.96155	-1.53859	0.06769
6	-0.55272	-1.62237	-0.53363
6	0.55272	-1.62237	0.53363
6	1.96155	-1.53859	-0.06769

6	2.32304	-0.18198	-0.69875
6	2.40073	0.98783	0.30088
1	1.20945	2.47812	1.47910
1	-1.20945	2.47812	-1.47910
1	-3.12191	1.73818	0.09913
1	-2.85561	0.61327	-1.24599
1	-1.62928	0.06799	1.53137
1	-3.32713	-0.29452	1.17353
1	-2.07431	-2.33982	0.83477
1	-2.70756	-1.77161	-0.72775
1	-0.46919	-2.55839	-1.13394
1	-0.40790	-0.78629	-1.25060
1	0.40790	-0.78629	1.25061
1	0.46919	-2.55839	1.13395
1	2.70756	-1.77161	0.72775
1	2.07431	-2.33982	-0.83476
1	3.32713	-0.29452	-1.17353
1	1.62928	0.06798	-1.53137
1	3.12191	1.73818	-0.09914
1	2.85561	0.61327	1.24599

FREE ENERGY AT 298.16 K = 114.213 KCAL/MOL

FREE ENERGY AT 173.16 K = 125.796 KCAL/MOL

FREE ENERGY AT 106.86 K = 130.897 KCAL/MOL

CONFORMER 1f STERIC ENERGY= -25.6658 KCAL/MOL

0	1		
6	-1.72749	1.67272	-0.34659
6	-0.48013	1.68263	0.06441
6	0.76800	1.74545	0.47049
6	1.92228	1.33927	-0.42465
6	2.81274	0.23146	0.16779
6	2.33235	-1.21383	-0.05361
6	0.90458	-1.53301	0.44159
6	-0.14557	-1.48926	-0.68331
6	-1.57154	-1.78864	-0.19882
6	-2.23628	-0.70481	0.67072
6	-2.71169	0.55038	-0.08797
1	-2.10576	2.56960	-0.86509
1	0.99511	2.15193	1.46911
1	1.55639	1.03372	-1.42938

1	2.54566	2.24800	-0.59117
1	3.82916	0.32182	-0.28440
1	2.95205	0.41446	1.25834
1	2.41386	-1.46767	-1.13531
1	3.04662	-1.89439	0.46776
1	0.89955	-2.55733	0.88259
1	0.63243	-0.84386	1.26996
1	-0.12660	-0.51096	-1.20708
1	0.13134	-2.24887	-1.45181
1	-2.22124	-1.98198	-1.08406
1	-1.55274	-2.74544	0.37390
1	-3.13494	-1.17016	1.14269
1	-1.57586	-0.41629	1.51797
1	-3.55419	0.99773	0.48975
1	-3.15030	0.23810	-1.06257

FREE ENERGY AT 298.16 K = 114.125 KCAL/MOL

FREE ENERGY AT 173.16 K = 125.818 KCAL/MOL

FREE ENERGY AT 106.86 K = 130.969 KCAL/MOL

CONFORMER 1g STERIC ENERGY= -25.5128 KCAL/MOL

0	1		
6	-1.30992	1.87903	0.09991
6	0.00000	1.90713	0.00000
6	1.30992	1.87903	-0.09991
6	2.09244	0.88878	0.74101
6	2.63908	-0.27485	-0.10570
6	1.54016	-1.09902	-0.80398
6	0.76295	-2.06229	0.13044
6	-0.76296	-2.06229	-0.13044
6	-1.54016	-1.09902	0.80398
6	-2.63908	-0.27485	0.10570
6	-2.09244	0.88878	-0.74101
1	-1.84323	2.52222	0.81699
1	1.84323	2.52222	-0.81699
1	2.93316	1.42316	1.23843
1	1.45029	0.48867	1.55655
1	3.32725	0.14027	-0.87907
1	3.25808	-0.94754	0.53171
1	0.83439	-0.40715	-1.31280
1	2.00397	-1.70036	-1.62078

1	1.15910	-3.09372	-0.02030
1	0.96171	-1.82091	1.19799
1	-0.96171	-1.82091	-1.19799
1	-1.15910	-3.09372	0.02030
1	-2.00397	-1.70036	1.62078
1	-0.83439	-0.40715	1.31280
1	-3.25808	-0.94754	-0.53171
1	-3.32725	0.14027	0.87907
1	-2.93316	1.42316	-1.23843
1	-1.45029	0.48867	-1.55655

FREE ENERGY AT 298.16 K = 113.926 KCAL/MOL
 FREE ENERGY AT 173.16 K = 125.510 KCAL/MOL
 FREE ENERGY AT 106.86 K = 130.613 KCAL/MOL

CONFORMER 1h STERIC ENERGY= -25.3889 KCAL/MOL

0	1		
6	1.90339	-1.50462	0.04863
6	0.61784	-1.71539	-0.13061
6	-0.67770	-1.88077	-0.28384
6	-1.62152	-1.27845	0.73788
6	-2.74604	-0.40579	0.15760
6	-2.32088	0.83156	-0.65618
6	-1.33474	1.79099	0.05920
6	0.13455	1.60700	-0.40529
6	1.13154	1.39249	0.74638
6	2.53622	0.96366	0.28033
6	2.56568	-0.30275	-0.59608
1	2.50693	-2.18409	0.67048
1	-1.08576	-2.48165	-1.11113
1	-2.08524	-2.11976	1.30303
1	-1.04835	-0.69505	1.49032
1	-3.39993	-1.04379	-0.48243
1	-3.39086	-0.06330	1.00129
1	-1.89884	0.50870	-1.63442
1	-3.24407	1.40440	-0.91069
1	-1.63868	2.84385	-0.14730
1	-1.41952	1.66642	1.16141
1	0.18223	0.74565	-1.10293
1	0.44958	2.49356	-1.00277
1	1.21128	2.33346	1.33891

1	0.73792	0.62331	1.44697
1	3.00348	1.80417	-0.28400
1	3.17720	0.79751	1.17771
1	3.62038	-0.56436	-0.84008
1	2.08027	-0.09189	-1.57450

FREE ENERGY AT 298.16 K = 114.275 KCAL/MOL
 FREE ENERGY AT 173.16 K = 125.924 KCAL/MOL
 FREE ENERGY AT 106.86 K = 131.054 KCAL/MOL

CONFORMER 1i STERIC ENERGY= -25.3198 KCAL/MOL

0	1		
6	0.54196	-1.59801	0.80369
6	-0.71766	-1.60420	0.42854
6	-1.98019	-1.60132	0.06475
6	-2.67869	-0.34466	-0.42336
6	-1.75437	0.84554	-0.73742
6	-1.20405	1.55791	0.51455
6	0.09501	2.36534	0.28363
6	1.38885	1.54835	0.49634
6	1.87432	0.73358	-0.72585
6	2.58797	-0.58410	-0.34806
6	1.63806	-1.79101	-0.22391
1	0.81638	-1.42572	1.85615
1	-2.55151	-2.54350	0.08417
1	-3.23114	-0.61055	-1.35431
1	-3.44860	-0.04040	0.32067
1	-0.92866	0.49058	-1.38822
1	-2.31494	1.59282	-1.34677
1	-1.99502	2.24909	0.89001
1	-1.04000	0.82827	1.33725
1	0.09062	2.83353	-0.72634
1	0.10377	3.21045	1.01258
1	2.20846	2.24684	0.78777
1	1.25201	0.88257	1.37573
1	1.03490	0.50440	-1.41318
1	2.57298	1.37227	-1.31544
1	3.34508	-0.81840	-1.13326
1	3.15988	-0.44621	0.59791
1	2.22606	-2.69586	0.05185
1	1.18528	-2.00425	-1.21889

