SUPPLEMENTARY MATERIAL

for

Poly[n]prismanes – a Family of Stable Cage Structures with Half-Planar Carbon Centers

Ruslan M. Minyaev,* Vladimir I. Minkin,*Tatyana N. Gribanova and Andrey G. Starikov

Institute of Physical and Organic Chemistry at Rostov State University, 344090 Rostov-on-Don, Russian Federation. Fax: +7 863 2 4346 67, E-mail: minkin@ipoc.rsu.ru; minyaev@ipoc.rsu.ru,

and Roald Hoffmann*

Department of Chemistry and Chemical Biology. Cornell University. Ithaca NY, 14853-1301. USA Fax: +1(607)255-5707, E-mail: rh34@cornell.edu

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8 RB3LYP/6-311G(2df,p) $E_{\text{Total}} = -232.122051862 \text{ a.u.}$ $\bar{\omega}_1 = 647.2 \text{ cm}^{-1}$

C	0.000000	0.876478	-0.778081
C	0.759052	-0.438239	-0.778081
C	-0.759052	-0.438239	-0.778081
H	0.000000	1.670514	-1.511143
H	1.446707	-0.835257	-1.511143
H	-1.446707	-0.835257	-1.511143
C	0.000000	0.876478	0.778081
C	0.759052	-0.438239	0.778081
C	-0.759052	-0.438239	0.778081
H	0.000000	1.670514	1.511143
H	1.446707	-0.835257	1.511143
H	-1.446707	-0.835257	1.511143

8a RB3LYP/6-311G(2df,p) $E_{\text{Total}} = -346.221499604 \text{ a.u.}$ $\bar{\omega}_1 = 240.6 \text{ cm}^{-1}$

C	0.000000	0.860074	0.000000
C	0.744846	-0.430037	0.000000
C	-0.744846	-0.430037	0.000000
C	0.000000	0.887177	1.575241
C	0.768318	-0.443589	1.575241
C	-0.768318	-0.443589	1.575241
H	0.000000	1.669579	2.323430
H	1.445898	-0.834789	2.323430
H	-1.445898	-0.834789	2.323430
C	0.000000	0.887177	-1.575241
C	0.768318	-0.443589	-1.575241
C	-0.768318	-0.443589	-1.575241
H	0.000000	1.669579	-2.323430
H	1.445898	-0.834789	-2.323430
H	-1.445898	-0.834789	-2.323430

8b RB3LYP/6-311G(d,p) $E_{\text{Total}} = -460.309893358 \text{ a.u.}$ $\bar{\omega}_1 = 132.6 \text{ cm}^{-1}$

C	0.803696	-0.435400	0.754136
C	0.803696	-0.435400	-0.754136
C	-0.803696	0.870801	0.000000
C	-0.803696	-0.435400	0.754136
C	-0.803696	-0.435400	-0.754136
C	0.803696	0.870801	0.000000
C	2.384339	-0.444354	0.769643
C	2.384339	-0.444354	-0.769643
C	-2.384339	0.888707	0.000000
C	-2.384339	-0.444354	0.769643
C	-2.384339	-0.444354	-0.769643
C	2.384339	0.888707	0.000000
H	3.134255	-0.835694	1.447464

H	3.134255	-0.835694	-1.447464
H	-3.134255	1.671388	0.000000
H	-3.134255	-0.835694	1.447464
H	-3.134255	-0.835694	-1.447464
H	3.134255	1.671388	0.000000

8c RB3LYP/6-311G(2df,p)

$E_{\text{Total}} = -346.302679173$ a.u. $\bar{\omega}_1 = 154.3$ cm⁻¹

C	-0.000001	0.000000	0.861021
C	0.745666	0.000000	-0.430510
C	-0.745665	0.000000	-0.430511
C	-0.000003	0.647646	2.199803
C	1.905087	0.647646	-1.099899
C	-1.905084	0.647646	-1.099904
C	-0.000003	-0.647646	2.199803
C	1.905087	-0.647646	-1.099899
C	-1.905084	-0.647646	-1.099904
H	-0.000003	1.566468	2.762164
H	2.392106	1.566468	-1.381079
H	-2.392102	1.566468	-1.381085
H	-0.000003	-1.566468	2.762164
H	2.392106	-1.566468	-1.381079
H	-2.392102	-1.566468	-1.381085

