

Supplementary Material

C₆H₄

CH₂CHCCCCCH b3lyp/6-311++g**

6	0	1.736581	2.288964	0.000000
6	0	0.448343	1.917988	0.000000
6	0	0.000000	0.575599	0.000000
6	0	-0.423146	-0.562828	0.000000
6	0	-0.887271	-1.841580	0.000000
6	0	-1.300388	-2.978046	0.000000
1	0	2.009964	3.336958	0.000000
1	0	2.538174	1.560137	0.000000
1	0	-0.329239	2.678777	0.000000
1	0	-1.663615	-3.976455	0.000000
Rotational constants (GHZ):		41.7003390	1.3646401	1.3213975
Frequencies --	107.3967	140.9090	258.4780	
Frequencies --	334.0452	493.0416	550.6421	
Frequencies --	562.2378	653.7017	657.5985	
Frequencies --	690.8129	698.9520	956.4864	
Frequencies --	1000.9052	1048.4704	1207.2611	
Frequencies --	1317.1400	1447.5522	1653.7937	
Frequencies --	2153.6181	2312.4813	3131.8462	
Frequencies --	3148.0649	3239.3854	3476.1754	

CHCCHCHCCH (CCCC trans) b3lyp/6-311++g**

6	0	0.000000	0.675032	0.000000
6	0	0.000000	-0.675032	0.000000
6	0	1.176117	1.462881	0.000000
6	0	-1.176117	-1.462881	0.000000
6	0	2.154600	2.168420	0.000000
6	0	-2.154600	-2.168420	0.000000
1	0	-0.946379	1.208288	0.000000
1	0	0.946379	-1.208288	0.000000
1	0	3.022972	2.780958	0.000000
1	0	-3.022972	-2.780958	0.000000
Rotational constants (GHZ):		47.7781260	1.4524990	1.4096445
Frequencies --	120.1772	129.6713	248.5499	
Frequencies --	363.9273	517.2285	527.3289	
Frequencies --	529.0298	651.3673	652.6260	
Frequencies --	690.8781	691.2763	868.2187	
Frequencies --	966.4510	1029.3319	1043.9776	
Frequencies --	1293.1561	1318.2669	1643.4759	
Frequencies --	2181.4811	2204.9182	3149.7304	
Frequencies --	3158.3732	3473.7979	3473.9149	

CHCCHCHCCH (CCCC cis) b3lyp/6-311++g**

6	0	0.000000	0.675675	1.077244
6	0	0.000000	-0.675675	1.077244
6	0	0.000000	1.497384	-0.074439
6	0	0.000000	-1.497384	-0.074439
6	0	0.000000	2.234850	-1.028643
6	0	0.000000	-2.234850	-1.028643
1	0	0.000000	1.188231	2.034630

1	0	0.000000	-1.188231	2.034630
1	0	0.000000	2.871251	-1.879606
1	0	0.000000	-2.871251	-1.879606
Rotational constants (GHZ):		7.3410881	2.4761216	1.8515879
Frequencies --	106.0531	226.7806		253.4570
Frequencies --	356.9603	447.6447		559.2579
Frequencies --	653.4343	658.6531		684.3371
Frequencies --	686.5208	740.5690		770.1493
Frequencies --	891.2711	964.6816		1038.5413
Frequencies --	1245.3732	1419.1529		1629.0201
Frequencies --	2185.5925	2204.1837		3147.7429
Frequencies --	3164.2023	3474.7690		3475.0065

CH₂C(CCH)CCH b3lyp/6-311++g**

6	0	0.000000	2.234314	-0.953088
6	0	0.000000	1.219622	-0.305524
6	0	0.000000	0.000000	0.447200
6	0	0.000000	0.000000	1.794727
6	0	0.000000	-1.219622	-0.305524
6	0	0.000000	-2.234314	-0.953088
1	0	0.000000	3.131939	-1.521893
1	0	0.000000	0.930136	2.347781
1	0	0.000000	-0.930136	2.347781
1	0	0.000000	-3.131939	-1.521893
Rotational constants (GHZ):		6.2518008	2.8548187	1.9598664
Frequencies --	137.5573	225.8336		250.4729
Frequencies --	343.5898	492.8421		587.9216
Frequencies --	646.1192	660.7248		669.1282
Frequencies --	697.9796	699.8103		730.5093
Frequencies --	759.0835	933.5026		955.4138
Frequencies --	1276.0411	1422.7501		1628.9810
Frequencies --	2204.0869	2210.8997		3157.7963
Frequencies --	3256.1630	3474.6543		3475.7614

CH₂CCCHCCH b3lyp/6-311++g**

6	0	2.157497	2.049244	0.000000
6	0	1.052605	1.332267	0.000000
6	0	0.000000	0.639179	0.000000
6	0	-1.120386	-0.073180	0.000000
6	0	-1.163501	-1.488864	0.000000
6	0	-1.241078	-2.692698	0.000000
1	0	3.134835	1.577386	0.000000
1	0	2.127072	3.134099	0.000000
1	0	-2.077176	0.446673	0.000000
1	0	-1.295553	-3.753843	0.000000
Rotational constants (GHZ):		19.5820305	1.5284638	1.4177984
Frequencies --	97.6629	207.9439		263.8297
Frequencies --	313.2297	367.0066		534.3084
Frequencies --	564.1439	605.6035		644.9543
Frequencies --	688.4977	849.0704		883.1917
Frequencies --	885.8547	1028.8983		1052.9409
Frequencies --	1311.4642	1445.1324		1666.4911
Frequencies --	2168.8967	2209.9050		3114.6997
Frequencies --	3122.8077	3200.8515		3475.4555

CH₂CCCCCH₂ b3lyp/6-311++g**

6	0	0.000000	0.000000	3.226275
6	0	0.000000	0.000000	1.910866
6	0	0.000000	0.000000	0.643181
6	0	0.000000	0.000000	-0.643181
6	0	0.000000	0.000000	-1.910866
6	0	0.000000	0.000000	-3.226275
1	0	0.000000	0.927244	3.791959
1	0	0.000000	-0.927244	3.791959
1	0	0.000000	0.927244	-3.791959
1	0	0.000000	-0.927244	-3.791959
Rotational constants (GHZ):		145.8089928	1.2468012	1.2362303
Frequencies --	107.8315	109.6692		260.5825
Frequencies --	265.2066	348.7757		485.0897
Frequencies --	517.2157	547.3726		640.6367
Frequencies --	642.8906	872.3601		872.5515
Frequencies --	1015.7399	1016.1078		1187.2243
Frequencies --	1424.0902	1465.6860		1701.8441
Frequencies --	2109.7852	2204.4093		3111.2825
Frequencies --	3111.4184	3186.6314		3186.6524

CH₂CHCCCCH⁺ (A'') b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =		-230.641649862	A.U. after	2 cycles
6	0	1.795985	2.204256	0.000000
6	0	0.453395	1.905041	0.000000
6	0	0.000000	0.604604	0.000000
6	0	-0.439762	-0.551515	0.000000
6	0	-0.909857	-1.795423	0.000000
6	0	-1.343909	-2.937655	0.000000
1	0	2.128506	3.236401	0.000000
1	0	2.549188	1.424261	0.000000
1	0	-0.288305	2.700890	0.000000
1	0	-1.724502	-3.937400	0.000000
Rotational constants (GHZ):		38.0407299	1.3903995	1.3413719
Frequencies --	108.0848	136.7023		239.9390
Frequencies --	311.2947	485.5991		501.1093
Frequencies --	541.3573	626.7968		681.7198
Frequencies --	714.2295	775.1114		913.7835
Frequencies --	1048.7265	1050.2710		1261.2701
Frequencies --	1287.1645	1451.9009		1549.2174
Frequencies --	2049.0311	2256.4049		3148.2136
Frequencies --	3151.9990	3257.6665		3410.0113

CHCCHCHCCH⁺ (A_u) (CCCC trans) b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =		-230.635058592	A.U. after	2 cycles
6	0	0.000000	0.699124	0.000000
6	0	0.000000	-0.699124	0.000000
6	0	1.165730	1.433738	0.000000
6	0	-1.165730	-1.433738	0.000000
6	0	2.176921	2.115308	0.000000
6	0	-2.176921	-2.115308	0.000000
1	0	-0.946469	1.234903	0.000000
1	0	0.946469	-1.234903	0.000000
1	0	3.067202	2.708326	0.000000
1	0	-3.067202	-2.708326	0.000000
Rotational constants (GHZ):		44.2563532	1.4776676	1.4299241
Frequencies --	100.2794	127.1380		234.6236

Frequencies --	336.2742	458.3901	510.1442
Frequencies --	527.0458	699.3925	700.2023
Frequencies --	772.3142	772.5936	893.0010
Frequencies --	925.2264	1069.3979	1110.3899
Frequencies --	1268.1846	1308.4571	1533.6419
Frequencies --	2108.4975	2138.2010	3155.5965
Frequencies --	3162.8537	3409.5125	3411.5886