FREE ENERGY AT 298.16 K = 114.364 KCAL/MOL
FREE ENERGY AT 173.16 K = 125.950 KCAL/MOL
FREE ENERGY AT 106.86 K = 131.047 KCAL/MOL

CONFORMER 1j STERIC ENERGY= -25.3041 KCAL/MOL

0	1		
6	2.00633	-1.21101	0.51201
6	1.97776	0.00000	0.00000
6	2.00632	1.21101	-0.51201
6	1.15789	2.34397	0.02909
6	-0.20250	1.92934	0.61131
6	-1.21329	1.49995	-0.47028
6	-2.44941	0.76390	0.10129
6	-2.44941	-0.76390	-0.10129
6	-1.21329	-1.49996	0.47028
6	-0.20249	-1.92934	-0.61131
6	1.15789	-2.34397	-0.02909
1	2.71589	-1.43166	1.32596
1	2.71589	1.43166	-1.32596
1	1.75039	2.88063	0.80473
1	0.98206	3.07840	-0.78972
1	-0.05193	1.12075	1.35878
1	-0.63404	2.78859	1.17643
1	-1.55277	2.41300	-1.01317
1	-0.71869	0.86670	-1.23651
1	-2.55281	0.99554	1.18601
1	-3.36551	1.17699	-0.38319
1	-3.36550	-1.17699	0.38319
1	-2.55280	-0.99554	-1.18601
1	-0.71869	-0.86670	1.23651
1	-1.55276	-2.41300	1.01317
1	-0.63403	-2.78859	-1.17643
1	-0.05193	-1.12075	-1.35878
1	1.75039	-2.88063	-0.80473
1	0.98206	-3.07840	0.78972

FREE ENERGY AT 298.16 K = 114.281 KCAL/MOL
FREE ENERGY AT 173.16 K = 125.835 KCAL/MOL
FREE ENERGY AT 106.86 K = 130.905 KCAL/MOL

CONFORMER 1k STERIC ENERGY= -25.2900 KCAL/MOL

0	1		
6	-0.30007	-1.79393	0.69368
6	0.91838	-1.56553	0.25650
6	2.15344	-1.34379	-0.13581
6	2.76514	0.04524	-0.16265
6	1.84708	1.18084	0.32193
6	0.73533	1.52149	-0.69013
6	-0.49456	2.20176	-0.06264
6	-1.37052	1.30189	0.84027
6	-2.46797	0.49531	0.11907
6	-2.02031	-0.59944	-0.86628
6	-1.49115	-1.89834	-0.23644
1	-0.46185	-1.95787	1.77153
1	2.79018	-2.19826	-0.41718
1	3.67531	0.02564	0.48012
1	3.11630	0.26704	-1.19564
1	1.41533	0.90523	1.30929
1	2.45587	2.09740	0.50297
1	1.16310	2.19322	-1.47090
1	0.43012	0.60403	-1.22999
1	-0.13797	3.07311	0.53528
1	-1.13183	2.62945	-0.87075
1	-0.73440	0.62502	1.44760
1	-1.88003	1.96365	1.58108
1	-3.12786	0.02567	0.88572
1	-3.11681	1.21718	-0.43090
1	-2.90393	-0.87183	-1.49214
1	-1.28246	-0.19180	-1.58664
1	-1.22002	-2.60031	-1.05883
1	-2.32032	-2.39587	0.31670

FREE ENERGY AT 298.16 K = 114.494 KCAL/MOL

FREE ENERGY AT 173.16 K = 126.219 KCAL/MOL

FREE ENERGY AT 106.86 K = 131.393 KCAL/MOL

CONFORMER 1l STERIC ENERGY= -25.2844 KCAL/MOL

0	1		
6	0.60928	-1.88444	-0.75636
6	-0.53491	-1.70040	-0.13406

6	-1.67869	-1.56727	0.49926
6	-2.46175	-0.27478	0.62070
6	-2.34686	0.78032	-0.49514
6	-0.94065	1.32781	-0.78961
6	-0.19012	1.86573	0.44169
6	1.31199	2.10816	0.19726
6	2.09512	0.87156	-0.28483
6	2.05763	-0.33445	0.68807
6	1.92952	-1.68680	-0.03378
1	0.62024	-2.19363	-1.81367
1	-2.07912	-2.45372	1.01923
1	-3.53844	-0.55897	0.68671
1	-2.22590	0.18638	1.60525
1	-2.76392	0.35025	-1.43618
1	-3.00854	1.63963	-0.23358
1	-0.35165	0.52672	-1.27953
1	-1.01721	2.14187	-1.54774
1	-0.66810	2.81819	0.76919
1	-0.30684	1.16372	1.29397
1	1.42666	2.92320	-0.55504
1	1.77657	2.48568	1.13795
1	1.72084	0.56387	-1.28538
1	3.15909	1.16038	-0.45280
1	2.98964	-0.33029	1.30009
1	1.22489	-0.23211	1.41619
1	2.05822	-2.51617	0.69850
1	2.76262	-1.78732	-0.76600

FREE ENERGY AT 298.16 K = 114.638 KCAL/MOL

FREE ENERGY AT 173.16 K = 126.263 KCAL/MOL

FREE ENERGY AT 106.86 K = 131.388 KCAL/MOL

CONFORMER 1m STERIC ENERGY= -25.2225 KCAL/MOL

0	1		
6	-0.42495	-1.70546	0.59591
6	0.82076	-1.57516	0.19558
6	2.04111	-1.42460	-0.26681
6	2.67391	-0.06243	-0.46366
6	2.29668	1.08768	0.48721
6	0.80035	1.41778	0.64365
6	-0.00544	1.46534	-0.66681

6	-1.51083	1.72689	-0.46734
6	-2.26973	0.78129	0.48789
6	-2.65682	-0.61594	-0.03431
6	-1.52033	-1.56786	-0.44417
1	-0.68692	-1.87306	1.65171
1	2.59214	-2.31303	-0.61610
1	3.77797	-0.20197	-0.39016
1	2.48892	0.25287	-1.51553
1	2.71489	0.86667	1.49758
1	2.82165	2.00841	0.13832
1	0.35517	0.67525	1.33833
1	0.70225	2.40032	1.16179
1	0.41660	2.26764	-1.31611
1	0.12702	0.52229	-1.23563
1	-1.62256	2.76789	-0.08114
1	-2.01771	1.71760	-1.46014
1	-1.71253	0.67746	1.44390
1	-3.22004	1.29477	0.77166
1	-3.25877	-1.12081	0.75857
1	-3.34666	-0.49384	-0.90210
1	-1.09291	-1.24473	-1.41863
1	-1.95172	-2.57916	-0.62552

