

Supplementary Materials

to the article

Polarizability of Kekulene, Septulene and Nearest Non-Planar Polycyclic Aromatic Hydrocarbons

Timur Lukmanov ¹, Arslan F. Akhmetov ² and Denis Sh. Sabirov ^{1,*}

¹ Institute of Petrochemistry and Catalysis UFRC RAS, 450075 Ufa, Russia

² Department of Oil and Gas Technology, Ufa State Petroleum Technological University, 450000 Ufa, Russia

* Correspondence: diozno@mail.ru

Computational results

The method is PBE/3 ζ . The coordinates and polarizability values are in Å and atomic units, respectively.

[11]helicene

Energy

E = -1766.979941 E0 = -1766.430329

ZPVE = 0.549612 a.u. = 344.8867 kcal/mol

H298 = 365.5537 kcal/mol

Dipole Polarizability

616.695625

-2.148694 644.130037

-9.965852 0.644019 362.07324

Coordinates

6	2.407872320	-1.785598530	-2.422098790
6	3.580952690	-0.981886540	-2.517909040
6	0.248506440	-2.286967440	1.061572760
6	1.523579210	-2.776803160	1.470506020
6	0.118362300	-0.943626180	0.595135150
6	1.190188080	-0.016395050	0.915071070
6	2.486162610	-0.573170080	1.149646610
6	2.626117500	-1.968524310	1.409544950
6	1.047635800	1.418913380	1.074275170
6	2.216868710	2.224438820	0.954380970
6	3.506839000	1.618431250	0.954490200
6	3.634503340	0.270456270	1.152189510
6	-0.174953760	2.087975680	1.496720220
6	-0.250539320	3.518748510	1.435666930
6	0.904456010	4.275003950	1.067512550
6	2.107380040	3.649904460	0.903335910
6	-1.256529620	1.407236480	2.111620720
6	-2.387772710	2.079066030	2.541141700
6	-2.501565730	3.473549070	2.370549650
6	-1.438529800	4.178611110	1.839024060
6	-0.902279890	-3.128345730	1.132462940
1	1.606715930	-3.819425110	1.781321310
6	-1.092985530	-0.602699770	-0.125623670
1	3.622088560	-2.360656630	1.622147590
1	4.386175590	2.260409020	0.879052720
1	4.616446810	-0.187829940	1.281116080
1	0.824005880	5.361763800	1.006426940
1	3.017173150	4.228608210	0.733194460
1	-1.181933620	0.336402900	2.280670860
1	-3.191968310	1.522058680	3.023199130
1	-3.403585930	3.994644780	2.693267410
1	-1.480735770	5.266660360	1.758296650
6	-2.259886980	-1.378422420	0.142769830
6	-2.135391940	-2.646703220	0.784761480
1	-0.785313070	-4.138743180	1.527405170
6	-1.216984500	0.484966460	-1.073047220

6	-3.544559600	-0.873760820	-0.216545920
1	-3.035773350	-3.242810030	0.941200380
6	-2.509628440	1.063363060	-1.246032760
6	-3.666095580	0.362552230	-0.792548520
6	-0.134609570	1.009786150	-1.883042890
1	-4.426243330	-1.466771940	0.031841530
6	-2.638410380	2.331553790	-1.887438510
1	-4.647427980	0.805949280	-0.968934210
6	-1.528138440	3.001251450	-2.325864920
6	-0.256182230	2.354028890	-2.349262270
6	1.043413730	0.263257500	-2.290311760
1	-3.631670290	2.775539350	-1.969995420
1	-1.604042670	4.015072830	-2.722063910
6	0.889289480	3.038152360	-2.852009420
6	2.107809990	2.416116980	-2.881468470
6	1.119543270	-1.177396530	-2.446739940
1	0.781205160	4.078885760	-3.161504150
1	3.009255200	2.960530400	-3.167677190
6	2.212228830	1.017881920	-2.620466060
6	3.476642010	0.367946300	-2.716635490
6	2.531187510	-3.209949730	-2.371121220
1	4.554480870	-1.475130990	-2.514506430
6	-0.009742860	-2.035411530	-2.777445370
1	4.360168160	0.976004230	-2.917907180
6	1.434166910	-4.019727580	-2.445323470
6	0.148480640	-3.459520500	-2.718595700
1	3.531968640	-3.635193170	-2.275378230
6	-1.229948810	-1.539817440	-3.303511440
1	1.532773390	-5.104988180	-2.384228100
6	-0.946870140	-4.302858480	-3.032204260
6	-2.146320780	-3.779737800	-3.476513480
6	-2.269472320	-2.386182240	-3.648043320
1	-1.340183700	-0.471932570	-3.471844060
1	-0.808950590	-5.383169470	-2.954370700
1	-2.976076670	-4.440027440	-3.731150860
1	-3.186717040	-1.967685460	-4.063850660

[11]helicene-exp

Energy

$$E = -1767.046503 \quad E0 = -1766.493489$$

$$ZPVE = 0.553014 \text{ a.u.} = 347.0214 \text{ kcal/mol}$$

$$H298 = 367.7624 \text{ kcal/mol}$$

Dipole Polarizability

$$651.805623$$

$$-261.744350 \quad 629.877925$$

$$202.954160 \quad 175.382275 \quad 803.157349$$

Coordinates

1	-5.751135360	1.030349440	-3.173881830
6	-5.217221750	1.424188660	-2.308592540
1	-3.738395050	-0.161901010	-2.293804190