CHCCHCHCCH⁺ (B₁) (CCCC cis) b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =	-230.632967543	A.U. after	2 cycles
6	0	0.000000	0.700673
6	0	0.000000	-0.700673
6	0	0.000000	1.483481
6	0	0.000000	-1.483481
6	0	0.000000	2.222906
6	0	0.000000	-2.222906
1	0	0.000000	1.209070
1	0	0.000000	-1.209070
1	0	0.000000	2.869223
1	0	0.000000	-2.869223
Rotational constants (GHZ):	7.3618309	2.4928483	1.8622552
Frequencies --	109.3018	182.1962	241.9892
Frequencies --	336.6066	439.7435	486.5046
Frequencies --	695.1122	698.4235	732.7993
Frequencies --	767.7403	777.2608	791.4011
Frequencies --	923.4874	978.2053	1086.2909
Frequencies --	1235.7761	1440.2069	1494.7593
Frequencies --	2107.2684	2142.2750	3153.2141
Frequencies --	3164.8386	3411.1258	3413.3445

CH₂C(CCH)CCH⁺ (B₁) b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =	-230.618706734	A.U. after	1 cycles
6	0	0.000000	2.271207
6	0	0.000000	1.215354
6	0	0.000000	0.000000
6	0	0.000000	0.000000
6	0	0.000000	-1.215354
6	0	0.000000	-2.271207
1	0	0.000000	3.201602
1	0	0.000000	0.935541
1	0	0.000000	-0.935541
1	0	0.000000	-3.201602
Rotational constants (GHZ):	6.5206477	2.7817552	1.9499097
Frequencies --	135.5705	204.6708	233.4588
Frequencies --	299.2087	478.0450	481.3618
Frequencies --	585.9858	618.5216	724.9865
Frequencies --	725.6707	770.9939	781.9224
Frequencies --	782.3010	975.7735	996.6114
Frequencies --	1330.2216	1352.7864	1504.2426
Frequencies --	2118.7229	2192.3233	3148.1958
Frequencies --	3266.7720	3417.4743	3419.9012

CH₂CCCHCCH⁺ (A'') b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =	-230.632783871	A.U. after	4 cycles
6	0	2.121910	2.101601
6	0	1.016490	1.339421
			0.000000
			0.000000

6	0	0.000000	0.633122	0.000000
6	0	-1.146749	-0.113808	0.000000
6	0	-1.135943	-1.491842	0.000000
6	0	-1.165917	-2.710764	0.000000
1	0	3.110431	1.649763	0.000000
1	0	2.049469	3.186154	0.000000
1	0	-2.109737	0.397656	0.000000
1	0	-1.188917	-3.779951	0.000000
Rotational constants (GHZ):		19.2447449	1.5338614	1.4206329
Frequencies --	-8.0895	108.0714		205.1414
Frequencies --	256.8261	344.6841		362.8473
Frequencies --	524.4098	554.3677		696.9811
Frequencies --	767.3557	862.2087		874.0988
Frequencies --	996.2173	1031.1656		1094.8948
Frequencies --	1300.9389	1436.8332		1518.3306
Frequencies --	2116.0422	2201.7358		3120.3725
Frequencies --	3122.5705	3219.3255		3414.1314

CH₂CCCCCH₂⁺ (B₃) b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =		-230.647191674	A.U. after	4 cycles
6	0	0.000000	0.000000	0.645357
6	0	0.000000	0.000000	-0.645357
6	0	0.000000	0.000000	1.909327
6	0	0.000000	0.000000	-1.909327
6	0	0.000000	0.000000	3.228682
6	0	0.000000	0.000000	-3.228682
1	0	0.332949	0.872104	3.788722
1	0	-0.332949	-0.872104	3.788722
1	0	-0.332949	0.872104	-3.788722
1	0	0.332949	-0.872104	-3.788722
Rotational constants (GHZ):		143.8614143	1.2448140	1.2368347
Frequencies --	105.2846	105.8186		260.9450
Frequencies --	261.1564	363.6801		441.5655
Frequencies --	530.6693	569.8266		602.8938
Frequencies --	638.3607	950.8648		951.0449
Frequencies --	978.2410	978.4642		1167.0626
Frequencies --	1393.3009	1433.0647		1620.8010
Frequencies --	1856.1532	2038.7431		3102.1877
Frequencies --	3103.0822	3192.4774		3192.5012

C7H4

CHCCCCCCH₃ b3lyp/6-311++g**

SCF Done: E(RB+HF-LYP) =		-269.046652962	A.U. after	2 cycles
6	0	0.000000	0.000000	-3.789266
6	0	0.000000	0.000000	-2.337825
6	0	0.000000	0.000000	-1.125066
6	0	0.000000	0.000000	0.229524
6	0	0.000000	0.000000	1.448217
6	0	0.000000	0.000000	2.803915
6	0	0.000000	0.000000	4.014363
1	0	0.000000	1.022102	-4.179993
1	0	0.885166	-0.511051	-4.179993
1	0	-0.885166	-0.511051	-4.179993

1	0	0.000000	0.000000	5.076804
Rotational constants (GHZ):		160.0008655	0.7818837	0.7818837
Frequencies --	80.2368	80.2423		204.7919
Frequencies --	204.7937	345.5099		345.5112
Frequencies --	507.8474	507.8479		522.1348
Frequencies --	651.2976	651.2976		652.4572
Frequencies --	652.4573	946.5806		1043.9933
Frequencies --	1043.9941	1316.8347		1413.4001
Frequencies --	1470.4645	1470.4647		2134.0075
Frequencies --	2277.2782	2325.1085		3019.8171
Frequencies --	3079.0039	3079.0040		3475.7773

CHCCCCCHCCH₂ b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-269.035941514	A.U. after	2 cycles	
	6	0	3.760836	0.073695	0.000000
	6	0	2.559109	0.208274	0.000000
	6	0	1.206934	0.359809	0.000000
	6	0	0.000000	0.488011	0.000000
	6	0	-1.402461	0.685032	0.000000
	6	0	-2.284696	-0.292675	0.000000
	6	0	-3.166342	-1.246007	0.000000
	1	0	4.816661	-0.044177	0.000000
	1	0	-1.761306	1.713757	0.000000
	1	0	-3.547815	-1.663202	0.927872
	1	0	-3.547815	-1.663202	-0.927872
Rotational constants (GHZ):		16.1159976	0.9447273	0.8979167	
Frequencies --	74.8447	140.2369	196.3237		
Frequencies --	304.1023	350.9807	352.7198		
Frequencies --	507.2522	535.6175	546.8815		
Frequencies --	633.6446	647.1861	663.1400		
Frequencies --	778.3880	878.0820	886.8710		
Frequencies --	998.7433	1068.2195	1215.3267		
Frequencies --	1363.1986	1464.0552	2027.1143		
Frequencies --	2155.0755	2316.4289	3107.0046		
Frequencies --	3111.0728	3182.4999	3476.5445		

CHCCCCCH₂CCH b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-269.020615192	A.U. after	2 cycles	
	6	0	3.635172	-0.483756	0.000000
	6	0	2.473866	-0.151550	0.000000
	6	0	1.162316	0.224061	0.000000
	6	0	0.000000	0.555578	0.000000
	6	0	-1.402090	0.970673	0.000000
	6	0	-2.346766	-0.150177	0.000000
	6	0	-3.131460	-1.058678	0.000000
	1	0	4.656385	-0.776814	0.000000
	1	0	-1.590786	1.603548	0.876397
	1	0	-1.590786	1.603548	-0.876397
	1	0	-3.821039	-1.867198	0.000000
Rotational constants (GHZ):		11.6884014	1.0132739	0.9377976	
Frequencies --	73.3381	141.5538	193.4617		
Frequencies --	310.7568	327.6507	333.5774		
Frequencies --	489.9667	537.5783	563.0289		
Frequencies --	661.7337	667.7848	680.1764		
Frequencies --	699.6932	744.2421	922.9779		
Frequencies --	944.1851	1170.6938	1239.0176		

Frequencies --	1341.0268	1449.9659	2163.7740
Frequencies --	2228.4260	2351.8088	3007.0803
Frequencies --	3029.9158	3476.2007	3477.4269

CHCCHCCHCCH b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-269.022108041	A.U. after	2 cycles
6	0	0.000000	3.226435	-0.829353
6	0	0.264062	2.265520	-0.153146
6	0	0.615335	1.157368	0.668841
6	0	0.000000	0.000000	0.655059
6	0	-0.615335	-1.157368	0.668841
6	0	-0.264062	-2.265520	-0.153146
6	0	0.000000	-3.226435	-0.829353
1	0	-0.240441	4.068026	-1.431859
1	0	1.456521	1.293770	1.348628
1	0	-1.456521	-1.293770	1.348628
1	0	0.240441	-4.068026	-1.431859
Rotational constants (GHZ):		9.4766642	1.1057387	1.0415216
Frequencies --	77.1274	135.1409	173.3987	
Frequencies --	336.1473	344.7044	356.4968	
Frequencies --	500.4588	552.0701	648.6914	
Frequencies --	650.0813	651.6201	696.8515	
Frequencies --	697.0460	788.6415	892.5456	
Frequencies --	920.2607	997.3723	1145.2852	
Frequencies --	1294.1350	1428.6897	2026.4997	
Frequencies --	2204.7756	2207.6958	3101.0125	
Frequencies --	3103.1788	3475.1050	3475.7344	