FREE ENERGY AT 298.16 K = 115.678 KCAL/MOL

FREE ENERGY AT 173.16 K = 127.117 KCAL/MOL

FREE ENERGY AT 106.86 K = 132.149 KCAL/MOL

CONFORMER 1n STERIC ENERGY= -25.2211 KCAL/MOL

0	1		
6	-0.35348	-2.02852	-0.42447
6	0.87829	-1.68981	-0.11762
6	2.10226	-1.30629	0.16849
6	2.62026	-0.00453	-0.41055
6	2.25761	1.23629	0.42103
6	0.74772	1.45103	0.63438
6	-0.06962	1.49846	-0.66861
6	-1.55951	1.80542	-0.46026
6	-2.34148	0.82559	0.43226
6	-2.50056	-0.62220	-0.09703
6	-1.51050	-1.66226	0.48376
1	-0.55619	-2.62621	-1.32731

1	2.75858	-1.91548	0.80909
1	3.72683	-0.07559	-0.51485
1	2.23107	0.11810	-1.44591
1	2.75733	1.16617	1.41551
1	2.68319	2.13893	-0.07666
1	0.35917	0.64493	1.29483
1	0.59689	2.40470	1.19191
1	0.36619	2.27787	-1.33647
1	0.02015	0.53808	-1.21941
1	-1.64834	2.82831	-0.02416
1	-2.05847	1.85686	-1.45629
1	-1.90862	0.81210	1.45680
1	-3.36637	1.24976	0.56049
1	-3.53009	-0.96099	0.17068
1	-2.46749	-0.63317	-1.20966
1	-2.06472	-2.60311	0.70651
1	-1.12528	-1.30669	1.46466

FREE ENERGY AT 298.16 K = 114.353 KCAL/MOL
 FREE ENERGY AT 173.16 K = 126.065 KCAL/MOL
 FREE ENERGY AT 106.86 K = 131.226 KCAL/MOL

CONFORMER 1o STERIC ENERGY= -25.1885 KCAL/MOL

0	1		
6	-0.05869	1.70452	-0.70933
6	1.13393	1.45223	-0.21800
6	2.32743	1.18515	0.26300
6	2.83269	-0.23706	0.42651
6	1.99286	-1.31567	-0.27926
6	0.59343	-1.51455	0.35289
6	-0.51956	-1.61769	-0.70322
6	-1.93350	-1.65005	-0.10658
6	-2.33877	-0.42350	0.73143
6	-2.43292	0.92734	-0.02356
6	-1.25786	1.90514	0.19499
1	-0.19162	1.82454	-1.79640
1	2.99595	2.01419	0.54621
1	3.86852	-0.27741	0.01705
1	2.91563	-0.47227	1.51146
1	1.89540	-1.04984	-1.35666
1	2.54032	-2.28668	-0.25408

1	0.59637	-2.43152	0.98600
1	0.37913	-0.67254	1.04455
1	-0.44905	-0.76826	-1.41730
1	-0.35735	-2.54040	-1.30797
1	-2.67081	-1.77824	-0.93332
1	-2.02668	-2.56189	0.52900
1	-3.34593	-0.64029	1.16168
1	-1.66985	-0.31932	1.61350
1	-2.59154	0.75258	-1.11152
1	-3.35867	1.44059	0.33165
1	-0.94090	1.87273	1.26137
1	-1.62520	2.94320	0.02155

FREE ENERGY AT 298.16 K = 114.377 KCAL/MOL

FREE ENERGY AT 173.16 K = 126.061 KCAL/MOL

FREE ENERGY AT 106.86 K = 131.206 KCAL/MOL

CONFORMER 1p STERIC ENERGY= -24.8678 KCAL/MOL

0	1		
6	-1.75055	-1.57418	0.45833
6	-0.50728	-1.77014	0.08375
6	0.74124	-1.96570	-0.27416
6	1.86590	-1.31082	0.50140
6	2.60456	-0.24019	-0.31376
6	1.75000	0.95766	-0.76845
6	1.21305	1.85216	0.36988
6	-0.17279	1.50431	0.95010
6	-1.37080	1.81218	0.02403
6	-1.90256	0.67716	-0.87315
6	-2.61004	-0.47569	-0.13170
1	-2.21162	-2.26936	1.17866
1	0.98614	-2.60633	-1.13582
1	1.48377	-0.86814	1.44641
1	2.58615	-2.10334	0.80805
1	3.46600	0.13887	0.28424
1	3.04964	-0.72401	-1.21501
1	2.38881	1.59127	-1.42903
1	0.91722	0.60930	-1.41349
1	1.96015	1.85597	1.19726
1	1.17590	2.90522	0.00426
1	-0.20992	0.45178	1.29247

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1	-0.30149	2.11334	1.87694
1	-2.21879	2.16535	0.65711
1	-1.10572	2.68292	-0.61949
1	-2.64763	1.13292	-1.56888
1	-1.10155	0.27710	-1.52988
1	-3.32801	-0.96315	-0.83119
1	-3.23085	-0.04151	0.68460

FREE ENERGY AT 298.16 K = 115.085 KCAL/MOL

FREE ENERGY AT 173.16 K = 126.776 KCAL/MOL

FREE ENERGY AT 106.86 K = 131.930 KCAL/MOL

CONFORMER 1q STERIC ENERGY= -24.5258 KCAL/MOL

0	1		
6	-0.54889	-1.90629	0.82348
6	-1.50648	-1.16312	0.31413
6	-2.47707	-0.42639	-0.17717
6	-2.37079	1.07627	-0.36684
6	-0.95627	1.65477	-0.55674
6	-0.10126	1.67754	0.72174
6	1.38192	2.01969	0.48779
6	2.18411	1.02133	-0.37295
6	2.11624	-0.44911	0.11961
6	1.30794	-1.37895	-0.81957
6	0.53093	-2.47701	-0.07500
1	-0.49302	-2.08115	1.90956
1	-3.41899	-0.91944	-0.46867
1	-2.96360	1.33372	-1.27553
1	-2.87763	1.58501	0.48362
1	-0.44214	1.08515	-1.36023
1	-1.04240	2.70030	-0.93560
1	-0.53595	2.42857	1.42237
1	-0.17234	0.70662	1.25300
1	1.44932	3.03110	0.02325
1	1.88261	2.10655	1.48095
1	1.85610	1.08549	-1.43419
1	3.25136	1.34601	-0.37609
1	3.15042	-0.85482	0.21409
1	1.69819	-0.47656	1.14917
1	0.59075	-0.78698	-1.42826
1	2.00598	-1.84885	-1.55097