6	-4.084778070	0.752951540	-1.812355240
6	-5.649391140	2.584229210	-1.688153640
6	-4.972044370	3.106478090	-0.561488670
6	-3.816215240	2.432218050	-0.056760170
6	-3.401109460	1.250446410	-0.712320970
6	-5.442670480	4.301555510	0.081462140
6	-4.815611760	4.805614610	1.181510970
6	-3.654181860	4.165546480	1.729714220
6	-3.129478180	2.981269430	1.109484580
6	-1.977838700	2.396668210	1.660717890
6	-3.024963030	4.670404940	2.876273690
6	-1.894287240	4.064503020	3.434419950
6	-1.335239050	2.902850490	2.798475170
6	-1.303106900	4.578425540	4.640230450
6	-0.226796050	3.971161320	5.210819830
6	0.382626990	2.817140180	4.607609840
6	-0.137611470	2.289810220	3.377403810
6	0.528951430	1.206121980	2.786691700
6	1.652156320	0.593484630	3.362888320
6	2.115255560	1.082035010	4.631336280
6	1.482097560	2.190904530	5.206486980
6	2.359941570	-0.525100050	2.738335510
6	3.418312140	-1.166055840	3.467225620
6	3.814304720	-0.661557040	4.753292530
6	3.207393160	0.428561470	5.298777520
6	2.062735160	-0.995582290	1.450249500
6	2.729706400	-2.079133430	0.859763620
6	3.733380310	-2.758915520	1.629567240
6	4.059567960	-2.275586350	2.902415380
6	2.450207930	-2.544046490	-0.500799520
6	3.127351950	-3.716293320	-0.984280670
6	4.089764670	-4.385452600	-0.151506500
6	4.392563750	-3.917188850	1.090164880
6	1.565682450	-1.885894750	-1.365730440
6	1.302967710	-2.328329700	-2.672317200
6	1.954882950	-3.523570560	-3.129372380
6	2.851072130	-4.180590300	-2.274671370
6	0.406249660	-1.621571450	-3.583135320
6	0.184199920	-2.156328590	-4.890834510
6	0.842875930	-3.368345040	-5.291111360
6	1.694576940	-4.020205080	-4.450251040
1	-6.528827260	3.113832390	-2.059616650
1	-2.530926890	0.704161120	-0.349847470
1	-6.325597490	4.795049790	-0.328763360
1	-5.187353340	5.708714070	1.668827540
1	-1.577294540	1.500022040	1.193103120
1	-3.438870380	5.560086940	3.356734380
1	-1.752356130	5.460764150	5.099366290
1	0.202393760	4.355693490	6.137705210
1	0.153532780	0.817138090	1.842558080
1	1.855480970	2.576840530	6.157987070
1	4.629099170	-1.164941390	5.276604210
1	3.528362000	0.818247000	6.266386620
1	1.285247320	-0.490889280	0.880646200
1	4.845244500	-2.777469090	3.472082030
1	4.587437850	-5.271931270	-0.548529270
1	5.139807270	-4.419260050	1.707202420
1	1.073385450	-0.981193840	-1.016105360

1	3.359708590	-5.078682290	-2.633021790
1	0.650713390	-3.753344020	-6.294220700
1	2.197966480	-4.935132840	-4.767684070
6	-0.678520640	-1.480275690	-5.785031420
6	-1.308092040	-0.302508590	-5.419108450
6	-1.088298970	0.231691260	-4.136317710
6	-0.250874830	-0.417598940	-3.240703880
1	-0.836389940	-1.904671830	-6.778429930
1	-1.967532850	0.210478620	-6.119732720
1	-1.578796320	1.159313040	-3.840270460
1	-0.097773940	0.024952090	-2.256971890

Kekulene

Energy

$E = -1842.022169$ $E_0 = -1841.476059$

$ZPVE = 0.546110 \text{ a.u.} = 342.6895 \text{ kcal/mol}$

$H_{298} = 362.8681 \text{ kcal/mol}$

Dipole Polarizability

1009.395977

0.120997 1008.834124

4.303218 -21.663623 232.507153

Coordinates

6	-4.145612880	-4.718428490	0.118165390
6	-2.975038090	-5.425973430	0.138382850
6	-1.692317580	-4.770056010	0.126208540
6	-4.160503140	-3.278268820	0.079932810
6	-2.907561550	-2.583822350	0.063763430
6	-1.659179790	-3.338243260	0.091569010
6	-0.474290420	-5.474679400	0.150962260
6	0.771302050	-4.819613480	0.141289820
6	0.796214160	-3.387619950	0.106561460
6	-0.418081070	-2.699728960	0.087535480
6	2.026359850	-5.526569420	0.168941850
6	3.224599040	-4.866667530	0.163170320
6	3.297844120	-3.428292430	0.125454980
6	2.074154830	-2.684038690	0.094311770
6	2.141942160	-1.290613330	0.049854020
6	4.517433490	-2.725973670	0.113798560
6	4.572919810	-1.320303860	0.073766100
6	3.344649960	-0.583041820	0.042734800
6	5.813054320	-0.587169210	0.058306150
6	5.840799630	0.779803390	0.014461930
6	4.631409550	1.562209480	-0.015147970
6	3.374205890	0.874947820	0.001870340
6	2.201091030	1.630310330	-0.019170910
6	2.189922750	3.025297730	-0.064905990
6	3.442822070	3.719724640	-0.082110240
6	4.632967550	2.968945820	-0.056018150
6	0.941544310	3.779684650	-0.092735000
6	0.974661160	5.211475510	-0.128614430

6	2.257366780	5.867389800	-0.141633510
6	3.427943370	5.159847490	-0.121265540
6	-0.299572760	3.141186680	-0.087920460
6	-1.513853210	3.829066730	-0.107579530
6	-1.488961710	5.261022960	-0.143500660
6	-0.243375610	5.916078210	-0.153881150
6	-2.791799090	3.125467450	-0.094972030
6	-4.015519050	3.869678870	-0.127480800
6	-3.942265570	5.308038760	-0.166106100
6	-2.744029010	5.967943460	-0.172008110
6	-2.859570460	1.732129900	-0.049567160
6	-4.062608520	1.024519680	-0.043329730
6	-5.290595480	1.761668050	-0.075712760
6	-5.235096400	3.167376900	-0.116095080
6	-4.092157680	-0.433501480	-0.002777170
6	-5.349079580	-1.120733480	0.013264290
6	-6.558531640	-0.338401230	-0.017178480
6	-6.530788040	1.028561100	-0.061060200
6	-2.918699830	-1.188872200	0.018659990
6	-5.350633090	-2.527531670	0.053497960
1	-5.101579520	-5.245372230	0.129588270
1	-2.997730420	-6.517032620	0.165728110
1	-0.496433350	-6.566747730	0.179682420
1	-0.396207660	-1.615334100	0.073646640
1	2.004839760	-6.617650800	0.196355440
1	4.158389540	-5.431631140	0.186086450
1	1.213856960	-0.730258760	0.014169860
1	5.452430430	-3.291000160	0.135241450
1	6.747484400	-1.151076350	0.081230260
1	6.797351030	1.305673590	0.002334420
1	1.250864620	1.107766230	0.005972170
1	5.590116960	3.495902010	-0.066795320
1	2.280055010	6.958426700	-0.169826120
1	4.383912830	5.686771430	-0.133399840
1	-0.321483870	2.056803080	-0.073227000
1	-0.221232340	7.008118260	-0.183659650
1	-4.876051780	5.872974570	-0.189843460
1	-2.722507490	7.059005000	-0.200206130
1	-1.931587060	1.171727300	-0.012424400
1	-6.170084320	3.732378010	-0.138472680
1	-7.515062090	-0.864320870	-0.005701300
1	-7.465195790	1.592467000	-0.084818420
1	-1.968543530	-0.666208450	-0.006060580
1	-6.307776510	-3.054510680	0.063425220