CH₂CC(CCH)₂ b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-269.017883258	A.U. after	2 cycles
6	0	0.000000	0.000000	2.600453
6	0	0.000000	0.000000	1.304053
6	0	0.000000	0.000000	-0.021072
6	0	0.000000	1.231543	-0.755335
6	0	0.000000	-1.231543	-0.755335
6	0	0.000000	2.254047	-1.389754
6	0	0.000000	-2.254047	-1.389754
1	0	-0.927774	0.000000	3.167082
1	0	0.927774	0.000000	3.167082
1	0	0.000000	3.158815	-1.946853
1	0	0.000000	-3.158815	-1.946853
Rotational constants (GHZ):		2.8047699	2.6441230	1.3738781
Frequencies --	129.8680	129.9702	163.9284	
Frequencies --	332.5019	342.5683	349.1709	
Frequencies --	566.6563	591.5227	610.6727	
Frequencies --	623.9854	644.8133	653.3436	
Frequencies --	657.9824	705.7548	707.5332	
Frequencies --	892.9267	991.1120	1181.4518	
Frequencies --	1248.3246	1449.4825	2021.1357	
Frequencies --	2204.7030	2211.8998	3104.5027	
Frequencies --	3175.0845	3476.1321	3477.2800	

CHCCHCCCCH₂ b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-269.028836602	A.U. after	7 cycles
6	0	3.518755	0.045794	0.000000
6	0	2.422307	0.548125	0.000000

6	0	1.153392	1.178538	0.000000
6	0	0.000000	0.527565	0.000000
6	0	-1.115123	-0.076750	0.000000
6	0	-2.236537	-0.688478	0.000000
6	0	-3.385336	-1.315636	0.000000
1	0	4.479346	-0.408216	0.000000
1	0	1.139284	2.267841	0.000000
1	0	-3.881691	-1.587288	0.927418
1	0	-3.881691	-1.587288	-0.927418
Rotational constants (GHZ):		16.0443808	0.9502774	0.9026978
Frequencies --	75.2380	142.6114		193.0483
Frequencies --	298.5360	335.2414		340.3493
Frequencies --	504.1308	519.1530		550.8557
Frequencies --	568.6296	635.7139		693.8930
Frequencies --	792.6101	813.0982		867.9103
Frequencies --	1001.3660	1011.9720		1252.2325
Frequencies --	1398.9129	1503.0689		1942.2835
Frequencies --	2178.8653	2226.1872		3108.4206
Frequencies --	3110.6014	3184.0408		3476.9630

CH₂CCCCCH₂ b3lyp/6-311++g**

SCF Done: E(RB+HF-LYP) =		-269.036594678	A.U. after	3 cycles
6	0	0.000000	0.000000	0.000000
6	0	0.000000	0.000000	1.278635
6	0	0.000000	0.000000	-1.278635
6	0	0.000000	0.000000	2.550566
6	0	0.000000	0.000000	-2.550566
6	0	0.000000	0.000000	3.863658
6	0	0.000000	0.000000	-3.863658
1	0	0.000000	0.927517	4.428915
1	0	0.000000	-0.927517	4.428915
1	0	0.927517	0.000000	-4.428915
1	0	-0.927517	0.000000	-4.428915
Rotational constants (GHZ):		145.7232050	0.7965691	0.7965691
Frequencies --	81.3494	81.3494		208.2198
Frequencies --	208.2198	336.5597		336.5597
Frequencies --	500.4230	500.4230		560.6233
Frequencies --	589.1259	589.1259		592.5839
Frequencies --	853.9520	853.9520		1002.9119
Frequencies --	1002.9119	1058.7527		1386.3267
Frequencies --	1439.5851	1558.8943		1908.2276
Frequencies --	2176.2355	2176.6390		3111.6792
Frequencies --	3111.8499	3186.3626		3186.3626

CH(CCH)₃ b3lyp/6-311++g**

SCF Done: E(RB+HF-LYP) =		-268.993434210	A.U. after	1 cycles
6	0	0.000000	0.000000	0.516425
1	0	0.000000	0.000000	1.616670
6	0	0.000000	1.408845	0.081814
6	0	1.220095	-0.704422	0.081814
6	0	-1.220095	-0.704422	0.081814
6	0	0.000000	2.561310	-0.251358
6	0	2.218160	-1.280655	-0.251358
6	0	-2.218160	-1.280655	-0.251358
1	0	0.000000	3.579908	-0.554477
1	0	3.100291	-1.789954	-0.554477

1	0	-3.100291	-1.789954	-0.554477
Rotational constants (GHZ):		2.7697127	2.7697127	1.4590575
Frequencies --	128.1072	128.1255	154.6251	
Frequencies --	324.8956	324.8977	328.9586	
Frequencies --	550.4285	550.4293	569.9015	
Frequencies --	691.4621	691.4621	693.9700	
Frequencies --	699.6840	702.7637	702.7639	
Frequencies --	838.4021	1029.1842	1029.2043	
Frequencies --	1285.3342	1285.3346	2226.6915	
Frequencies --	2226.6922	2234.2634	2983.2179	
Frequencies --	3476.4809	3476.4809	3477.7524	

CHCCCCCH₃⁺ b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-268.731537095	A.U. after	4 cycles
6	0	3.769730	0.000525	-0.001015
6	0	2.340461	0.002149	-0.008927
6	0	1.106989	0.001502	-0.003571
6	0	-0.211434	0.000630	-0.002192
6	0	-1.453932	0.000254	-0.000449
6	0	-2.779052	-0.000319	0.001016
6	0	-4.002422	-0.000782	0.002296
1	0	4.162606	-0.835792	-0.589720
1	0	4.171608	0.948701	-0.371548
1	0	4.115565	-0.135487	1.034931
1	0	-5.071825	-0.001178	0.003391
Rotational constants (GHZ):		157.9373399	0.7887424	0.7886692
Frequencies --	76.1457	79.0665	187.4720	
Frequencies --	196.6512	284.5781	349.2722	
Frequencies --	438.0094	468.6378	521.6323	
Frequencies --	535.1056	535.8657	549.5827	
Frequencies --	666.3003	765.4560	956.5453	
Frequencies --	988.9976	1324.9357	1364.7230	
Frequencies --	1390.8457	1436.0008	2025.7836	
Frequencies --	2160.4684	2275.8476	2991.1898	
Frequencies --	3044.1253	3068.5625	3411.6630	

CHCCCCCHCCH₂⁺ b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-268.726701351	A.U. after	2 cycles
6	0	3.722093	-0.181025	0.000000
6	0	2.522145	0.045405	0.000000
6	0	1.215035	0.294990	0.000000
6	0	0.000000	0.524060	0.000000
6	0	-1.343300	0.816430	0.000000
6	0	-2.273502	-0.168585	0.000000
6	0	-3.172082	-1.083122	0.000000
1	0	4.772909	-0.377622	0.000000
1	0	-1.659092	1.859621	0.000000
1	0	-3.568074	-1.485460	0.932483
1	0	-3.568074	-1.485460	-0.932483
Rotational constants (GHZ):		14.7312464	0.9712063	0.9169313
Frequencies --	74.7804	135.8168	189.2824	
Frequencies --	271.6497	330.5017	348.2540	
Frequencies --	444.0613	501.2689	544.5805	
Frequencies --	572.8288	685.4498	758.6695	
Frequencies --	787.7246	811.4307	901.2099	
Frequencies --	908.2744	1046.5889	1260.4108	

Frequencies --	1344.9128	1434.1863	1962.9891
Frequencies --	2056.2058	2244.7837	3089.2809
Frequencies --	3119.9143	3164.2352	3415.6380

CHCCCCCH₂CCH⁺ (A') b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-268.685851209	A.U. after	2 cycles
6	0	3.285413	-1.141834	0.000000
6	0	2.216679	-0.547495	0.000000
6	0	1.053462	0.102147	0.000000
6	0	0.000000	0.741048	0.000000
6	0	-1.299433	1.388751	0.000000
6	0	-2.146486	0.196675	0.000000
6	0	-2.770006	-0.841926	0.000000
1	0	4.220544	-1.661294	0.000000
1	0	-1.449948	2.005047	0.892632
1	0	-1.449948	2.005047	-0.892632
1	0	-3.358427	-1.732997	0.000000
Rotational constants (GHZ):		8.2022969	1.2133304	1.0641252
Frequencies --	72.2091	144.2713	171.6155	
Frequencies --	301.9173	320.9972	330.6059	
Frequencies --	449.5265	521.3001	549.8144	
Frequencies --	681.0702	705.3867	713.2319	
Frequencies --	754.8350	766.5740	941.2069	
Frequencies --	942.1425	1201.0516	1203.1717	
Frequencies --	1296.8581	1441.4335	2038.0042	
Frequencies --	2117.0750	2269.0810	3035.5713	
Frequencies --	3078.7370	3410.2213	3430.3274	

CHCCCCCH₂CCH⁺ (A'') b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-268.686063955	A.U. after	3 cycles
6	0	3.680076	-0.385205	0.000000
6	0	2.491568	-0.096267	0.000000
6	0	1.195628	0.217920	0.000000
6	0	0.000000	0.503005	0.000000
6	0	-1.386841	0.876708	0.000000
6	0	-2.367619	-0.186447	0.000000
6	0	-3.219253	-1.041341	0.000000
1	0	4.719844	-0.636945	0.000000
1	0	-1.554706	1.552333	0.862685
1	0	-1.554706	1.552333	-0.862685
1	0	-3.971791	-1.797954	0.000000
Rotational constants (GHZ):		13.3742388	0.9833856	0.9210400
Frequencies --	74.2164	133.4298	189.1386	
Frequencies --	275.8072	319.6785	325.8695	
Frequencies --	488.9254	510.0467	548.6250	
Frequencies --	685.6171	716.0322	738.2345	
Frequencies --	743.2266	751.5647	764.2304	
Frequencies --	964.1475	1150.4465	1177.7003	
Frequencies --	1295.6824	1317.4481	2043.9457	
Frequencies --	2145.0525	2280.9710	2911.3238	
Frequencies --	2920.3560	3408.6333	3440.0089	