1 1.23492 -3.09032 0.53122
1 0.05988 -3.16860 -0.81005

FREE ENERGY AT 298.16 K = 114.983 KCAL/MOL

FREE ENERGY AT 173.16 K = 126.591 KCAL/MOL

FREE ENERGY AT 106.86 K = 131.695 KCAL/MOL

CONFORMER 1r STERIC ENERGY= -24.4616 KCAL/MOL

0	1			
6	1.79680	1.40829	-0.35774	
6	0.56553	1.83301	-0.17483	
6	-0.68219	2.19829	0.02407	
6	-1.79114	1.30409	-0.49659	
6	-2.33374	0.36055	0.61021	
6	-2.48771	-1.11887	0.19550	
6	-1.24402	-1.76729	-0.44803	
6	0.06217	-1.58609	0.35682	
6	1.31116	-1.56804	-0.54449	
6	2.56907	-0.97921	0.12239	
6	2.40095	0.45724	0.65835	
1	2.38149	1.70033	-1.24368	
1	-0.93492	3.10149	0.60054	
1	-2.61382	1.93138	-0.90689	
1	-1.40638	0.71342	-1.35415	
1	-1.67703	0.41892	1.50726	
1	-3.32222	0.74422	0.95560	
1	-2.77530	-1.71182	1.09518	
1	-3.34203	-1.20449	-0.51621	
1	-1.42992	-2.85612	-0.59872	
1	-1.11299	-1.34932	-1.47067	
1	0.01455	-0.63273	0.91797	
1	0.15322	-2.38765	1.12485	
1	1.52471	-2.60500	-0.89337	
1	1.09537	-0.97458	-1.46235	
1	2.88785	-1.64503	0.95778	
1	3.40193	-0.99075	-0.61950	
1	3.39234	0.85438	0.97414	
1	1.77653	0.44129	1.57930	

FREE ENERGY AT 298.16 K = 115.201 KCAL/MOL
FREE ENERGY AT 173.16 K = 126.836 KCAL/MOL
FREE ENERGY AT 106.86 K = 131.963 KCAL/MOL

CONFORMER 1s STERIC ENERGY= -24.1370 KCAL/MOL

0	1		
6	1.25408	-1.86360	-0.39055
6	0.00000	-1.85523	0.00000
6	-1.25408	-1.86360	0.39055
6	-2.29680	-0.98660	-0.27521
6	-2.51277	0.37559	0.42788
6	-1.94475	1.58365	-0.34016
6	-0.43552	1.54502	-0.63231
6	0.43552	1.54502	0.63231
6	1.94475	1.58365	0.34016
6	2.51277	0.37559	-0.42788
6	2.29680	-0.98660	0.27521
1	1.57061	-2.53281	-1.20654
1	-1.57061	-2.53280	1.20654
1	-2.02098	-0.81810	-1.33967
1	-3.25690	-1.55063	-0.30202
1	-3.60932	0.53590	0.55740
1	-2.09381	0.34309	1.45870
1	-2.49170	1.67674	-1.30781
1	-2.17647	2.51339	0.23023
1	-0.20116	0.65553	-1.25661
1	-0.16896	2.43360	-1.25102
1	0.16896	2.43360	1.25102
1	0.20116	0.65553	1.25661
1	2.17647	2.51339	-0.23023
1	2.49170	1.67674	1.30781
1	2.09381	0.34309	-1.45870
1	3.60932	0.53590	-0.55740
1	2.02098	-0.81810	1.33967
1	3.25690	-1.55063	0.30202

FREE ENERGY AT 298.16 K = 115.343 KCAL/MOL
FREE ENERGY AT 173.16 K = 126.951 KCAL/MOL
FREE ENERGY AT 106.86 K = 132.049 KCAL/MOL

CONFORMER 1t STERIC ENERGY= -24.1106 KCAL/MOL

0	1	
6	-1.07228	-1.49754 -0.72923
6	0.12928	-1.70374 -0.23640
6	1.30282	-1.90428 0.31882
6	2.22391	-0.76375 0.70408
6	2.55812	0.28971 -0.36338
6	1.42234	1.20079 -0.86273
6	0.70794	2.05554 0.21579
6	-0.57222	1.42750 0.80014
6	-1.71915	1.32876 -0.22994
6	-2.76716	0.23653 0.05509
6	-2.18606	-1.17927 0.25035
1	-1.26973	-1.48149 -1.81190
1	1.59561	-2.93117 0.59192
1	1.81728	-0.26549 1.61162
1	3.18638	-1.22166 1.03251
1	3.36729	0.94438 0.03912
1	3.00516	-0.23263 -1.24199
1	1.86308	1.89986 -1.61314
1	0.68769	0.59489 -1.43273
1	1.42503	2.27842 1.03889
1	0.43719	3.04274 -0.22680
1	-0.32921	0.42804 1.21396
1	-0.92121	2.03423 1.66782
1	-2.23034	2.31764 -0.29431
1	-1.30232	1.15156 -1.24529
1	-3.35938	0.51581 0.95726
1	-3.48926	0.21398 -0.79499
1	-2.99675	-1.93391 0.13513
1	-1.81451	-1.28683 1.29441

FREE ENERGY AT 298.16 K = 116.128 KCAL/MOL

FREE ENERGY AT 173.16 K = 127.617 KCAL/MOL

FREE ENERGY AT 106.86 K = 132.668 KCAL/MOL

CONFORMER 1u STERIC ENERGY= -23.8946 KCAL/MOL

0	1	
6	0.55183	1.45330 0.75199
6	-0.67690	1.53529 0.29115

6	-1.90268	1.57223	-0.18134
6	-2.56578	0.32463	-0.73232
6	-2.57141	-0.93863	0.14960
6	-1.20900	-1.41776	0.68350
6	-0.09020	-1.48634	-0.37155
6	1.30824	-1.66893	0.26161
6	2.43252	-0.95526	-0.52280
6	2.79138	0.46309	-0.03089
6	1.72674	1.56444	-0.19933
1	0.74291	1.29979	1.82562
1	-2.42709	2.53728	-0.26843
1	-3.62662	0.58233	-0.95892
1	-2.10875	0.09157	-1.72025
1	-3.24854	-0.76452	1.01882
1	-3.03290	-1.76950	-0.43450
1	-0.90045	-0.74450	1.51399
1	-1.33080	-2.42391	1.14822
1	-0.29419	-2.31812	-1.08427
1	-0.08818	-0.56196	-0.98495
1	1.31445	-1.30496	1.31313
1	1.52869	-2.76043	0.31862
1	3.35372	-1.58080	-0.44631
1	2.17998	-0.92721	-1.60715
1	3.09822	0.41217	1.03953
1	3.70346	0.78824	-0.58657
1	1.37057	1.58116	-1.25380
1	2.20907	2.55285	-0.01873

FREE ENERGY AT 298.16 K = 116.033 KCAL/MOL

FREE ENERGY AT 173.16 K = 127.595 KCAL/MOL

FREE ENERGY AT 106.86 K = 132.679 KCAL/MOL

CONFORMER 1v STERIC ENERGY= -23.8517 KCAL/MOL

0	1		
6	-1.38713	-1.77913	0.55150
6	-0.25374	-1.69624	-0.10581
6	0.88904	-1.62405	-0.74908
6	2.16969	-1.24008	-0.03320
6	2.63653	0.20366	-0.31001
6	2.07196	1.26917	0.64870
6	0.54252	1.33303	0.78176

6	-0.18263	1.63948	-0.53682
6	-1.71691	1.68491	-0.40904
6	-2.46102	0.34096	-0.53568
6	-2.37369	-0.63246	0.66346
1	-1.64427	-2.73336	1.04010
1	0.93344	-1.85874	-1.82454
1	2.05282	-1.38486	1.06421
1	2.96358	-1.95353	-0.35247
1	3.74917	0.23277	-0.22772
1	2.40921	0.47591	-1.36559
1	2.50438	1.09430	1.66211
1	2.44580	2.27003	0.32892
1	0.17096	0.38443	1.22079
1	0.28443	2.12583	1.52250
1	0.17393	2.63082	-0.90327
1	0.09712	0.90577	-1.32346
1	-2.00076	2.18259	0.54611
1	-2.09961	2.35299	-1.21768
1	-3.54076	0.58429	-0.68495
1	-2.14996	-0.17866	-1.47035
1	-3.38057	-1.09657	0.78581
1	-2.19080	-0.07260	1.60684