[12]helicene

Energy

$$E = -1920.473679 \quad E_0 = -1919.878970$$

$$ZPVE = 0.594709 \text{ a.u.} = 373.1858 \text{ kcal/mol}$$

$$H_{298} = 395.5848 \text{ kcal/mol}$$

Dipole Polarizability

$$663.218848$$

1.73149 664.720861

-41.864468 -19.010896 419.771788

Coordinates

6	2.524570330	-1.698583020	-2.511540370
6	3.699637400	-0.897244360	-2.605328400
6	0.398261850	-2.267967670	0.914517160
6	1.673898930	-2.767628380	1.312679860
6	0.264624870	-0.906208050	0.509625510
6	1.331011610	0.008334460	0.872511800
6	2.628239010	-0.547545310	1.091284820
6	2.772937560	-1.952060710	1.297798310
6	1.175611040	1.439004330	1.076308540
6	2.341489410	2.251375780	0.914973030
6	3.635008910	1.651153830	0.924912940
6	3.771548270	0.303770810	1.120331690
6	-0.042263250	2.108779030	1.494877260
6	-0.159540620	3.505481600	1.237897030
6	0.981328060	4.257938800	0.832988420
6	2.212711710	3.664000510	0.778270480
6	-1.089668210	1.494736150	2.299178700
6	-2.323549290	2.197267750	2.502290640
6	-2.473055020	3.527773610	2.003797030
6	-1.404456480	4.176107740	1.453923130
6	-0.751220550	-3.112363370	0.952078390
1	1.760868150	-3.822278080	1.578761580
6	-0.953297100	-0.529527810	-0.176780310
1	3.768825490	-2.348074510	1.503273580
1	4.509662710	2.298326690	0.840640730
1	4.756101300	-0.149434190	1.246792110
1	0.865837720	5.328677390	0.656208310
1	3.113475610	4.253502740	0.599196250
6	-0.902785680	0.290723870	3.025139960
6	-3.349695550	1.607224410	3.281899170
1	-3.425988650	4.039923240	2.148440960
1	-1.476015300	5.228275270	1.172089600
6	-2.118966840	-1.311669190	0.074155240
6	-1.988275470	-2.611064770	0.647924390
1	-0.630636210	-4.142207680	1.291977520
6	-1.078821320	0.579980180	-1.098524630
6	-3.405231310	-0.787604110	-0.250803730
1	-2.887591080	-3.213099780	0.786317430
6	-2.371413190	1.164177300	-1.253826690
6	-3.526080660	0.462648720	-0.795225100
6	-0.004479540	1.101763200	-1.922415550
1	-4.287435080	-1.380857420	-0.005580140
6	-2.504795930	2.430332340	-1.897651120
1	-4.506750140	0.915458110	-0.949830040
6	-1.399430850	3.093796720	-2.357253870
6	-0.129368100	2.444249090	-2.393351100
6	1.167357810	0.353082310	-2.345216980
1	-3.497735800	2.877209970	-1.968500560
1	-1.478549550	4.104940740	-2.759956650
6	1.010280910	3.124652380	-2.913931530
6	2.228682400	2.503083110	-2.951601670
6	1.237724530	-1.086568360	-2.516704670
1	0.898794590	4.163658340	-3.228202620

1	3.127529370	3.045739300	-3.249179030
6	2.334483500	1.105976650	-2.686086480
6	3.597126500	0.454100650	-2.793600560
6	2.644806010	-3.123745210	-2.484982890
1	4.671728610	-1.393275420	-2.612962540
6	0.103207530	-1.936414350	-2.850819440
1	4.480318930	1.061522970	-2.998461590
6	1.545688370	-3.929753620	-2.567947790
6	0.259528510	-3.361885830	-2.821745940
1	3.645231550	-3.552817950	-2.403214630
6	-1.122383610	-1.429340370	-3.353197960
1	1.642661130	-5.016169100	-2.527989400
6	-0.839219480	-4.197432210	-3.143487690
6	-3.154922620	0.397698010	3.921174050
6	-1.904030180	-0.242959370	3.817814940
1	-4.289057540	2.151095100	3.400201930
1	-3.946574890	-0.037949980	4.531771180
6	-2.042176750	-3.664337500	-3.565723370
6	-2.166039510	-2.267533450	-3.705120270
1	-1.234438270	-0.358039110	-3.496297870
1	-0.701724660	-5.279239290	-3.088921910
1	-2.874975150	-4.318502120	-3.826197150
1	-3.087692250	-1.839328020	-4.100760080
1	-1.716197930	-1.163448310	4.371669750
1	0.061148610	-0.209166920	2.984440630

[12]helicene-exp

Energy

$$E = -1920.545798 \quad E0 = -1919.947468$$

$$ZPVE = 0.598330 \text{ a.u.} = 375.4575 \text{ kcal/mol}$$

$$H298 = 397.9545 \text{ kcal/mol}$$

Dipole Polarizability

$$707.413182$$

$$-235.662434 \quad 701.836676$$

$$246.222780 \quad 211.717185 \quad 871.448508$$

Coordinates

6	-5.834978150	-0.544913140	-3.719655960
6	-6.194246740	0.678880660	-3.198740920
6	-5.450389080	1.261271700	-2.132574910
6	-4.713782810	-1.246087340	-3.201016090
6	-3.970357830	-0.710407650	-2.172294220
6	-4.310566740	0.552769920	-1.608712320
6	-5.789515600	2.500505260	-1.558446010
6	-5.058907520	3.052370390	-0.504551400
6	-3.905563880	2.353462930	0.016376610
6	-3.569746020	1.125084200	-0.552992020
6	-5.456445020	4.306536730	0.079961990
6	-4.782517140	4.841891830	1.133110820
6	-3.629989660	4.186478110	1.693061950
6	-3.159672260	2.954107360	1.128112870