CHCCHCCHCCH⁺ (B) b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-268.697335408	A.U. after	2 cycles
6	0	0.000000	3.359082	-0.593995
6	0	0.334451	2.298593	-0.112118

6	0	0.742481	1.100268	0.478487
6	0	0.000000	0.000000	0.461838
6	0	-0.742481	-1.100268	0.478487
6	0	-0.334451	-2.298593	-0.112118
6	0	0.000000	-3.359082	-0.593995
1	0	-0.288857	4.290956	-1.029282
1	0	1.698571	1.071224	1.009523
1	0	-1.698571	-1.071224	1.009523
1	0	0.288857	-4.290956	-1.029282
Rotational constants (GHZ):		12.8025020	1.0356428	1.0302547
Frequencies --	76.2742	92.1423		153.7683
Frequencies --	315.3365	320.7234		330.6226
Frequencies --	442.3081	479.6369		653.2573
Frequencies --	720.3633	720.8360		761.7517
Frequencies --	761.7881	818.1233		849.5943
Frequencies --	898.8119	1035.5339		1116.0370
Frequencies --	1265.4626	1396.4022		1700.2983
Frequencies --	2119.6368	2178.9175		3075.9549
Frequencies --	3078.4257	3426.5645		3427.9716

CHCCHCCHCCH⁺ (A) b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =		-268.697143525	A.U. after	2 cycles
6	0	0.000000	3.015940	-1.026666
6	0	0.200911	2.180308	-0.172347
6	0	0.477898	1.238367	0.821291
6	0	0.000000	0.000000	0.799390
6	0	-0.477898	-1.238367	0.821291
6	0	-0.200911	-2.180308	-0.172347
6	0	0.000000	-3.015940	-1.026666
1	0	-0.187136	3.757745	-1.772279
1	0	1.147237	1.518482	1.640444
1	0	-1.147237	-1.518482	1.640444
1	0	0.187136	-3.757745	-1.772279
Rotational constants (GHZ):		7.3270103	1.2281984	1.0850920
Frequencies --	63.3737	141.9009		153.7177
Frequencies --	302.1478	325.4290		330.6417
Frequencies --	453.8573	533.6742		540.3283
Frequencies --	719.8199	720.0594		761.6327
Frequencies --	762.0500	823.3851		869.4036
Frequencies --	928.2490	1027.1274		1123.9638
Frequencies --	1243.8498	1405.3962		1698.0133
Frequencies --	2119.7429	2179.6042		3072.1362
Frequencies --	3076.8994	3425.8373		3427.2687

CH₂CC(CCH)₂⁺ b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =		-268.702770916	A.U. after	1 cycles
6	0	0.000000	0.000000	2.578583
6	0	0.000000	0.000000	1.299112
6	0	0.000000	0.000000	-0.077056
6	0	0.000000	1.225250	-0.760821
6	0	0.000000	-1.225250	-0.760821
6	0	0.000000	2.284060	-1.351600
6	0	0.000000	-2.284060	-1.351600
1	0	-0.933043	0.000000	3.145043
1	0	0.933043	0.000000	3.145043
1	0	0.000000	3.217160	-1.872437

1	0	0.000000	-3.217160	-1.872437
Rotational constants (GHZ):		2.7488220	2.7092938	1.3775096
Frequencies --	124.8615	128.1167		158.8154
Frequencies --	253.2886	322.8133		327.8437
Frequencies --	378.0450	561.2260		561.8844
Frequencies --	609.8385	671.2175		729.1567
Frequencies --	729.8858	755.8684		756.0024
Frequencies --	864.9319	903.5258		1204.4083
Frequencies --	1260.6091	1356.0590		1950.5300
Frequencies --	2102.5904	2187.5479		3075.2094
Frequencies --	3147.9817	3422.9980		3425.6254

CHCCHCCCCH₂⁺ b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-268.725565300	A.U. after	2 cycles	
	6	0	-3.401333	-0.844999	0.032277
	6	0	-2.468790	-0.065134	0.010262
	6	0	-1.436885	0.854820	-0.032649
	6	0	-0.127148	0.497515	-0.015877
	6	0	1.085532	0.201759	-0.008427
	6	0	2.344937	-0.107340	0.002610
	6	0	3.604098	-0.416868	0.013370
	1	0	-4.219565	-1.531571	0.055864
	1	0	-1.684728	1.915663	-0.100210
	1	0	4.254212	-0.105830	0.830782
	1	0	4.047617	-0.996778	-0.795839
Rotational constants (GHZ):		16.0355855	0.9538953	0.9047654	
Frequencies --	73.9022	133.3367	184.5372		
Frequencies --	243.4722	322.0603	340.6887		
Frequencies --	384.2956	461.3910	510.3707		
Frequencies --	537.4114	705.9270	752.4613		
Frequencies --	779.9419	835.2762	908.5170		
Frequencies --	921.9549	1057.1738	1226.1409		
Frequencies --	1362.4922	1446.1968	1891.3838		
Frequencies --	2047.4812	2138.9291	3090.9565		
Frequencies --	3107.2327	3171.3801	3424.0005		

CH₂CCCCCCH₂⁺ b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-268.743371800	A.U. after	2 cycles
	6	0	0.000000	0.000000
	6	0	0.000000	0.000000
	6	0	0.000000	0.000000
	6	0	0.000000	0.000000
	6	0	0.000000	0.000000
	6	0	0.000000	0.000000
	6	0	0.000000	0.000000
	6	0	0.000000	0.000000
	1	0	-0.366471	0.858207
	1	0	0.366471	-0.858207
	1	0	-0.366471	-0.858207
	1	0	0.366471	0.858207
Rotational constants (GHZ):		143.9606696	0.7988554	0.7958015
Frequencies --	77.5582	80.4318		196.9127
Frequencies --	204.2087	342.8526		345.0629
Frequencies --	431.1349	501.7154		555.6247
Frequencies --	558.9021	563.8159		582.5326
Frequencies --	923.4667	923.4961		959.5130
Frequencies --	959.6262	1042.0863		1358.6795

Frequencies --	1405.3798	1533.8240	1660.1346
Frequencies --	1915.1696	2098.3577	3102.6270
Frequencies --	3104.1182	3190.0000	3190.0190

CH(CCH)₃⁺ b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-268.639432346	A.U. after	1 cycles
6	0	0.000000	0.000000	0.272117
1	0	0.000000	0.000000	1.416256
6	0	0.000000	1.424549	0.011179
6	0	1.233696	-0.712275	0.011179
6	0	-1.233696	-0.712275	0.011179
6	0	0.000000	2.626226	-0.132727
6	0	2.274378	-1.313113	-0.132727
6	0	-2.274378	-1.313113	-0.132727
1	0	0.000000	3.683792	-0.287034
1	0	3.190258	-1.841896	-0.287034
1	0	-3.190258	-1.841896	-0.287034
Rotational constants (GHZ):		2.7320096	2.7320096	1.3946110
Frequencies --	127.5354	127.5409	157.7378	
Frequencies --	310.7012	310.7047	315.4051	
Frequencies --	549.2790	549.2803	598.6835	
Frequencies --	719.5937	738.0306	739.8947	
Frequencies --	739.8947	748.6576	748.6578	
Frequencies --	756.8182	932.2088	932.2151	
Frequencies --	1145.2826	1145.2953	2105.2541	
Frequencies --	2105.2548	2202.6900	2602.0635	
Frequencies --	3422.8448	3422.8448	3427.0021	

C₈H₄

-CCCHC(CCH)CHCH- b3lyp/6-311++g**

6	0	0.000000	0.469883	0.000000
6	0	-1.107511	-0.415390	0.000000
6	0	-0.963431	-1.813631	0.000000
6	0	0.374293	-2.164158	0.000000
6	0	1.352920	-1.395868	0.000000
6	0	1.338165	-0.019450	0.000000
6	0	-0.220953	1.881027	0.000000
6	0	-0.393410	3.073355	0.000000
1	0	-2.104130	0.011287	0.000000
1	0	-1.813455	-2.483115	0.000000
1	0	2.185523	0.652624	0.000000
1	0	-0.548373	4.124593	0.000000
Rotational constants (GHZ):		6.0111647	1.6541324	1.2971790
Frequencies --	152.6450	165.0490	376.5994	
Frequencies --	405.9936	418.6685	483.7968	
Frequencies --	531.2182	548.3408	647.6664	
Frequencies --	661.8777	665.5734	704.3551	
Frequencies --	831.6375	884.8885	920.0852	
Frequencies --	949.2068	1071.5049	1131.5197	
Frequencies --	1189.5568	1264.0661	1284.5977	
Frequencies --	1369.4723	1440.4062	1497.0417	
Frequencies --	2008.9399	2202.0615	3181.9467	
Frequencies --	3202.7314	3208.0246	3475.5867	