FREE ENERGY AT 298.16 K = 115.750 KCAL/MOL

FREE ENERGY AT 173.16 K = 127.442 KCAL/MOL

FREE ENERGY AT 106.86 K = 132.584 KCAL/MOL

CONFORMER 1w STERIC ENERGY= -23.5002 KCAL/MOL

0	1		
6	0.97057	-1.62486	0.88488
6	0.00000	-1.60351	0.00000
6	-0.97057	-1.62486	-0.88488
6	-2.23164	-0.78866	-0.78285
6	-2.47536	0.01152	0.51285
6	-1.88858	1.43443	0.57919
6	-0.35598	1.53549	0.68123
6	0.35598	1.53549	-0.68123
6	1.88859	1.43443	-0.57919
6	2.47536	0.01152	-0.51285
6	2.23164	-0.78866	0.78285
1	0.88414	-2.31848	1.73766

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1	-0.88414	-2.31848	-1.73766
1	-2.28580	-0.10312	-1.65785
1	-3.08520	-1.49612	-0.90510
1	-3.58061	0.11207	0.63770
1	-2.13498	-0.58081	1.39258
1	-2.24600	2.02902	-0.29234
1	-2.32174	1.93269	1.47943
1	-0.09512	2.48546	1.20465
1	0.02307	0.72303	1.33480
1	-0.02307	0.72303	-1.33480
1	0.09512	2.48546	-1.20466
1	2.32174	1.93269	-1.47944
1	2.24600	2.02902	0.29234
1	2.13499	-0.58081	-1.39258
1	3.58061	0.11206	-0.63770
1	2.28580	-0.10312	1.65785
1	3.08520	-1.49612	0.90511

FREE ENERGY AT 298.16 K = 116.931 KCAL/MOL

FREE ENERGY AT 173.16 K = 129.399 KCAL/MOL

FREE ENERGY AT 106.86 K = 133.428 KCAL/MOL

CONFORMER 1x STERIC ENERGY= -23.3963 KCAL/MOL

0	1		
6	-2.37878	0.79019	0.19469
6	-1.30194	1.44880	-0.17546
6	-0.25694	2.15317	-0.55453
6	0.97742	2.29076	0.31869
6	1.60260	0.95078	0.73841
6	2.18007	0.15408	-0.45269
6	2.27947	-1.36846	-0.21993
6	0.99236	-2.03059	0.31319
6	-0.27873	-1.64826	-0.47713
6	-1.55710	-1.65067	0.38557
6	-2.63273	-0.67355	-0.12386
1	-3.15503	1.33662	0.75547
1	-0.27699	2.67410	-1.52532
1	1.74013	2.89580	-0.22193
1	0.70345	2.87526	1.22648
1	2.41491	1.13145	1.48016
1	0.82859	0.36002	1.27310

1	1.57130	0.34431	-1.36409
1	3.19268	0.55268	-0.69560
1	2.56823	-1.85869	-1.17898
1	3.10999	-1.57245	0.49563
1	1.11058	-3.13892	0.30535
1	0.86938	-1.75567	1.38447
1	-0.15756	-0.64086	-0.91879
1	-0.40444	-2.33535	-1.34517
1	-1.96961	-2.68614	0.40952
1	-1.31593	-1.38755	1.44062
1	-3.60922	-0.95609	0.33316
1	-2.76458	-0.79381	-1.22259

FREE ENERGY AT 298.16 K = 116.435 KCAL/MOL

FREE ENERGY AT 173.16 K = 127.677 KCAL/MOL

FREE ENERGY AT 106.86 K = 132.648 KCAL/MOL

CONFORMER 1y STERIC ENERGY= -23.3949 KCAL/MOL

0	1		
6	0.26206	2.14862	0.55606
6	1.30723	1.44402	0.17797
6	2.38416	0.78443	-0.19011
6	2.63159	-0.68200	0.12108
6	1.54979	-1.65196	-0.38895
6	0.27360	-1.64787	0.47693
6	-0.99984	-2.02796	-0.31096
6	-2.28454	-1.36083	0.22181
6	-2.18053	0.16181	0.45196
6	-1.59952	0.95470	-0.74002
6	-0.96823	2.29233	-0.32188
1	0.27785	2.66293	1.53045
1	3.16525	1.33180	-0.74321
1	3.60495	-0.96730	-0.34091
1	2.76701	-0.80775	1.21875
1	1.30689	-1.38335	-1.44223
1	1.95755	-2.68918	-0.41845
1	0.40029	-2.33578	1.34417
1	0.15490	-0.64063	0.91961
1	-0.87726	-1.75600	-1.38305
1	-1.12145	-3.13590	-0.30050
1	-3.11610	-1.56351	-0.49291

1	-2.57427	-1.84856	1.18184
1	-3.19200	0.56410	0.69352
1	-1.57180	0.35143	1.36351
1	-0.82799	0.35985	-1.27377
1	-2.41080	1.13806	-1.48222
1	-1.72900	2.90366	0.21433
1	-0.68734	2.87236	-1.23042

FREE ENERGY AT 298.16 K = 116.437 KCAL/MOL

FREE ENERGY AT 173.16 K = 127.678 KCAL/MOL

FREE ENERGY AT 106.86 K = 132.650 KCAL/MOL

Optimized Coordinates of 1,2 - Cycloundecadiene

Gaussian 94: SGI-G94RevE.3 1-Dec-1997

17-Oct-2002

% chk=1b.chk

HF/6-311G* opt test direct

Cycloundecadiene 1a

OPTIMIZED COORDINATES :

6	-0.638745	-1.863572	0.541288
6	0.599064	-1.805332	0.158651
6	1.840134	-1.737242	-0.212644
6	2.742848	-0.522144	-0.118781
6	2.079469	0.747086	0.418195
6	1.178824	1.459341	-0.602699
6	0.100547	2.344813	0.036744
6	-1.064237	1.550008	0.642622
6	-2.011258	0.949137	-0.413112
6	-2.678938	-0.378695	-0.023695
6	-1.847705	-1.635222	-0.339224
1	-0.834557	-2.112095	1.574610
1	2.296595	-2.635251	-0.601776

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1	3.581179	-0.791800	0.519881
1	3.174252	-0.331794	-1.100067
1	1.519369	0.492012	1.311133
1	2.854745	1.436767	0.741750
1	1.805581	2.066132	-1.252072
1	0.710080	0.726863	-1.250384
1	0.558674	2.963258	0.806159
1	-0.290372	3.035768	-0.707552
1	-0.671619	0.767970	1.279521
1	-1.640167	2.199425	1.297404
1	-2.784702	1.680531	-0.632555
1	-1.484273	0.801510	-1.351179
1	-2.952743	-0.367250	1.029834
1	-3.613091	-0.472279	-0.571421
1	-1.534711	-1.604596	-1.377582
1	-2.494259	-2.504232	-0.239777

Dipole moment (Debye):