6	-2.009518450	2.369945940	1.676162370
6	-2.963948920	4.727768020	2.798382990
6	-1.839550170	4.114993560	3.367436730
6	-1.322727310	2.915597890	2.772536780
6	-1.219619000	4.659181700	4.544077760
6	-0.155468470	4.041776190	5.128318880
6	0.418405100	2.853974480	4.558702240
6	-0.126020610	2.302408500	3.349180150
6	0.520783040	1.197598920	2.775003500
6	1.640563780	0.583125370	3.354627110
6	2.114220510	1.083655600	4.614800570
6	1.507480320	2.217928290	5.167822370
6	2.336314600	-0.548680980	2.741215850
6	3.376213620	-1.205225230	3.482336560
6	3.773703950	-0.696262850	4.766411850
6	3.190454790	0.415590500	5.294003920
6	2.048839290	-1.011975560	1.448863220
6	2.706430770	-2.105161880	0.866051120
6	3.681834030	-2.807708160	1.651239230
6	4.000713660	-2.329898390	2.928388830
6	2.446139560	-2.555151850	-0.502709640
6	3.103314110	-3.741595400	-0.978495540
6	4.030791620	-4.438079220	-0.128477030
6	4.322325180	-3.980342810	1.120075400
6	1.601832950	-1.866268320	-1.383451020
6	1.359224450	-2.291394710	-2.699353490
6	1.987354010	-3.502118350	-3.149278650
6	2.844319150	-4.189886370	-2.278278070
6	0.505943630	-1.551579770	-3.625382670
6	0.298410780	-2.070925340	-4.941490490
6	0.931757240	-3.298545750	-5.335285470
6	1.744468320	-3.981096800	-4.479975420
1	-6.412744970	-0.982995200	-4.534304150
1	-7.056950850	1.218880760	-3.593349370
1	-6.657332800	3.043261740	-1.940742320
1	-2.717211690	0.559065620	-0.176172290
1	-6.328260580	4.813809560	-0.337054320
1	-5.104638530	5.785351580	1.577338610
1	-1.644404370	1.439239590	1.246944350
1	-3.342098740	5.651846660	3.242004240
1	-1.639027780	5.570381680	4.974161450
1	0.292113280	4.446404390	6.037769820
1	0.133085180	0.795667330	1.841162570
1	1.893834380	2.618024740	6.108219260
1	4.574157870	-1.211150890	5.300567040
1	3.517459520	0.811398360	6.257108180
1	1.290227170	-0.491035590	0.868486850
1	4.769307120	-2.846194110	3.508396580
1	4.514048390	-5.335547250	-0.518605570
1	5.046043670	-4.502115830	1.748714000
1	1.129292320	-0.948869800	-1.039780210
1	3.336813270	-5.098958070	-2.631517780
1	0.752815190	-3.670567640	-6.345769010
1	2.228972310	-4.907605610	-4.793123300
6	-0.525113820	-1.364340670	-5.849094660
6	-1.130795940	-0.172867220	-5.487206550
6	-0.924540550	0.345728890	-4.196125430
6	-0.123808910	-0.331557470	-3.288433260

1	-4.440623580	-2.212930180	-3.624552440
1	-3.105117740	-1.246785530	-1.779261000
1	-0.672758880	-1.776762950	-6.849118300
1	-1.763152690	0.361681840	-6.196362660
1	-1.398554530	1.282834310	-3.903326990
1	0.019286020	0.099309330	-2.298090430

[13]circulene

Energy

E = -1995.499558 E0 = -1994.909429

ZIPVE = 0.590129 a.u. = 370.3115 kcal/mol

H298 = 392.1335 kcal/mol

Dipole Polarizability

1087.760948

-35.637678 1135.064686

-9.393373 -5.070336 271.399082

Coordinates

6	-7.541327700	1.102963310	0.253250010
6	-7.338578950	2.452927940	0.334658760
6	-6.038886230	3.042866170	0.106283870
6	-4.978833360	2.194249940	-0.331198750
6	-5.743621670	4.390400650	0.355504260
6	-4.429708210	4.891975360	0.278684200
6	-3.346389820	3.996169860	-0.022095930
6	-3.668744410	2.680259360	-0.356492860
6	-1.964082170	4.470940320	0.035333340
6	-1.753121620	5.874120650	0.233669460
6	-2.869419030	6.751921630	0.461331500
6	-4.147115740	6.280344670	0.514920500
6	-0.444433490	6.362608510	0.213013260
6	0.666007190	5.525717070	0.058944380
6	0.485320910	4.097147590	-0.042482530
6	-0.839205070	3.623817390	-0.072959360
6	1.688250760	3.239377630	-0.102882570
6	2.966493310	3.899576590	-0.146796490
6	3.076935090	5.330544650	-0.111058250
6	1.974692660	6.111616790	0.009996920
6	4.133899640	3.137173050	-0.183710770
6	4.124197170	1.742904820	-0.146291100
6	2.867596970	1.042389430	-0.102544640
6	1.686200560	1.823246500	-0.090801760
6	2.917770150	-0.434180460	-0.042057840
6	4.208204980	-1.072953910	0.060310670
6	5.419706610	-0.305967540	0.011857990
6	5.377888370	1.044261320	-0.109802490
6	1.791388710	-1.276573800	-0.073251020
6	1.875754020	-2.682228230	0.035173370
6	3.161671920	-3.281686210	0.234807050
6	4.291986300	-2.460876230	0.214727230
6	0.716177120	-3.571956180	-0.022900320

6	0.864067200	-4.969804750	0.278238380
6	2.177246970	-5.501424780	0.515406210
6	3.276334340	-4.697101660	0.462706110
6	-0.558610800	-3.113534280	-0.357786410
6	-1.687642220	-3.936884340	-0.332624470
6	-1.566181440	-5.289338590	0.104902960
6	-0.279972970	-5.787801150	0.354556200
6	-3.005964520	-3.389733840	-0.601931760
6	-4.184698110	-4.095271640	-0.158721090
6	-4.013184110	-5.469565780	0.252184320
6	-2.776030820	-6.046572660	0.333392510
6	-3.150690930	-2.135259330	-1.158958620
6	-4.341583430	-1.412448370	-0.998638010
6	-5.500846970	-2.034846500	-0.408260450
6	-5.410918870	-3.418857570	-0.101697010
6	-4.285833050	-0.020414360	-1.158313230
6	-5.251299230	0.793216520	-0.600783110
6	-6.490715740	0.200608490	-0.157759180
6	-6.604593460	-1.195186190	-0.101238460
1	-8.514610950	0.681470240	0.511526450
1	-8.154402540	3.107567950	0.647014370
1	-6.547396780	5.070091280	0.648283270
1	-2.862961080	1.993601580	-0.600979180
1	-2.663192790	7.812206120	0.618116990
1	-4.980221120	6.954096030	0.722525110
1	-0.277322710	7.436240070	0.326864240
1	-1.002544810	2.551216140	-0.170945380
1	4.075288600	5.768716780	-0.156222040
1	2.056850330	7.198195760	0.067012120
1	5.096164630	3.653709550	-0.209867900
1	0.726750790	1.308196340	-0.031784020
1	6.370722660	-0.837824490	0.069615460
1	6.294784160	1.634196800	-0.154768310
1	0.807219940	-0.820066650	-0.172086620
1	5.279067210	-2.914849820	0.329407050
1	2.278262460	-6.568069920	0.723182350
1	4.273884530	-5.111067360	0.620299120
1	-0.685590110	-2.062511150	-0.602356480
1	-0.157700530	-6.833289170	0.647425550
1	-4.902297560	-6.047829810	0.510507380
1	-2.681177560	-7.088298320	0.645636040
1	-2.294826120	-1.614763640	-1.587196460
1	-6.292517330	-3.944972660	0.271509730
1	-3.379175370	0.405439690	-1.586608930
1	-7.530194580	-1.639370400	0.271945970