-CCC(CCH)CHCHCH- b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-307.137915057	A.U. after	2 cycles
6	0	0.000000	0.620416	0.000000
6	0	-1.044693	-0.345885	0.000000
6	0	-0.799859	-1.724807	0.000000
6	0	0.504716	-2.266134	0.000000
6	0	1.432983	-1.244480	0.000000
6	0	1.238105	-0.017173	0.000000
6	0	-0.248606	2.019928	0.000000
6	0	-0.470121	3.203744	0.000000
1	0	-2.068190	0.012436	0.000000
1	0	-1.645433	-2.405138	0.000000
1	0	0.697186	-3.330521	0.000000
1	0	-0.658719	4.249568	0.000000
Rotational constants (GHZ):		7.0262833	1.5065637	1.2405640
Frequencies --	136.9316	161.9735	360.2050	
Frequencies --	421.7245	444.2492	497.1993	
Frequencies --	541.3303	564.8053	628.1994	
Frequencies --	662.8707	708.3170	763.4164	
Frequencies --	774.9426	887.9280	895.8798	
Frequencies --	950.4013	1041.6539	1132.4931	
Frequencies --	1165.7298	1226.9143	1286.3150	
Frequencies --	1437.7356	1449.6140	1482.7750	
Frequencies --	2014.4453	2207.8332	3165.9743	
Frequencies --	3185.4958	3206.8956	3475.3931	

CHCCCCCHCH₂ b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-307.138571814	A.U. after	5 cycles
6	0	-1.365140	-4.354400	0.000000
6	0	-1.045147	-3.186719	0.000000
6	0	-0.681550	-1.881936	0.000000
6	0	-0.358178	-0.705431	0.000000
6	0	0.000000	0.596304	0.000000
6	0	0.332399	1.767814	0.000000
6	0	0.673253	3.139189	0.000000
6	0	1.928901	3.611274	0.000000
1	0	-1.648371	-5.378591	0.000000
1	0	-0.162306	3.836130	0.000000
1	0	2.785683	2.948230	0.000000
1	0	2.117774	4.677667	0.000000
Rotational constants (GHZ):		37.4140653	0.5714899	0.5628919
Frequencies --	64.1109	76.9312	158.2404	
Frequencies --	196.9326	281.0083	337.4981	
Frequencies --	443.1813	486.5474	497.0046	
Frequencies --	589.6279	597.5529	634.8494	
Frequencies --	652.2952	654.3131	694.3476	
Frequencies --	918.2333	956.7084	997.9332	
Frequencies --	1089.4440	1315.6337	1320.2799	
Frequencies --	1452.6137	1650.7071	2128.6967	
Frequencies --	2266.2677	2287.4183	3129.8712	
Frequencies --	3148.6251	3240.8267	3473.3392	

CHCCCCCHCHCH (trans) b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-307.129066150	A.U. after	5 cycles
6	0	2.057379	3.893746	0.000000

6	0	1.397552	2.879957	0.000000
6	0	0.655669	1.741236	0.000000
6	0	0.000000	0.717193	0.000000
6	0	-0.799491	-0.440993	0.000000
6	0	-0.302681	-1.700366	0.000000
6	0	-1.108397	-2.862109	0.000000
6	0	-1.764042	-3.875141	0.000000
1	0	2.636696	4.784693	0.000000
1	0	-1.876693	-0.295415	0.000000
1	0	0.773506	-1.848060	0.000000
1	0	-2.349449	-4.762358	0.000000
Rotational constants (GHZ):		38.3786093	0.6068745	0.5974275
Frequencies --	69.0840	73.8482	177.8495	
Frequencies --	187.9997	256.1693	355.3107	
Frequencies --	448.3415	489.9059	497.3335	
Frequencies --	550.3431	568.0890	653.1081	
Frequencies --	655.7675	662.1617	691.6095	
Frequencies --	797.2010	867.5895	960.6681	
Frequencies --	1035.0979	1221.2927	1301.8473	
Frequencies --	1313.8783	1630.5164	2150.2857	
Frequencies --	2189.2057	2302.5509	3143.8449	
Frequencies --	3156.4806	3471.1057	3472.1078	

CHCCCCCHCCH (cis) b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-307.128248311	A.U. after	5 cycles
6	0	3.778764	0.685909	0.000000
6	0	2.571002	0.750277	0.000000
6	0	1.214088	0.824382	0.000000
6	0	0.000000	0.881867	0.000000
6	0	-1.401722	1.000709	0.000000
6	0	-2.277941	-0.032451	0.000000
6	0	-1.928225	-1.401616	0.000000
6	0	-1.668336	-2.579485	0.000000
1	0	4.839727	0.628541	0.000000
1	0	-1.801610	2.011025	0.000000
1	0	-3.339318	0.196769	0.000000
1	0	-1.424579	-3.613886	0.000000
Rotational constants (GHZ):		4.5867401	0.9623042	0.7954233
Frequencies --	59.5539	120.0443	158.4206	
Frequencies --	253.0832	267.8413	349.4887	
Frequencies --	423.8884	524.0294	539.3414	
Frequencies --	585.7729	635.6586	657.4689	
Frequencies --	658.2378	662.4372	685.7991	
Frequencies --	766.1520	784.3769	969.2643	
Frequencies --	976.4399	1179.2381	1255.9064	
Frequencies --	1426.4717	1615.9578	2151.4794	
Frequencies --	2191.9282	2303.2390	3143.7775	
Frequencies --	3162.0933	3473.9476	3475.6122	

CHCCCCCHCCCH₂ b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-307.121627757	A.U. after	5 cycles
6	0	3.388001	2.605006	0.000000
6	0	2.304005	2.068023	0.000000
6	0	1.086394	1.465581	0.000000
6	0	0.000000	0.919374	0.000000
6	0	-1.279442	0.332485	0.000000

6	0	-1.499282	-0.980086	0.000000
6	0	-1.726178	-2.218502	0.000000
6	0	-1.956635	-3.516181	0.000000
1	0	4.340169	3.076489	0.000000
1	0	-2.132318	1.010579	0.000000
1	0	-2.968090	-3.909348	0.000000
1	0	-1.140942	-4.231922	0.000000
Rotational constants (GHZ):		9.5103682	0.6673341	0.6235782
Frequencies --	53.6860	140.2034		162.5042
Frequencies --	210.4323	270.7695		330.3135
Frequencies --	361.7861	483.8991		516.5832
Frequencies --	537.6383	553.8474		607.6885
Frequencies --	654.7728	660.5942		772.2571
Frequencies --	846.2740	887.0021		917.1135
Frequencies --	1029.3063	1220.5891		1318.8537
Frequencies --	1447.1504	1659.5620		2148.0480
Frequencies --	2177.2223	2303.5992		3106.4085
Frequencies --	3123.9596	3203.8204		3475.9009

CHCCHCCCHCCH (trans) b3lyp/6-311++g**

SCF Done: E(RB+HF-LYP) =		-307.111578568	A.U. after	5 cycles
6	0	2.081971	-3.510631	0.000000
6	0	1.123908	-2.776903	0.000000
6	0	-0.028263	-1.958141	0.000000
6	0	-0.000780	-0.627263	0.000000
6	0	0.000000	0.626873	0.000000
6	0	0.028099	1.957741	0.000000
6	0	-1.123691	2.777059	0.000000
6	0	-2.081387	3.511265	0.000000
1	0	2.932008	-4.148372	0.000000
1	0	-0.993041	-2.462422	0.000000
1	0	0.993120	2.461538	0.000000
1	0	-2.931225	4.149262	0.000000
Rotational constants (GHZ):		15.4391038	0.6736741	0.6455078
Frequencies --	66.3788	74.7688		126.6652
Frequencies --	255.9497	291.4131		356.8266
Frequencies --	365.5644	498.8886		520.7390
Frequencies --	525.9052	626.7780		643.7436
Frequencies --	643.9633	689.9310		690.5302
Frequencies --	786.1786	856.9058		874.7378
Frequencies --	1001.5973	1087.9594		1278.8701
Frequencies --	1368.9594	1655.3199		2145.9538
Frequencies --	2190.2661	2216.1139		3119.5922
Frequencies --	3121.1161	3473.5339		3474.2446

CHCCHCCCHCCH (cis) b3lyp/6-311++g**

SCF Done: E(RB+HF-LYP) =		-307.111368211	A.U. after	2 cycles
6	0	-1.997815	-3.140971	0.000000
6	0	-2.005842	-1.934313	0.000000
6	0	-2.065258	-0.522260	0.000000
6	0	-0.996753	0.271833	0.000000
6	0	0.000000	1.032978	0.000000
6	0	1.047070	1.855121	0.000000
6	0	2.393819	1.426527	0.000000
6	0	3.555867	1.101340	0.000000
1	0	-1.977517	-4.203438	0.000000

1	0	-3.055405	-0.069749	0.000000
1	0	0.870844	2.929417	0.000000
1	0	4.575556	0.802238	0.000000
Rotational constants (GHZ):		5.5668697	0.8086168	0.7060582
Frequencies --	56.7793	138.6781	144.2163	
Frequencies --	205.2570	290.3264	358.6427	
Frequencies --	370.7666	470.5593	488.1042	
Frequencies --	550.5317	644.0809	645.0011	
Frequencies --	646.6745	690.2215	691.1374	
Frequencies --	785.6764	853.9869	881.6002	
Frequencies --	995.5579	1088.1946	1273.8877	
Frequencies --	1375.2668	1654.4145	2145.5728	
Frequencies --	2190.5877	2215.2621	3118.2812	
Frequencies --	3119.9175	3474.4541	3475.0045	