X= -0.0444 Y= 0.1970 Z= -0.0333 Tot= 0.2046

Low frequencies --- 84.9256 117.5890 160.6182

- Thermochemistry -

Temperature 298.150 Kelvin

Zero-point correction=	0.283864 (Hartree/Particle)
Thermal correction to Energy=	0.294253
Thermal correction to Enthalpy=	0.295197
Thermal correction to Gibbs Free Energy=	0.248443
Sum of electronic and zero-point Energies=	-426.761571
Sum of electronic and thermal Energies=	-426.751181
Sum of electronic and thermal Enthalpies=	-426.750237
Sum of electronic and thermal Free Energies=	-426.796992

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	184.647	40.835	98.403

- Thermochemistry -

Temperature 173.150 Kelvin

Zero-point correction= 0.283864 (Hartree/Particle)
 Thermal correction to Energy= 0.287767
 Thermal correction to Enthalpy= 0.288315
 Thermal correction to Gibbs Free Energy= 0.266235
 Sum of electronic and zero-point Energies= -426.761571
 Sum of electronic and thermal Energies= -426.757667
 Sum of electronic and thermal Enthalpies= -426.757119
 Sum of electronic and thermal Free Energies= -426.779199

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	180.577	24.819	80.019

 - Thermochemistry -

Temperature 106.850 Kelvin.

Zero-point correction= 0.283864 (Hartree/Particle)
 Thermal correction to Energy= 0.285566
 Thermal correction to Enthalpy= 0.285905
 Thermal correction to Gibbs Free Energy= 0.274128
 Sum of electronic and zero-point Energies= -426.761571
 Sum of electronic and thermal Energies= -426.759868
 Sum of electronic and thermal Enthalpies= -426.759529
 Sum of electronic and thermal Free Energies= -426.771306

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	179.196	16.662	69.163

Gaussian 94: SGI-G94RevE.3 1-Dec-1997
 21-Oct-2002

% chk=2b.chk

 # HF/6-311G* opt test direct

Cycloundecadiene 1b

OPTIMIZED COORDINATES :

6	0.702924	-1.852651	0.480883
6	-0.565297	-1.817105	0.213176
6	-1.831865	-1.773489	-0.064898
6	-2.735694	-0.548793	-0.038331
6	-2.073545	0.768215	-0.464987
6	-1.211971	1.445560	0.614247
6	-0.101327	2.341015	0.044327
6	1.066951	1.563292	-0.580235
6	1.965279	0.870605	0.456839
6	2.705886	-0.374603	-0.045001
6	1.802118	-1.534550	-0.507745
1	1.002832	-2.079173	1.494035
1	-2.299976	-2.699831	-0.361887
1	-3.563111	-0.754278	-0.710519
1	-3.180381	-0.444259	0.949623
1	-1.487291	0.573905	-1.356341
1	-2.852239	1.463208	-0.769502
1	-1.861395	2.043693	1.249194
1	-0.776642	0.698300	1.265026
1	-0.530696	3.007423	-0.701327
1	0.282666	2.984169	0.833617
1	0.673732	0.836661	-1.281254
1	1.673186	2.241933	-1.175419
1	2.698815	1.585794	0.821612
1	1.378695	0.590668	1.324162
1	3.371678	-0.110962	-0.864021
1	3.347757	-0.732493	0.757322
1	2.424134	-2.414517	-0.653342
1	1.357485	-1.315219	-1.470627

Dipole moment (Debye):

X= 0.0411 Y= 0.2887 Z= -0.0757 Tot= 0.3013

Low frequencies --- 87.9764 128.0712 166.4885

- Thermochemistry -

Temperature 298.150 Kelvin

Zero-point correction= 0.283948 (Hartree/Particle)
 Thermal correction to Energy= 0.294322
 Thermal correction to Enthalpy= 0.295266
 Thermal correction to Gibbs Free Energy= 0.248619
 Sum of electronic and zero-point Energies= -426.759731
 Sum of electronic and thermal Energies= -426.749358
 Sum of electronic and thermal Enthalpies= -426.748413
 Sum of electronic and thermal Free Energies= -426.795060

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	184.690	40.874	98.176

 - Thermochemistry -

Temperature 173.150 Kelvin

Zero-point correction= 0.283948 (Hartree/Particle)
 Thermal correction to Energy= 0.287833
 Thermal correction to Enthalpy= 0.288382
 Thermal correction to Gibbs Free Energy= 0.266366
 Sum of electronic and zero-point Energies= -426.759731
 Sum of electronic and thermal Energies= -426.755846
 Sum of electronic and thermal Enthalpies= -426.755298
 Sum of electronic and thermal Free Energies= -426.777314

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	180.618	24.806	79.787

 - Thermochemistry -

Temperature 106.850 Kelvin

Zero-point correction= 0.283948 (Hartree/Particle)
 Thermal correction to Energy= 0.285635
 Thermal correction to Enthalpy= 0.285974
 Thermal correction to Gibbs Free Energy= 0.274234

Sum of electronic and zero-point Energies= -426.759731
 Sum of electronic and thermal Energies= -426.758044
 Sum of electronic and thermal Enthalpies= -426.757706
 Sum of electronic and thermal Free Energies= -426.769445

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	179.239	16.622	68.942

Gaussian 94: Cray-C90-Unicos-G94RevE.3 1-Dec-1997
 10-Oct-2002

%chk=three.chk
 %mem=32000000

 # HF/6-311G* opt geom=check guess=check test direct

 Cycloundecadiene 1c

OPTIMIZED COORDINATES :

6	0.497079	-2.091833	0.214947
6	-0.747786	-1.847878	-0.053937
6	-1.983353	-1.557211	-0.320581
6	-2.727198	-0.334188	0.188261
6	-1.827562	0.813308	0.655200
6	-1.157337	1.557612	-0.511201
6	0.094486	2.391807	-0.168516
6	1.430521	1.658347	-0.375101
6	1.825867	0.651018	0.723390
6	2.553595	-0.598666	0.214617
6	1.671323	-1.574015	-0.585499
1	0.723917	-2.675903	1.095209
1	-2.542227	-2.240114	-0.941973
1	-3.386807	0.015872	-0.602705
1	-3.381335	-0.644886	0.999973
1	-2.425270	1.519313	1.226337
1	-1.093540	0.421625	1.346860
1	-0.898063	0.849235	-1.291376
1	-1.905799	2.212061	-0.951588
1	0.102066	3.269026	-0.809664

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1	0.029157	2.772770	0.849428
1	1.392682	1.165670	-1.342492
1	2.223401	2.396881	-0.462557
1	2.463665	1.154839	1.445064
1	0.955566	0.334071	1.280204
1	3.400252	-0.308773	-0.404426
1	2.973274	-1.130630	1.065974
1	2.284970	-2.414773	-0.899922
1	1.306282	-1.106097	-1.491818

Dipole moment (Debye):

X= 0.0601 Y= 0.3133 Z= 0.0534 Tot= 0.3234

Low frequencies --- 69.8268 124.8662 162.6947

- Thermochemistry -

Temperature 298.150 Kelvin

Zero-point correction=	0.283822 (Hartree/Particle)
Thermal correction to Energy=	0.294278
Thermal correction to Enthalpy=	0.295222
Thermal correction to Gibbs Free Energy=	0.248224
Sum of electronic and zero-point Energies=	-426.759242
Sum of electronic and thermal Energies=	-426.748786
Sum of electronic and thermal Enthalpies=	-426.747841
Sum of electronic and thermal Free Energies=	-426.794839