[13]helicene

Energy

$$E = -2073.966964 \quad E0 = -2073.327277$$

$$ZPVE = 0.639688 \text{ a.u.} = 401.4102 \text{ kcal/mol}$$

$$H298 = 425.5488 \text{ kcal/mol}$$

Dipole Polarizability

690.751465

1.970171 697.514448

-32.189521 -55.242445 483.434429

Coordinates

6	0.699808130	-2.606477710	-3.426148260
6	1.878075170	-1.812134900	-3.535758440
6	-1.383554310	-3.157342170	0.026752300
6	-0.096183440	-3.672973890	0.359467670
6	-1.519761580	-1.792063150	-0.362981620
6	-0.431760360	-0.892751480	-0.037706580
6	0.867990060	-1.459779990	0.123093750
6	1.009491010	-2.867969610	0.300589870
6	-0.572153120	0.531282500	0.205333520
6	0.587569950	1.346179580	0.028843180
6	1.879345150	0.741533490	-0.011814340
6	2.015184680	-0.611750150	0.141085880
6	-1.782505900	1.189926210	0.668703470
6	-1.922489780	2.581865400	0.371300280
6	-0.784187580	3.344008490	-0.025626560
6	0.452488460	2.761298370	-0.082381030
6	-2.826236920	0.578291460	1.470776390
6	-4.107805390	1.201363910	1.489572260
6	-4.275251980	2.512629180	0.956834450
6	-3.190968990	3.216274270	0.508129110
6	-2.539300090	-3.991554090	0.095765990
1	-0.007293580	-4.731258970	0.609811960
6	-2.747351180	-1.405480240	-1.026460300
1	2.009901430	-3.276338000	0.453543740
1	2.754148730	1.387451540	-0.103436600
1	3.001495690	-1.071017760	0.225234600
1	-0.911599260	4.411875580	-0.211083910
1	1.347992940	3.357852070	-0.264111930
6	-2.621105670	-0.536598350	2.385633300
6	-5.219592580	0.545532300	2.105971140
1	-5.264892100	2.971047360	0.996982770
1	-3.281646480	4.265071430	0.220374400
6	-3.912278350	-2.184843440	-0.762326270
6	-3.778645190	-3.481955880	-0.182663150
1	-2.419051000	-5.021709950	0.434369930
6	-2.876784500	-0.306582160	-1.961307330
6	-5.199267990	-1.668233660	-1.094744320
1	-4.678887550	-4.078068200	-0.026003200
6	-4.171091830	0.271732590	-2.125750320
6	-5.323731400	-0.427622730	-1.659910430
6	-1.806271920	0.207751380	-2.795584990
1	-6.079959910	-2.260526390	-0.841510860
6	-4.308169530	1.528870060	-2.786392160
1	-6.306088870	0.018498460	-1.823997670
6	-3.204367540	2.192996040	-3.248787710
6	-1.932194990	1.546880930	-3.276128590
6	-0.642171750	-0.547029150	-3.229744150
1	-5.302978260	1.970371480	-2.865411790
1	-3.286121440	3.199844240	-3.661651730
6	-0.793162650	2.223626940	-3.802747400

6	0.423174790	1.598401750	-3.846523940
6	-0.583214040	-1.986478850	-3.406359250
1	-0.903910250	3.261966370	-4.119645850
1	1.321823180	2.137526250	-4.151062800
6	0.524558350	0.200062970	-3.584782640
6	1.781199140	-0.459013550	-3.714238430
6	0.811967660	-4.032372380	-3.407489840
1	2.846764360	-2.314185240	-3.562758990
6	-1.728237900	-2.828953660	-3.724383710
1	2.664851050	0.143857820	-3.930353980
6	-0.293098690	-4.831650950	-3.472709310
6	-1.580150900	-4.255445640	-3.701609630
1	1.811148380	-4.467454340	-3.344542260
6	-2.957734740	-2.313694780	-4.208481330
1	-0.202007170	-5.918718940	-3.437175260
6	-2.689044190	-5.083663520	-4.006718610
6	-5.065047690	-0.634698560	2.774839060
6	-3.757672880	-1.168652040	2.990646490
6	-1.339015440	-0.942392800	2.836275970
1	-6.200268430	1.019212790	2.031438900
1	-5.920979880	-1.140472350	3.225220780
6	-3.568575540	-2.256013450	3.879790940
6	-1.180562040	-1.976756900	3.742257120
6	-2.300940220	-2.669179700	4.243174150
1	-0.460159300	-0.407244480	2.487385310
1	-4.451266350	-2.737156290	4.305876880
1	-0.178334620	-2.249695040	4.074548270
1	-2.168671310	-3.496691160	4.941073970
6	-3.895163590	-4.542465300	-4.409274160
6	-4.011922600	-3.144840050	-4.545699840
1	-3.064929520	-1.241744210	-4.349656060
1	-2.557303830	-6.166371200	-3.955949170
1	-4.736150040	-5.190983820	-4.657276800
1	-4.936479800	-2.710229380	-4.927374240

[13]helicene-exp

Energy

E = -2074.050594 E0 = -2073.406860

ZPVE = 0.643734 a.u. = 403.9494 kcal/mol

H298 = 428.2465 kcal/mol

Dipole Polarizability

727.092356

-239.613461 784.174951

246.721796 225.249818 902.734886

Coordinates

6	-5.866874180	-0.586208950	-3.705506440
6	-6.142062010	0.662029190	-3.231848410
6	-5.394043130	1.220727430	-2.142036930
6	-4.829216490	-1.392253510	-3.125238610
6	-4.055626050	-0.882797700	-2.036192020