CHCCHCCCCCH₂ b3lyp/6-311++g**

SCF Done: E(RB+HF-LYP) =		-307.116058888	A.U. after	2 cycles
6	0	-1.462825	-3.821798	0.000000
6	0	-1.622986	-2.625632	0.000000
6	0	-1.857663	-1.231579	0.000000
6	0	-0.896485	-0.312026	0.000000
6	0	0.000000	0.574678	0.000000
6	0	0.917061	1.481842	0.000000
6	0	1.817553	2.371043	0.000000
6	0	2.754501	3.295863	0.000000
1	0	-1.310274	-4.873443	0.000000
1	0	-2.897178	-0.905391	0.000000
1	0	3.807815	3.031843	0.000000
1	0	2.504705	4.352640	0.000000
Rotational constants (GHZ):		14.1949331	0.6292099	0.6025032
Frequencies --	59.9963	103.3846	146.5311	
Frequencies --	253.5762	287.5589	312.9440	
Frequencies --	351.0600	484.1470	487.6690	
Frequencies --	518.1488	533.6936	584.2090	
Frequencies --	641.2953	690.6046	723.9603	
Frequencies --	810.3323	870.1561	989.2028	
Frequencies --	1014.3867	1182.4555	1352.0077	
Frequencies --	1452.4366	1686.4169	2110.9495	
Frequencies --	2161.4323	2213.9665	3107.2643	
Frequencies --	3114.8074	3191.7746	3474.9029	

CH₂CCCCCCH₂ b3lyp/6-311++g**

SCF Done: E(RB+HF-LYP) =		-307.123794367	A.U. after	5 cycles
6	0	0.000000	0.000000	0.635030
6	0	0.000000	0.000000	-0.635030
6	0	0.000000	0.000000	1.919521
6	0	0.000000	0.000000	-1.919521
6	0	0.000000	0.000000	3.188179
6	0	0.000000	0.000000	-3.188179
6	0	0.000000	0.000000	4.503745
6	0	0.000000	0.000000	-4.503745
1	0	0.000000	0.927274	5.069614
1	0	0.000000	-0.927274	5.069614
1	0	0.000000	0.927274	-5.069614
1	0	0.000000	-0.927274	-5.069614
Rotational constants (GHZ):		145.7992983	0.5419771	0.5399698

Frequencies --	62.6705	63.0716	162.6639
Frequencies --	167.0403	281.2235	292.9428
Frequencies --	342.2262	469.8454	490.9858
Frequencies --	496.0462	554.7412	557.8250
Frequencies --	559.5499	653.5761	866.0044
Frequencies --	866.2003	949.4043	1009.2665
Frequencies --	1009.3432	1320.1052	1430.7256
Frequencies --	1483.2627	1726.0716	2044.2298
Frequencies --	2138.0031	2205.4126	3110.1982
Frequencies --	3110.4756	3185.3874	3185.3895

CH₂C(CCH)CCCCH b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-307.120713166	A.U. after	3 cycles	
	6	0	-2.416694	0.535671	0.000000
	6	0	-1.308263	-0.234264	0.000000
	6	0	-1.383957	-1.666063	0.000000
	6	0	-1.425848	-2.868847	0.000000
	6	0	0.000000	0.334878	0.000000
	6	0	1.121569	0.795935	0.000000
	6	0	2.376974	1.320885	0.000000
	6	0	3.492076	1.787413	0.000000
	1	0	-3.400917	0.085964	0.000000
	1	0	-2.341011	1.615121	0.000000
	1	0	-1.466101	-3.930829	0.000000
	1	0	4.472880	2.196090	0.000000
Rotational constants (GHZ):		5.1513843	0.9428162	0.7969558	
Frequencies --	71.2160	111.7854	180.1739		
Frequencies --	253.3547	261.0268	338.9654		
Frequencies --	450.3662	505.4894	535.9440		
Frequencies --	572.5821	645.5138	661.0891		
Frequencies --	665.0897	667.5093	672.0255		
Frequencies --	701.1612	724.2623	896.4387		
Frequencies --	937.2571	1082.6184	1319.2577		
Frequencies --	1424.6776	1620.9276	2157.0598		
Frequencies --	2208.2824	2320.3690	3158.5158		
Frequencies --	3257.8153	3475.4656	3476.2913		

CH₂CCC(CCH)CCH b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-307.105201065	A.U. after	2 cycles	
	6	0	0.000000	0.000000	3.396254
	6	0	0.000000	0.000000	2.077345
	6	0	0.000000	0.000000	0.821020
	6	0	0.000000	0.000000	-0.518338
	6	0	0.000000	1.224237	-1.253118
	6	0	0.000000	2.248228	-1.887496
	6	0	0.000000	-1.224237	-1.253118
	6	0	0.000000	-2.248228	-1.887496
	1	0	0.000000	-0.927896	3.958662
	1	0	0.000000	0.927896	3.958662
	1	0	0.000000	3.153623	-2.443824
	1	0	0.000000	-3.153623	-2.443824
Rotational constants (GHZ):		2.8223905	1.3724271	0.9234073	
Frequencies --	82.3312	124.1962	128.2721		
Frequencies --	259.5661	271.0910	336.6247		
Frequencies --	365.1060	516.2466	545.7798		
Frequencies --	546.9036	572.9223	615.0977		

Frequencies --	634.4648	650.6357	661.8921
Frequencies --	699.4521	701.6788	881.0299
Frequencies --	1026.8237	1082.4300	1189.2863
Frequencies --	1435.5813	1645.2728	2165.2902
Frequencies --	2191.1414	2217.8996	3125.6964
Frequencies --	3206.0652	3474.6561	3475.8339

CHCC(CCH)CHCCH b3lyp/6-311++g**

SCF Done:	E(RB+HF-LYP) =	-307.113166147	A.U. after	1 cycles	
	6	0	-0.176515	3.117382	0.000000
	6	0	-0.105509	1.915050	0.000000
	6	0	0.000000	0.491135	0.000000
	6	0	1.314166	-0.061859	0.000000
	6	0	2.432308	-0.508517	0.000000
	6	0	-1.122020	-0.283645	0.000000
	6	0	-1.131494	-1.692477	0.000000
	6	0	-1.188746	-2.897849	0.000000
	1	0	-0.240330	4.178207	0.000000
	1	0	3.416191	-0.910155	0.000000
	1	0	-2.085031	0.216604	0.000000
	1	0	-1.223979	-3.959981	0.000000
Rotational constants (GHZ):		3.4296694	1.4561456	1.0221627	
Frequencies --	107.5928	117.8690	135.7741		
Frequencies --	234.0826	252.6491	354.6014		
Frequencies --	438.5438	494.1315	524.5453		
Frequencies --	593.4152	640.8353	655.4297		
Frequencies --	658.1329	669.6983	686.6286		
Frequencies --	695.9475	702.1451	794.3146		
Frequencies --	879.5256	1048.6701	1182.3526		
Frequencies --	1353.8294	1592.1499	2182.3563		
Frequencies --	2198.3998	2213.5790	3166.8876		
Frequencies --	3474.5132	3474.5925	3476.2095		

-CCCHC(CCH)CHCH-⁺ b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-306.812698957	A.U. after	1 cycles	
	6	0	0.000000	0.476311	0.000000
	6	0	-1.138776	-0.427240	0.000000
	6	0	-0.989694	-1.807154	0.000000
	6	0	0.368612	-2.126875	0.000000
	6	0	1.367073	-1.372896	0.000000
	6	0	1.379873	-0.018372	0.000000
	6	0	-0.218170	1.842727	0.000000
	6	0	-0.390163	3.052794	0.000000
	1	0	-2.130296	0.011810	0.000000
	1	0	-1.821754	-2.497924	0.000000
	1	0	2.224384	0.659007	0.000000
	1	0	-0.544864	4.111340	0.000000
Rotational constants (GHZ):		5.7546404	1.6888068	1.3056418	
Frequencies --	124.2376	160.1013	334.6166		
Frequencies --	378.3835	426.0831	492.2124		
Frequencies --	522.8824	545.2306	612.8414		
Frequencies --	625.3284	709.5025	746.1352		
Frequencies --	822.5471	870.7121	880.6039		
Frequencies --	979.1819	1057.8313	1129.3887		
Frequencies --	1208.3063	1225.4618	1279.8302		
Frequencies --	1366.7284	1428.9906	1486.3297		

Frequencies --	1921.8634	2102.2892	3194.6449
Frequencies --	3214.0763	3226.4841	3408.8750