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	184.662	40.931	98.915

- Thermochemistry -

Temperature 173.150 Kelvin

Zero-point correction=	0.283822 (Hartree/Particle)
Thermal correction to Energy=	0.287772
Thermal correction to Enthalpy=	0.288320
Thermal correction to Gibbs Free Energy=	0.266114

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Sum of electronic and zero-point Energies= -426.759242
 Sum of electronic and thermal Energies= -426.755292
 Sum of electronic and thermal Enthalpies= -426.754744
 Sum of electronic and thermal Free Energies= -426.776949

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	180.579	24.945	80.474

 - Thermochemistry -

Temperature 106.850 Kelvin

Zero-point correction= 0.283822 (Hartree/Particle)
 Thermal correction to Energy= 0.285554
 Thermal correction to Enthalpy= 0.285893
 Thermal correction to Gibbs Free Energy= 0.274051
 Sum of electronic and zero-point Energies= -426.759242
 Sum of electronic and thermal Energies= -426.757509
 Sum of electronic and thermal Enthalpies= -426.757171
 Sum of electronic and thermal Free Energies= -426.769012

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	179.188	16.856	69.540

Gaussian 94: Cray-C90-Unicos-G94RevE.3 1-Dec-1997
 10-Oct-2002

%chk=four.chk
 %mem=32000000

 # HF/6-311G* opt geom=check guess=check test direct

 Cycloundecadiene 1d

OPTIMIZED COORDINATES :

6	0.914799	2.008360	-0.157237
6	-0.361707	1.883623	0.033923
6	-1.624856	1.697611	0.258356
6	-2.515690	0.726394	-0.495792
6	-2.591889	-0.708432	0.061697
6	-1.362243	-1.584156	-0.234963
6	-0.222476	-1.488765	0.791136
6	1.142756	-1.930989	0.243785
6	1.794437	-1.001272	-0.799478
6	2.667955	0.137268	-0.253889
6	1.972055	1.218148	0.587208
1	1.259837	2.724589	-0.887995
1	-2.087992	2.279792	1.040709
1	-3.518267	1.143946	-0.504735
1	-2.199089	0.680445	-1.532526
1	-2.790279	-0.684848	1.131292
1	-3.462051	-1.175365	-0.392606
1	-1.676740	-2.623340	-0.295410
1	-0.999700	-1.335956	-1.227903
1	-0.160964	-0.485265	1.181119
1	-0.475263	-2.118641	1.641710
1	1.832681	-2.068444	1.074272
1	1.023960	-2.916943	-0.201010
1	2.436901	-1.606542	-1.434085
1	1.039882	-0.588994	-1.460776
1	3.468371	-0.289918	0.347169
1	3.156692	0.619066	-1.098694
1	2.731558	1.915996	0.931133
1	1.541604	0.783684	1.479862

Dipole moment (Debye):

X= 0.0253 Y= -0.2826 Z= 0.0053 Tot= 0.2837

Low frequencies --- 54.4559 119.5246 180.3395

- Thermochemistry -

Temperature 298.150 Kelvin

Zero-point correction=

0.283858 (Hartree/Particle)

Thermal correction to Energy=

0.294348

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Thermal correction to Enthalpy= 0.295293
 Thermal correction to Gibbs Free Energy= 0.248086
 Sum of electronic and zero-point Energies= -426.758032
 Sum of electronic and thermal Energies= -426.747542
 Sum of electronic and thermal Enthalpies= -426.746598
 Sum of electronic and thermal Free Energies= -426.793805

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	184.706	40.983	99.355

 - Thermochemistry -

Temperature 173.150 Kelvin

Zero-point correction= 0.283858 (Hartree/Particle)
 Thermal correction to Energy= 0.287831
 Thermal correction to Enthalpy= 0.288379
 Thermal correction to Gibbs Free Energy= 0.266060
 Sum of electronic and zero-point Energies= -426.758032
 Sum of electronic and thermal Energies= -426.754060
 Sum of electronic and thermal Enthalpies= -426.753511
 Sum of electronic and thermal Free Energies= -426.775830

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	180.616	24.989	80.884

 - Thermochemistry -

Temperature 106.850 Kelvin

Zero-point correction= 0.283858 (Hartree/Particle)
 Thermal correction to Energy= 0.285610
 Thermal correction to Enthalpy= 0.285948
 Thermal correction to Gibbs Free Energy= 0.274040
 Sum of electronic and zero-point Energies= -426.758032
 Sum of electronic and thermal Energies= -426.756280
 Sum of electronic and thermal Enthalpies= -426.755942
 Sum of electronic and thermal Free Energies= -426.767850

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	179.223	16.879	69.936

Gaussian 94: Cray-C90-Unicos-G94RevE.3 1-Dec-1997
10-Oct-2002

%chk=five.chk
%mem=32000000

HF/6-311G* opt geom=check guess=check test direct

Cycloundecadiene 1e

OPTIMIZED COORDINATES :

6	-1.125030	-1.798259	0.644091
6	0.000003	-1.773044	-0.000010
6	1.125036	-1.798235	-0.644111
6	2.386825	-1.011149	-0.351262
6	2.303363	0.111361	0.694417
6	1.959934	1.499090	0.133242
6	0.575891	1.647610	-0.505184
6	-0.575898	1.647614	0.505178
6	-1.959942	1.499085	-0.133245
6	-2.303370	0.111350	-0.694408
6	-2.386816	-1.011155	0.351278
1	-1.199879	-2.491581	1.469574
1	1.199926	-2.491615	-1.469542
1	3.135223	-1.735141	-0.036316
1	2.760657	-0.608439	-1.290549
1	1.611609	-0.170382	1.480937
1	3.275196	0.190824	1.173794
1	2.061927	2.229361	0.934119
1	2.716643	1.761382	-0.603685
1	0.546160	2.584880	-1.057438
1	0.434201	0.866312	-1.242611
1	-0.434206	0.866325	1.242614
1	-0.546169	2.584890	1.057422
1	-2.716650	1.761382	0.603680

1	-2.061938	2.229349	-0.934129
1	-3.275210	0.190806	-1.173773
1	-1.611626	-0.170395	-1.480935
1	-3.135230	-1.735140	0.036354
1	-2.760618	-0.608438	1.290573

Dipole moment (Debye):

X= 0.0000 Y= 0.0465 Z= 0.0001 Tot= 0.0465

Low frequencies --- 92.2170 106.5601 146.3669

- Thermochemistry -

Temperature 298.150 Kelvin

Zero-point correction= 0.283810 (Hartree/Particle)

Thermal correction to Energy= 0.294241

Thermal correction to Enthalpy= 0.295186

Thermal correction to Gibbs Free Energy= 0.248309

Sum of electronic and zero-point Energies= -426.761145

Sum of electronic and thermal Energies= -426.750714

Sum of electronic and thermal Enthalpies= -426.749770

Sum of electronic and thermal Free Energies= -426.796646

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	184.639	40.827	98.660

- Thermochemistry -

Temperature 173.150 Kelvin

Zero-point correction= 0.283810 (Hartree/Particle)