6	-4.331362250	0.463287260	-1.541759410
6	-5.691607190	2.495376760	-1.638825250
6	-4.981357000	3.062097480	-0.574816230
6	-3.887113780	2.331976200	0.004096470
6	-3.604427680	1.053659350	-0.495539440
6	-5.346171350	4.347993530	-0.044262090
6	-4.688374250	4.883813840	1.020630100
6	-3.577163530	4.202977270	1.628339720
6	-3.135799710	2.941491360	1.103158790
6	-2.002471890	2.345938490	1.675183090
6	-2.918372800	4.747451920	2.738050630
6	-1.819516410	4.118097570	3.337038210
6	-1.315080640	2.902505970	2.763697620
6	-1.208369010	4.659725770	4.520016870
6	-0.163922100	4.028754740	5.125656820
6	0.406964940	2.833195790	4.568000770
6	-0.126825860	2.285490790	3.352593030
6	0.524824250	1.184582180	2.778376760
6	1.639063480	0.567535130	3.364983050
6	2.096116150	1.056251710	4.635568560
6	1.485334490	2.189274460	5.188345520
6	2.345535440	-0.553417450	2.745457840
6	3.376009360	-1.218793050	3.491272140
6	3.753410320	-0.726427850	4.787971950
6	3.162752640	0.379239680	5.321273770
6	2.078767250	-0.994893090	1.441197640
6	2.748130960	-2.075762860	0.849578120
6	3.713265100	-2.789398340	1.637734370
6	4.011471120	-2.332862440	2.927903260
6	2.510399340	-2.500708260	-0.531308650
6	3.179512320	-3.675569630	-1.018751700
6	4.095717060	-4.384743760	-0.166843470
6	4.365720780	-3.950109190	1.094889090
6	1.677068870	-1.798345300	-1.412166520
6	1.457059260	-2.198474080	-2.739981770
6	2.096207250	-3.399013490	-3.202088210
6	2.942176590	-4.100057840	-2.330686340
6	0.614926240	-1.444755190	-3.664743540
6	0.424994190	-1.943210280	-4.991212320
6	1.069253500	-3.160860410	-5.397863910
6	1.874107300	-3.855160960	-4.544447650
1	-6.440202170	-1.002737810	-4.535788610
1	-6.939964290	1.261626440	-3.673620960
1	-6.514663910	3.059261530	-2.084305610
1	-2.798508180	0.483179000	-0.039443280
1	-6.181870910	4.877646180	-0.505055160
1	-4.988875330	5.849359220	1.431262420
1	-1.648929370	1.401308320	1.267329740
1	-3.280756670	5.689096940	3.157238010
1	-1.619623370	5.580104580	4.938249210
1	0.273882720	4.431760870	6.040584580
1	0.149260360	0.791756210	1.835789870
1	1.862605420	2.583889900	6.134736340
1	4.546458370	-1.247471770	5.327172130
1	3.477160990	0.763058650	6.293390210
1	1.329772470	-0.463916760	0.857475570
1	4.773201840	-2.856797780	3.510135720
1	4.588520450	-5.273058200	-0.565966260

1	5.081217780	-4.481583710	1.724808700
1	1.193832670	-0.890269260	-1.058802440
1	3.443085540	-5.000935600	-2.693107350
1	0.904916040	-3.515915520	-6.416906650
1	2.367071910	-4.773797160	-4.867585180
6	-0.391893620	-1.226413010	-5.896441250
6	-1.008175260	-0.044544900	-5.521392950
6	-0.817406200	0.454648080	-4.220269060
6	-0.022636990	-0.232829050	-3.315287000
1	-0.526520970	-1.623211550	-6.904555010
1	-1.635134370	0.498584970	-6.228894780
1	-1.296755450	1.386322350	-3.918483680
1	0.107730340	0.182806020	-2.316844350
6	-3.058774300	-1.718757210	-1.484080720
6	-2.823790270	-2.991717970	-1.981700770
6	-3.581798010	-3.485010940	-3.059008810
6	-4.570233270	-2.692560040	-3.617854560
1	-5.170024410	-3.064054140	-4.450987870
1	-3.392471500	-4.485811440	-3.447825640
1	-2.045778620	-3.610882970	-1.534266740
1	-2.456712010	-1.368265990	-0.646639300

Septulene

Energy

$$E = -2149.011634 \quad E0 = -2148.376322$$

$$ZPVE = 0.635312 \text{ a.u.} = 398.6643 \text{ kcal/mol}$$

$$H298 = 422.3387 \text{ kcal/mol}$$

Dipole Polarizability

$$351.232210$$

$$0.614085 \quad 1195.763829$$

$$0.000041 \quad -0.000027 \quad 1195.726050$$

Coordinates

6	-1.519046040	0.905671660	6.559958890
6	-1.255647890	2.213982450	6.315727800
6	-0.636788790	-3.789277740	5.653404560
6	-0.051243710	-4.764705820	4.912768410
6	0.724942680	5.760464050	3.602385820
6	1.195205470	6.253451400	2.428539000
6	1.541401140	-6.580750940	0.678333090
6	1.541401490	-6.580750790	-0.678332720
6	1.195203080	6.253451740	-2.428539220
6	0.724939500	5.760464380	-3.602385710
6	-0.051247580	-4.764707490	-4.912766790
6	-0.636787340	-3.789277810	-5.653405020
6	-1.255648890	2.213982030	-6.315727790
6	-1.519045870	0.905671110	-6.559959270
6	-1.228466050	-1.440687750	5.964493920
6	-0.301980860	3.950962540	4.886646190
6	0.848723780	-5.561186860	2.784109220
6	1.363218060	6.099798950	-0.000000220