-CCC(CCH)CHCHCH-⁺ b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-306.812445834	A.U. after	1 cycles
6	0	0.000000	0.621710	0.000000
6	0	-1.071462	-0.373869	0.000000
6	0	-0.809231	-1.727044	0.000000
6	0	0.531497	-2.242428	0.000000
6	0	1.443908	-1.200559	0.000000
6	0	1.285750	0.023735	0.000000
6	0	-0.265843	1.977347	0.000000
6	0	-0.501101	3.175783	0.000000
1	0	-2.094487	-0.015669	0.000000
1	0	-1.630670	-2.434706	0.000000
1	0	0.746327	-3.304228	0.000000
1	0	-0.702281	4.226543	0.000000
Rotational constants (GHZ):		6.7133037	1.5354312	1.2496238
Frequencies --	86.4855	157.5137	244.1785	
Frequencies --	335.6379	423.4884	451.8254	
Frequencies --	498.7499	541.1523	635.5128	
Frequencies --	712.3943	737.4615	758.0682	
Frequencies --	777.9452	860.8721	902.4443	
Frequencies --	983.6169	1013.2584	1089.4691	
Frequencies --	1144.0090	1195.9089	1304.9245	
Frequencies --	1316.4063	1415.4791	1505.2269	
Frequencies --	2032.6109	2119.1725	3191.1661	
Frequencies --	3204.4661	3213.1089	3409.4374	

CHCCCCCHCH₂⁺ b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-306.834800830	A.U. after	2 cycles
6	0	-1.416674	-4.315190	0.000000
6	0	-1.076299	-3.144405	0.000000
6	0	-0.705514	-1.867019	0.000000
6	0	-0.360915	-0.677379	0.000000
6	0	0.000000	0.589955	0.000000
6	0	0.347311	1.777834	0.000000
6	0	0.688140	3.117077	0.000000
6	0	1.990138	3.532977	0.000000
1	0	-1.715444	-5.340972	0.000000
1	0	-0.122563	3.842153	0.000000
1	0	2.811328	2.825566	0.000000
1	0	2.229547	4.590157	0.000000
Rotational constants (GHZ):		34.9706864	0.5795230	0.5700759
Frequencies --	64.2566	75.3419	154.7129	
Frequencies --	192.0337	265.4012	327.2160	
Frequencies --	440.6705	467.6210	483.1677	
Frequencies --	589.6585	597.3827	621.8550	
Frequencies --	653.1269	683.2300	765.7244	
Frequencies --	931.0322	947.0584	1042.0618	
Frequencies --	1095.2415	1293.0951	1364.4651	
Frequencies --	1473.2433	1561.9380	2053.2006	
Frequencies --	2171.3157	2235.6212	3148.3735	
Frequencies --	3153.0660	3257.4429	3421.2528	

CHCCCCCHCHCH⁺ (trans) b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) = -306.826024766 A.U. after 7 cycles

6	0	2.226515	3.768910	0.000000
6	0	1.510397	2.783904	0.000000
6	0	0.723089	1.705929	0.000000
6	0	0.000000	0.706583	0.000000
6	0	-0.839266	-0.376567	0.000000
6	0	-0.362132	-1.686475	0.000000
6	0	-1.200400	-2.785649	0.000000
6	0	-1.910524	-3.772568	0.000000
1	0	2.853330	4.634027	0.000000
1	0	-1.912217	-0.198050	0.000000
1	0	0.710686	-1.863065	0.000000
1	0	-2.537876	-4.637311	0.000000

Rotational constants (GHZ): 35.4657291 0.6164591 0.6059270

Frequencies --	67.1999	69.4509	173.0419
Frequencies --	176.5222	241.8934	334.9869
Frequencies --	435.1909	448.8612	493.4042
Frequencies --	535.1192	567.2680	685.8900
Frequencies --	701.5065	764.3538	767.2367
Frequencies --	814.3824	898.0312	916.2428
Frequencies --	1076.3598	1252.4132	1272.5316
Frequencies --	1344.1530	1543.4489	2077.8798
Frequencies --	2131.2165	2233.9354	3150.6525
Frequencies --	3161.6150	3421.9622	3423.8132

CHCCCCCHCCH⁺ (cis) b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) = -306.823905152 A.U. after 27 cycles

6	0	3.779315	0.650393	0.000000
6	0	2.563542	0.721088	0.000000
6	0	1.231010	0.804550	0.000000
6	0	0.000000	0.876945	0.000000
6	0	-1.361486	1.028742	0.000000
6	0	-2.275523	-0.026811	0.000000
6	0	-1.941158	-1.368697	0.000000
6	0	-1.705518	-2.560812	0.000000
1	0	4.846079	0.591705	0.000000
1	0	-1.754462	2.043002	0.000000
1	0	-3.334258	0.221624	0.000000
1	0	-1.498450	-3.608725	0.000000

Rotational constants (GHZ): 4.6247454 0.9648348 0.7982917

Frequencies --	61.2421	112.1414	157.7938
Frequencies --	222.7400	252.9203	333.2810
Frequencies --	414.1624	461.6327	522.8302
Frequencies --	556.7003	646.5151	685.4543
Frequencies --	700.0870	763.7993	770.5413
Frequencies --	778.0458	787.0161	973.0925
Frequencies --	998.2162	1193.9855	1279.0261
Frequencies --	1455.0071	1507.1473	2079.5451
Frequencies --	2131.5430	2235.1228	3148.6032
Frequencies --	3161.9740	3422.9154	3425.9210

CHCCCCCHCCCH₂⁺ b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) = -306.823306466 A.U. after 2 cycles

6	0	3.447587	2.488053	0.000000
6	0	2.339203	1.983865	0.000000
6	0	1.122350	1.435094	0.000000

6	0	0.000000	0.923454	0.000000
6	0	-1.266454	0.401425	0.000000
6	0	-1.506781	-0.943250	0.000000
6	0	-1.764534	-2.156833	0.000000
6	0	-2.038189	-3.465217	0.000000
1	0	4.418956	2.932390	0.000000
1	0	-2.111962	1.090069	0.000000
1	0	-3.065406	-3.819122	0.000000
1	0	-1.240681	-4.202879	0.000000
Rotational constants (GHZ):		9.2623196	0.6748249	0.6289980
Frequencies --	55.6195	133.0532		160.5766
Frequencies --	188.6044	256.0345		257.2362
Frequencies --	351.4660	375.0767		479.5460
Frequencies --	506.3506	533.0099		564.4701
Frequencies --	685.6635	767.6696		783.8389
Frequencies --	848.7513	898.0566		984.7556
Frequencies --	1029.2025	1262.9967		1325.0068
Frequencies --	1450.1966	1549.2870		2080.0287
Frequencies --	2167.3372	2230.3400		3115.5848
Frequencies --	3124.0540	3220.2322		3425.9780

CHCCHCCCHCCH⁺ (trans) b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =		-306.814386096	A.U. after	3 cycles
6	0	2.060344	-3.503833	0.000000
6	0	1.089352	-2.772421	0.000000
6	0	-0.042960	-1.979883	0.000000
6	0	-0.000553	-0.616439	0.000000
6	0	0.000000	0.616169	0.000000
6	0	0.042860	1.979608	0.000000
6	0	-1.089239	2.772475	0.000000
6	0	-2.059908	3.504315	0.000000
1	0	2.915203	-4.144351	0.000000
1	0	-1.016225	-2.470902	0.000000
1	0	1.016277	2.470297	0.000000
1	0	-2.914629	4.145006	0.000000
Rotational constants (GHZ):		15.0837495	0.6780389	0.6488711
Frequencies --	53.8377	67.4561		126.6431
Frequencies --	218.8236	279.7184		330.6550
Frequencies --	354.6041	385.2015		492.1920
Frequencies --	516.1489	619.0762		699.9611
Frequencies --	700.5532	759.4455		759.8483
Frequencies --	850.2132	868.4116		871.2542
Frequencies --	1047.4177	1115.5775		1265.7892
Frequencies --	1383.3774	1526.2608		2111.2926
Frequencies --	2135.1889	2225.1377		3123.8857
Frequencies --	3124.4924	3424.3618		3424.9703

CHCCHCCCHCCH⁺ (cis) b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =		-306.814236903	A.U. after	2 cycles
6	0	-1.990271	-3.147310	0.000000
6	0	-2.005791	-1.931799	0.000000
6	0	-2.075877	-0.551499	0.000000
6	0	-0.975536	0.254612	0.000000
6	0	0.000000	1.008001	0.000000
6	0	1.057699	1.869297	0.000000
6	0	2.375648	1.453174	0.000000

6	0	3.547874	1.131294	0.000000
1	0	-1.973880	-4.215340	0.000000
1	0	-3.061577	-0.085763	0.000000
1	0	0.855814	2.940639	0.000000
1	0	4.577173	0.845839	0.000000
Rotational constants (GHZ):		5.6948185	0.8049095	0.7052316
Frequencies --	57.9920	89.5472	141.1089	
Frequencies --	193.8389	276.5803	332.2279	
Frequencies --	359.9749	380.9136	478.1347	
Frequencies --	482.4892	643.9240	699.9406	
Frequencies --	700.6529	759.0534	760.1037	
Frequencies --	848.5796	867.9276	874.1968	
Frequencies --	1041.9344	1116.6980	1261.9601	
Frequencies --	1388.5104	1523.8482	2111.3771	
Frequencies --	2137.8265	2220.2653	3123.3581	
Frequencies --	3123.7695	3425.0046	3426.6026	