Thermal correction to Energy= 0.287756

Thermal correction to Enthalpy= 0.288304

Thermal correction to Gibbs Free Energy= 0.266154

Sum of electronic and zero-point Energies= -426.761145

Sum of electronic and thermal Energies= -426.757200

Sum of electronic and thermal Enthalpies= -426.756651

Sum of electronic and thermal Free Energies= -426.778802

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	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	180.570	24.845	80.276

- Thermochemistry -

Temperature 106.850 Kelvin

Zero-point correction= 0.283810 (Hartree/Particle)
 Thermal correction to Energy= 0.285544
 Thermal correction to Enthalpy= 0.285883
 Thermal correction to Gibbs Free Energy= 0.274071
 Sum of electronic and zero-point Energies= -426.761145
 Sum of electronic and thermal Energies= -426.759411
 Sum of electronic and thermal Enthalpies= -426.759073
 Sum of electronic and thermal Free Energies= -426.770884

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	179.182	16.879	69.366

Gaussian 94: SGI-G94RevE.3 1-Dec-1997
19-Oct-2002

% chk=6.chk
% mem=32000000

HF/6-311G* opt test direct

Cycloundecadiene 1f

OPTIMIZED COORDINATES :

6	-1.715583	1.730208	-0.324808
6	-0.479603	1.771744	0.061371
6	0.760122	1.806671	0.436437
6	1.950336	1.386953	-0.398470
6	2.779351	0.239636	0.206535

6	2.310515	-1.193051	-0.084720
6	0.902076	-1.578669	0.406051
6	-0.179215	-1.498817	-0.677880
6	-1.599343	-1.748707	-0.159762
6	-2.249594	-0.631343	0.671152
6	-2.712048	0.609840	-0.108331
1	-2.104792	2.598908	-0.835591
1	0.980054	2.184332	1.424630
1	1.629401	1.136924	-1.403529
1	2.596647	2.256273	-0.494447
1	3.796364	0.327423	-0.167604
1	2.849346	0.382026	1.283469
1	2.382121	-1.377145	-1.155280
1	3.038566	-1.857979	0.372576
1	0.924735	-2.601988	0.773805
1	0.633249	-0.965433	1.259175
1	-0.136278	-0.547187	-1.192777
1	0.046848	-2.252482	-1.429976
1	-2.250378	-1.964338	-1.004611
1	-1.590874	-2.656047	0.441676
1	-3.132508	-1.058559	1.138902
1	-1.602317	-0.329938	1.488323
1	-3.558567	1.050024	0.414050
1	-3.103699	0.308396	-1.078237

Dipole moment (Debye):

X= 0.0174 Y= -0.1977 Z= -0.0078 Tot= 0.1986

Low frequencies --- 80.4187 117.6221 139.8968

- Thermochemistry -

Temperature 298.150 Kelvin

Zero-point correction=	0.283699 (Hartree/Particle)
Thermal correction to Energy=	0.294207
Thermal correction to Enthalpy=	0.295151
Thermal correction to Gibbs Free Energy=	0.248056
Sum of electronic and zero-point Energies=	-426.759268
Sum of electronic and thermal Energies=	-426.748759
Sum of electronic and thermal Enthalpies=	-426.747815
Sum of electronic and thermal Free Energies=	-426.794911

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	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	184.618	40.961	99.121

- Thermochemistry -

Temperature 173.150 Kelvin

Zero-point correction= 0.283699 (Hartree/Particle)
 Thermal correction to Energy= 0.287683
 Thermal correction to Enthalpy= 0.288232
 Thermal correction to Gibbs Free Energy= 0.265983
 Sum of electronic and zero-point Energies= -426.759268
 Sum of electronic and thermal Energies= -426.755283
 Sum of electronic and thermal Enthalpies= -426.754735
 Sum of electronic and thermal Free Energies= -426.776983

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	180.524	25.088	80.630

- Thermochemistry -

Temperature 106.850 Kelvin

Zero-point correction= 0.283699 (Hartree/Particle)
 Thermal correction to Energy= 0.285447
 Thermal correction to Enthalpy= 0.285786
 Thermal correction to Gibbs Free Energy= 0.273933
 Sum of electronic and zero-point Energies= -426.759268
 Sum of electronic and thermal Energies= -426.757519
 Sum of electronic and thermal Enthalpies= -426.757181
 Sum of electronic and thermal Free Energies= -426.769034

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	179.121	17.070	69.609

Gaussian 94: SGI-G94RevE.3 1-Dec-1997
19-Oct-2002

% chk=7.chk
% mem=32000000-----
HF/6-311G* opt test direct

Cycloundecadiene 1g

OPTIMIZED COORDINATES :

6	-1.293369	-1.927370	-0.053693
6	0.000000	-1.996062	0.000000
6	1.293369	-1.927370	0.053693
6	2.104164	-0.926452	-0.743773
6	2.629469	0.229288	0.127933
6	1.537971	1.069194	0.802731
6	0.762645	2.044360	-0.115149
6	-0.762645	2.044360	0.115149
6	-1.537971	1.069194	-0.802731
6	-2.629469	0.229288	-0.127933
6	-2.104164	-0.926451	0.743773
1	-1.825563	-2.563215	-0.745006
1	1.825562	-2.563214	0.745007
1	2.950391	-1.431110	-1.202400
1	1.499097	-0.541140	-1.556106
1	3.274801	-0.187153	0.898551
1	3.265384	0.866848	-0.482770
1	0.845522	0.396031	1.292378
1	1.995360	1.642717	1.604293
1	1.150267	3.046288	0.043616
1	0.960793	1.824797	-1.160943
1	-0.960792	1.824797	1.160943
1	-1.150267	3.046288	-0.043616
1	-1.995360	1.642717	-1.604293
1	-0.845522	0.396031	-1.292378
1	-3.265383	0.866848	0.482770
1	-3.274801	-0.187152	-0.898551
1	-2.950391	-1.431109	1.202400
1	-1.499097	-0.541140	1.556106

Dipole moment (Debye):

X= 0.0000 Y= 0.4685 Z= 0.0000 Tot= 0.4685

Low frequencies --- 38.4844 103.9805 161.4770

- Thermochemistry -

Temperature 298.150 Kelvin

Zero-point correction= 0.283781 (Hartree/Particle)
 Thermal correction to Energy= 0.294281
 Thermal correction to Enthalpy= 0.295225
 Thermal correction to Gibbs Free Energy= 0.247648
 Sum of electronic and zero-point Energies= -426.755728
 Sum of electronic and thermal Energies= -426.745228
 Sum of electronic and thermal Enthalpies= -426.744284
 Sum of electronic and thermal Free Energies= -426.791862

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	184.664	40.890	100.136

- Thermochemistry -

Temperature 173.150 Kelvin

Zero-point correction= 0.283781 (Hartree/Particle)
 Thermal correction to Energy= 0.287788
 Thermal correction to Enthalpy= 0.288337
 Thermal correction to Gibbs Free Energy= 0.265784
 Sum of electronic and zero-point Energies= -426.755728
 Sum of electronic and thermal Energies= -426.751721
 Sum of electronic and thermal Enthalpies= -426.751173
 Sum of electronic and thermal Free Energies= -426.773726

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	180.590	24.850	81.734