6	0.848724070	-5.561186780	-2.784108810
6	-0.301983530	3.950962460	-4.886645770
6	-1.228464840	-1.440688080	-5.964494460
6	-0.342385570	-0.786976590	3.406296440
6	-0.085853870	2.192356760	2.739721290
6	0.239814250	-3.150745030	1.530589710
6	0.379192330	3.494064160	0.000000080
6	0.239813430	-3.150745260	-1.530589250
6	-0.085855450	2.192356690	-2.739720990
6	-0.342387600	-0.786977010	-3.406295900
6	-1.182046800	-0.097155580	5.590415350
6	-0.776161640	-2.461106190	5.128173750
6	-0.697144340	2.624202450	5.059791690
6	0.215249470	4.421864830	3.679916760
6	0.310348230	-4.524108470	3.545380580
6	1.043305010	-5.449519610	1.406806050
6	1.086035280	5.485011560	1.221338390
6	1.043305370	-5.449519450	-1.406805680
6	1.086034120	5.485011680	-1.221338640
6	0.310347100	-4.524108940	-3.545379970
6	0.215246780	4.421864960	-3.679916440
6	-0.776161200	-2.461106540	-5.128173900
6	-0.697146240	2.624202170	-5.059791330
6	-1.182046760	-0.097155990	-5.590415560
6	-0.693991320	0.258960080	4.283989370
6	-0.366482660	-2.142682090	3.786330120
6	-0.499980220	1.684168840	3.987474860
6	0.237373490	3.548063660	2.536476400
6	0.072488030	-3.247911880	2.925062480
6	0.663444040	-4.234652110	0.734290750
6	0.587930940	4.135081700	1.237282410
6	0.587929910	4.135081760	-1.237282380
6	0.663443970	-4.234652090	-0.734290350
6	0.072487000	-3.247912190	-2.925062020
6	0.237371610	3.548063710	-2.536476170
6	-0.499981920	1.684168590	-3.987474490
6	-0.366483940	-2.142682550	-3.786329720
6	-0.693992620	0.258959730	-4.283989080
1	-1.931034910	0.581275920	7.516836080
1	-1.447155350	2.979175460	7.069716520
1	-0.956862870	-3.974705650	6.679934810
1	0.118445580	-5.761166540	5.323764840
1	0.737148260	6.361514140	4.513017490
1	1.600893260	7.264213320	2.362435570
1	1.876462690	-7.451988520	1.243399660
1	1.876463380	-7.451988220	-1.243399310
1	1.600890620	7.264213770	-2.362435980
1	0.737144240	6.361514540	-4.513017340
1	0.118458610	-5.761163080	-5.323768640
1	-0.956855220	-3.974703990	-6.679937520
1	-1.447156450	2.979175050	-7.069716480
1	-1.931033730	0.581275170	-7.516836840
1	-1.554285270	-1.693756620	6.976006740
1	-0.382005410	4.639314430	5.731127730
1	1.073747190	-6.512344410	3.271980780
1	1.724667130	7.130680980	-0.000000350
1	1.073747900	-6.512344230	-3.271980380
1	-0.382008430	4.639314310	-5.731127310

1	-1.554282550	-1.693756870	-6.976007780
1	0.045704340	-0.534302580	2.419498980
1	0.008268370	1.504503270	1.899368160
1	-0.026627700	-2.212981290	1.043014980
1	-0.051055270	2.492448730	0.000000230
1	-0.026629190	-2.212981750	-1.043014440
1	0.008267410	1.504503200	-1.899367920
1	0.045701310	-0.534303030	-2.419498030

[14]helicene

Energy

$$E = -2227.460097 \quad E0 = -2226.775419$$

$$ZPVE = 0.684678 \text{ a.u.} = 429.6419 \text{ kcal/mol}$$

$$H298 = 455.5316 \text{ kcal/mol}$$

Dipole Polarizability

$$742.777397$$

$$-0.664173 \quad 719.461812$$

$$-0.885220 \quad -70.384028 \quad 533.481450$$

Coordinates

6	0.625853170	-2.540792380	-3.466529010
6	1.808643960	-1.755720480	-3.603067050
6	-1.378532930	-3.151039970	0.029689380
6	-0.089309750	-3.668041080	0.353223620
6	-1.516300820	-1.786113790	-0.361001960
6	-0.424982980	-0.889489960	-0.037314240
6	0.876435490	-1.457847710	0.105633150
6	1.017915340	-2.866357040	0.280659280
6	-0.562679450	0.530608180	0.230609630
6	0.594505040	1.349061390	0.053780180
6	1.885564470	0.745482450	-0.019569890
6	2.023794240	-0.609602300	0.114389800
6	-1.765635890	1.178408690	0.726680870
6	-1.908991720	2.577626880	0.467091700
6	-0.776472200	3.348546980	0.071084900
6	0.458282340	2.766299310	-0.022170230
6	-2.798178620	0.548164460	1.529334920
6	-4.079672440	1.169349610	1.579260910
6	-4.253604830	2.493787890	1.082532510
6	-3.174777170	3.208922420	0.638983270
6	-2.534679550	-3.983090290	0.108687250
1	-0.000915840	-4.726087980	0.605090240
6	-2.748317810	-1.396749710	-1.015835950
1	2.019257830	-3.276228620	0.423288870
1	2.758774830	1.392943890	-0.115398540
1	3.011285990	-1.069565040	0.179417650
1	-0.905475940	4.420958340	-0.084952890
1	1.351123700	3.366740090	-0.204349900
6	-2.579242330	-0.583571630	2.419810790
6	-5.183024620	0.497760790	2.193857870
1	-5.242631970	2.950791570	1.146457840

1	-3.268826220	4.264720290	0.379289060
6	-3.911451450	-2.178177330	-0.748408210
6	-3.774786320	-3.474277200	-0.167924920
1	-2.414203880	-5.011870290	0.451814750
6	-2.890256930	-0.274969820	-1.921359440
6	-5.201644460	-1.656959380	-1.063507600
1	-4.674418410	-4.069923800	-0.005526070
6	-4.183507270	0.313760270	-2.045959730
6	-5.331926340	-0.402426040	-1.594903430
6	-1.828882100	0.274496540	-2.740662000
1	-6.079906040	-2.255681830	-0.817165150
6	-4.319462520	1.605625990	-2.634640090
1	-6.316045150	0.046246190	-1.739286580
6	-3.216488200	2.288569870	-3.071609790
6	-1.951768940	1.634516900	-3.156031600
6	-0.687491630	-0.471555660	-3.238817360
1	-5.312342420	2.056232830	-2.677675230
1	-3.296541080	3.317614120	-3.426119650
6	-0.819488980	2.317758280	-3.691956930
6	0.386370030	1.680114650	-3.803808500
6	-0.656402710	-1.907070430	-3.464688810
1	-0.925521880	3.369806830	-3.961908120
1	1.281234300	2.220461150	-4.117079080
6	0.478608220	0.271017550	-3.597554240
6	1.723505370	-0.400917010	-3.775625510
6	0.720427040	-3.959179830	-3.368425950
1	2.771914800	-2.267535410	-3.638035730
6	-1.804736210	-2.742596570	-3.765877720
1	2.609427760	0.194304650	-4.002971330
6	-0.409385320	-4.728293230	-3.304323660
6	-1.687108650	-4.145865620	-3.547953860
1	1.712008710	-4.411786700	-3.314534400
6	-3.015815270	-2.277680370	-4.428341760
1	-0.346397820	-5.807551270	-3.154843680
6	-2.838378300	-4.989396100	-3.644078650
6	-5.018049810	-0.695638950	2.836397970
6	-3.706747180	-1.229616910	3.026947410
6	-1.290631000	-0.992911050	2.848162940
1	-6.165423750	0.970696310	2.140507080
1	-5.867226100	-1.213000240	3.286415890
6	-3.503861300	-2.331563630	3.894805120
6	-1.118459920	-2.041737780	3.734761750
6	-2.230764860	-2.746252550	4.236829490
1	-0.417625360	-0.449596250	2.497204330
1	-4.380005870	-2.822914000	4.322764550
1	-0.111539540	-2.317055930	4.050511450
1	-2.087819990	-3.584764160	4.919358480
6	-4.046547230	-4.497092710	-4.046921830
6	-4.149962230	-3.151376760	-4.515310760
1	-2.723202360	-6.045066830	-3.391266420
1	-4.926035330	-5.141332370	-4.099244450
6	-3.087908320	-1.051033960	-5.136671490
6	-5.332802280	-2.708075300	-5.157988540
1	-6.191120710	-3.382343250	-5.187174120
6	-5.388437860	-1.475330820	-5.780074520
1	-6.298953820	-1.152794220	-6.286345730
6	-4.239149290	-0.660201390	-5.798194310
1	-4.249944700	0.284530380	-6.342949650