CHCCHCCCCCH₂⁺ (A) b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =		-306.823131072	A.U. after	2 cycles
6	0	3.972468	0.953705	0.036266
6	0	3.076454	0.135869	0.001421
6	0	2.085755	-0.832027	-0.027247
6	0	0.759891	-0.545524	-0.020967
6	0	-0.461846	-0.317399	-0.012465
6	0	-1.748470	-0.075825	-0.003814
6	0	-2.978661	0.153445	0.004617
6	0	-4.285334	0.396049	0.013520
1	0	4.759490	1.674898	0.063818
1	0	2.388369	-1.880472	-0.046290
1	0	-4.685397	1.318285	-0.401035
1	0	-4.984004	-0.322465	0.435524
Rotational constants (GHZ):		14.4020217	0.6284067	0.6026902
Frequencies --	59.9141	98.1801	142.7941	
Frequencies --	215.5037	261.3976	279.2778	
Frequencies --	348.3162	363.6271	432.2611	
Frequencies --	486.5089	510.4151	563.0292	
Frequencies --	702.8884	716.9561	762.2406	
Frequencies --	847.6559	956.7461	1002.4016	
Frequencies --	1017.5071	1159.7443	1350.4441	
Frequencies --	1437.5443	1589.1991	2036.2613	
Frequencies --	2081.8371	2159.0647	3107.9475	
Frequencies --	3112.6034	3205.4488	3430.2395	

CHCCHCCCCCH₂⁺ (A") b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =		-306.822650196	A.U. after	2 cycles
6	0	-1.478696	-3.807366	0.000000
6	0	-1.644332	-2.603051	0.000000
6	0	-1.878454	-1.240702	0.000000
6	0	-0.880359	-0.311959	0.000000
6	0	0.000000	0.557822	0.000000
6	0	0.937524	1.481384	0.000000
6	0	1.823770	2.357642	0.000000
6	0	2.771617	3.296424	0.000000
1	0	-1.330022	-4.865039	0.000000
1	0	-2.913158	-0.895309	0.000000
1	0	3.824868	3.027063	0.000000

1	0	2.511888	4.352124	0.000000
Rotational constants (GHZ):		14.3551082	0.6284318	0.6020744
Frequencies --	-202.2407	60.6027		99.1222
Frequencies --	143.9742	249.0780		278.6069
Frequencies --	328.9551	343.5397		448.1034
Frequencies --	471.0482	504.5842		574.4902
Frequencies --	698.5260	718.4314		757.5402
Frequencies --	842.9396	971.3489		1015.1974
Frequencies --	1018.6996	1157.9710		1353.7442
Frequencies --	1443.7785	1575.2684		2071.2870
Frequencies --	2133.5357	2221.0495		3114.2753
Frequencies --	3115.0732	3209.2317		3426.9394

CHCCHCCCCCH₂⁺ (A') b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-306.798499490	A.U. after	2 cycles
6	0	-1.366780	-3.852391	0.000000
6	0	-1.559158	-2.662284	0.000000
6	0	-1.827728	-1.285048	0.000000
6	0	-0.896601	-0.350348	0.000000
6	0	0.000000	0.583501	0.000000
6	0	0.868418	1.490094	0.000000
6	0	1.771804	2.430451	0.000000
6	0	2.668492	3.364454	0.000000
1	0	-1.199790	-4.905759	0.000000
1	0	-2.869441	-0.947722	0.000000
1	0	3.732320	3.125226	0.000000
1	0	2.386221	4.417687	0.000000
Rotational constants (GHZ):		14.2693554	0.6285109	0.6019953
Frequencies --	53.3455	100.9730		128.4840
Frequencies --	238.2718	280.9527		303.1357
Frequencies --	359.5455	444.0134		454.1742
Frequencies --	513.8011	519.1417		683.8220
Frequencies --	730.8180	730.9134		748.2314
Frequencies --	870.5392	884.0195		986.0961
Frequencies --	1053.7757	1134.5034		1307.0270
Frequencies --	1372.7054	1735.1100		1949.5078
Frequencies --	2169.7326	2226.1375		3063.4679
Frequencies --	3082.7736	3160.9185		3445.1136

CH₂CCCCCCH₂⁺ b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-306.838063075	A.U. after	4 cycles
6	0	0.000000	0.000000	-0.633065
6	0	0.000000	0.000000	0.633065
6	0	0.000000	0.000000	-1.919538
6	0	0.000000	0.000000	1.919538
6	0	0.000000	0.000000	-3.185459
6	0	0.000000	0.000000	3.185459
6	0	0.000000	0.000000	-4.501876
6	0	0.000000	0.000000	4.501876
1	0	-0.339465	0.868591	-5.062263
1	0	0.339465	-0.868591	-5.062263
1	0	0.339465	0.868591	5.062263
1	0	-0.339465	-0.868591	5.062263
Rotational constants (GHZ):		144.1480563	0.5423923	0.5408964
Frequencies --	61.5898	61.6401		158.2972
Frequencies --	160.6810	281.4787		286.1412

Frequencies --	356.1345	413.4825	489.2075
Frequencies --	494.2018	518.9990	538.0818
Frequencies --	558.8867	608.6013	942.6977
Frequencies --	942.8163	943.4281	976.6546
Frequencies --	976.7152	1300.8559	1406.9030
Frequencies --	1456.0537	1667.7047	1694.6606
Frequencies --	2039.5608	2124.1279	3106.7429
Frequencies --	3107.6732	3195.1234	3195.1322

CH₂C(CCH)CCCCH⁺ b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =	-306.808316143	A.U. after	3 cycles	
6	0	-2.404138	0.412046	0.000000
6	0	-1.234603	-0.347846	0.000000
6	0	-1.287515	-1.758367	0.000000
6	0	-1.338722	-2.965146	0.000000
6	0	0.000000	0.299571	0.000000
6	0	1.091370	0.862548	0.000000
6	0	2.279830	1.477167	0.000000
6	0	3.361317	2.034664	0.000000
1	0	-3.372991	-0.073959	0.000000
1	0	-2.357863	1.494657	0.000000
1	0	-1.385937	-4.031724	0.000000
1	0	4.311550	2.523204	0.000000
Rotational constants (GHZ):	5.3548728	0.9331251	0.7946513	
Frequencies --	72.1531	106.1042	176.2553	
Frequencies --	236.8214	244.5769	308.7926	
Frequencies --	441.0491	493.6996	501.9400	
Frequencies --	559.9975	561.3889	617.4728	
Frequencies --	672.2873	695.8947	733.8174	
Frequencies --	764.9292	774.0237	917.1409	
Frequencies --	992.3925	1091.4036	1351.7657	
Frequencies --	1396.2638	1506.5683	2091.4892	
Frequencies --	2162.4831	2268.7068	3151.5011	
Frequencies --	3267.6498	3424.1444	3435.0602	

CH₂CCC(CCH)CCH⁺ b3lyp/6-311++g**

SCF Done: E(UB+HF-LYP) =	-306.803891208	A.U. after	2 cycles	
6	0	0.000000	0.000000	3.400110
6	0	0.000000	0.000000	2.057793
6	0	0.000000	0.000000	0.821822
6	0	0.000000	0.000000	-0.561110
6	0	0.000000	1.216436	-1.256766
6	0	0.000000	2.264938	-1.862314
6	0	0.000000	-1.216436	-1.256766
6	0	0.000000	-2.264938	-1.862314
1	0	0.000000	-0.933108	3.956553
1	0	0.000000	0.933108	3.956553
1	0	0.000000	3.188988	-2.397917
1	0	0.000000	-3.188988	-2.397917
Rotational constants (GHZ):	2.7939195	1.3822590	0.9247498	
Frequencies --	82.2357	120.9725	126.5341	
Frequencies --	177.4219	239.4722	259.7852	
Frequencies --	339.3433	354.2819	463.0484	
Frequencies --	533.7928	557.9196	627.2990	
Frequencies --	668.3243	722.5990	723.7594	
Frequencies --	766.1702	766.5053	973.5124	

Frequencies --	1028.0779	1074.6481	1261.9551
Frequencies --	1408.0516	1504.7162	2126.6886
Frequencies --	2179.1208	2184.5926	3123.9085
Frequencies --	3222.3585	3428.7464	3430.6272

CHCC(CCH)CHCCH⁺ b3lyp/6-311++g**

SCF Done:	E(UB+HF-LYP) =	-306.806064018	A.U. after	2 cycles
6	0	-0.423574	3.084576	0.000000
6	0	-0.229574	1.888808	0.000000
6	0	0.000000	0.507304	0.000000
6	0	1.317044	0.030239	0.000000
6	0	2.464283	-0.354592	0.000000
6	0	-1.112551	-0.370361	0.000000
6	0	-1.011298	-1.741504	0.000000
6	0	-0.976613	-2.959141	0.000000
1	0	-0.595084	4.139144	0.000000
1	0	3.476376	-0.696024	0.000000
1	0	-2.105264	0.072372	0.000000
1	0	-0.942326	-4.027474	0.000000
Rotational constants (GHZ):		3.4001102	1.4728758	1.0276943
Frequencies --	98.1032	110.0863	133.8647	
Frequencies --	213.1568	240.2540	328.7108	
Frequencies --	418.9057	428.0551	517.3170	
Frequencies --	599.6576	632.9213	699.0376	
Frequencies --	724.2808	725.4277	760.2152	
Frequencies --	771.7046	773.6583	796.5803	
Frequencies --	888.5533	1099.7311	1221.1141	
Frequencies --	1350.2798	1472.4974	2117.4876	
Frequencies --	2131.4573	2186.8416	3164.9195	
Frequencies --	3418.5122	3426.0798	3429.2055	