1 -2.207659270 -0.416277450 -5.189028250

[14]helicene-exp

Energy

E = -2227.550737 E0 = -2226.861612

ZPVE = 0.689125 a.u. = 432.4322 kcal/mol

H298 = 458.4746 kcal/mol

Dipole Polarizability

768.897467

-262.505205 882.865538

242.260124 252.430177 938.928305

Coordinates

6	-5.803633660	-0.584423190	-3.763590200
6	-6.087812980	0.652284840	-3.273386260
6	-5.348236770	1.205238200	-2.169334690
6	-4.762785710	-1.397483340	-3.190868470
6	-3.991538470	-0.892345870	-2.077992470
6	-4.282557310	0.452996050	-1.570941710
6	-5.661304130	2.469521960	-1.657260020
6	-4.963103610	3.035023850	-0.581775050
6	-3.865696440	2.312191820	-0.004746480
6	-3.567222340	1.039846410	-0.518124630
6	-5.346474560	4.310858650	-0.043083210
6	-4.701846900	4.843892480	1.031827340
6	-3.588176690	4.169140180	1.639359590
6	-3.127987350	2.917981780	1.104144640
6	-1.990494460	2.330402050	1.678624360
6	-2.945191260	4.708738160	2.760790840
6	-1.844248650	4.086307790	3.361557420
6	-1.318148110	2.884233270	2.777755010
6	-1.253111420	4.621729610	4.557387020
6	-0.206512850	3.997700660	5.165731280
6	0.387904300	2.818816710	4.597304320
6	-0.124407580	2.278940420	3.369105060
6	0.552770280	1.197943840	2.786272870
6	1.672944290	0.592870250	3.375281500
6	2.107560000	1.071602160	4.657460960
6	1.470484330	2.185034580	5.219910220
6	2.408789960	-0.504447790	2.747317950
6	3.446766740	-1.157569380	3.493969540
6	3.800179130	-0.677708040	4.801896270
6	3.180329480	0.406677900	5.345212010
6	2.164264880	-0.934207180	1.434654480
6	2.864224940	-1.990923730	0.834294920
6	3.839956630	-2.691693900	1.621157900
6	4.114135650	-2.247525350	2.920749000
6	2.647743930	-2.404042990	-0.553764070
6	3.351554710	-3.554185810	-1.051393860
6	4.280229370	-4.250077850	-0.202146490
6	4.527520410	-3.826938080	1.068077820

6	1.799179960	-1.715468550	-1.430863190
6	1.594164480	-2.108150460	-2.763089970
6	2.271062880	-3.282825570	-3.236743890
6	3.134202910	-3.968370080	-2.370086560
6	0.725893740	-1.374733920	-3.679553250
6	0.551892030	-1.866183650	-5.010760220
6	1.238348820	-3.055848680	-5.430573430
6	2.066340050	-3.731016130	-4.584310890
1	-6.370027970	-0.992122020	-4.602898920
1	-6.886911230	1.253579210	-3.710635870
1	-6.486882460	3.029761750	-2.102661910
1	-2.756316270	0.474298150	-0.064170450
1	-6.185090190	4.835171470	-0.504657770
1	-5.015942050	5.801704140	1.450274030
1	-1.622006850	1.394596460	1.263441750
1	-3.323081140	5.640649450	3.187949950
1	-1.682037070	5.530702340	4.982759460
1	0.216166150	4.394286070	6.090496120
1	0.194005570	0.812574970	1.833928540
1	1.831178500	2.572889230	6.175489490
1	4.598680020	-1.190013730	5.341452550
1	3.475845170	0.782525540	6.326326730
1	1.408702590	-0.412282530	0.851146490
1	4.882617360	-2.761567890	3.502938270
1	4.800059830	-5.119032060	-0.609603860
1	5.251309620	-4.348196220	1.697016080
1	1.288370920	-0.825820600	-1.069386900
1	3.663123340	-4.849703460	-2.740720860
1	1.085775730	-3.405511940	-6.453247010
1	2.590163970	-4.629017690	-4.916748190
6	-0.290987320	-1.169591080	-5.907827980
6	-0.948205550	-0.014008460	-5.520279660
6	-0.773469900	0.478525870	-4.214409660
6	0.046350200	-0.189695070	-3.317219610
1	-0.412967320	-1.560872940	-6.919673070
1	-1.594882840	0.513719220	-6.221679120
1	-1.285159410	1.389499660	-3.902613850
1	0.162942810	0.220093200	-2.314612060
6	-3.007347290	-1.716101710	-1.533114040
6	-2.736592020	-3.005191100	-2.036547280
6	-3.500929470	-3.498761590	-3.153223270
6	-4.500851410	-2.671674560	-3.697504510
1	-5.092693800	-3.037667040	-4.539849630
1	-2.412734000	-1.376118870	-0.684708320
6	-1.726631600	-3.837987460	-1.474854300
6	-1.481589380	-5.092194270	-1.989454710
6	-2.235736850	-5.578015500	-3.090821690
6	-3.221621720	-4.800952280	-3.658280650
1	-3.803909610	-5.172340680	-4.503632300
1	-2.029811740	-6.573723540	-3.485233290
1	-0.703533800	-5.718352710	-1.551811370
1	-1.144166140	-3.463817390	-0.631033740

Ethylene

Energy

E = -78.502240 E0 = -78.452690

ZPVE = 0.049549 a.u. = 31.0927 kcal/mol

H298 = 33.6131 kcal/mol

Dipole Polarizability

17.210355

0.000000 23.560396

0.000000 -0.000000 35.154584

Coordinates

6	4.326189530	2.838997860	-0.584507270
6	4.326189530	2.838997860	0.749354470
1	4.326189530	3.767347070	-1.157373990
1	4.326189530	1.910648650	-1.157373990
1	4.326189530	3.767347110	1.322221200
1	4.326189530	1.910648620	1.322221200