9 RB3LYP/6-311G(2df,p)

$E_{\text{Total}} = -309.544168863$ a.u. $\bar{\omega}_1 = 624.7$ cm⁻¹

C	0.783804	-0.783804	-0.783804
C	-0.783804	0.783804	-0.783804
C	-0.783804	-0.783804	0.783804
C	0.783804	0.783804	0.783804
C	-0.783804	-0.783804	-0.783804
C	0.783804	0.783804	-0.783804
C	0.783804	-0.783804	0.783804
C	-0.783804	0.783804	0.783804
H	1.411935	-1.411935	-1.411935
H	-1.411935	1.411935	-1.411935
H	-1.411935	-1.411935	1.411935
H	1.411935	1.411935	1.411935
H	-1.411935	-1.411935	-1.411935
H	1.411935	1.411935	-1.411935
H	1.411935	-1.411935	1.411935
H	-1.411935	1.411935	1.411935

9a RB3LYP/6-311G(2df,p)

$E_{\text{Total}} = -461.668143238$ a.u. $\bar{\omega}_1 = 337.0$ cm⁻¹

C	0.000000	1.076199	0.000000
C	0.000000	-1.076199	0.000000

C	1.076199	0.000000	0.000000
C	-1.076199	0.000000	0.000000
C	0.000000	1.133205	1.584479
C	0.000000	-1.133205	1.584479
C	1.133205	0.000000	1.584479
C	-1.133205	0.000000	1.584479
C	0.000000	1.133205	-1.584479
C	0.000000	-1.133205	-1.584479
C	1.133205	0.000000	-1.584479
C	-1.133205	0.000000	-1.584479
H	0.000000	1.995531	2.251151
H	0.000000	-1.995531	2.251151
H	1.995531	0.000000	2.251151
H	-1.995531	0.000000	2.251151
H	0.000000	1.995531	-2.251151
H	0.000000	-1.995531	-2.251151
H	1.995531	0.000000	-2.251151
H	-1.995531	0.000000	-2.251151

9b RB3LYP/6-311G(d,p)

E_{Total}= -613.795686475 a.u. $\bar{\omega}_1 = 190.6 \text{ cm}^{-1}$

C	0.000000	1.095546	0.815723
C	-1.095546	0.000000	0.815723
C	0.000000	-1.095546	0.815723
C	1.095546	0.000000	-0.815723
C	0.000000	1.095546	-0.815723
C	-1.095546	0.000000	-0.815723
C	0.000000	-1.095546	-0.815723
C	1.095546	0.000000	0.815723
C	0.000000	1.132582	2.407445
C	-1.132582	0.000000	2.407445
C	0.000000	-1.132582	2.407445
C	1.132582	0.000000	-2.407445
C	0.000000	1.132582	-2.407445
C	-1.132582	0.000000	-2.407445
C	0.000000	-1.132582	-2.407445
C	1.132582	0.000000	2.407445
H	0.000000	1.992432	3.076407
H	-1.992432	0.000000	3.076407
H	0.000000	-1.992432	3.076407
H	1.992432	0.000000	-3.076407
H	0.000000	1.992432	-3.076407
H	-1.992432	0.000000	-3.076407
H	0.000000	-1.992432	-3.076407
H	1.992432	0.000000	3.076407

9c RB3LYP/6-311G(2df,p)

E_{Total}= -461.808062898 a.u. $\bar{\omega}_1 = 45.3 \text{ cm}^{-1}$

C	1.085377	0.000000	0.000000
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C	-1.085377	0.000000	0.000000
C	0.000000	1.085377	0.000000
C	0.000000	-1.085377	0.000000
C	2.431689	0.000000	0.646158
C	-2.431689	0.000000	0.646158
C	0.000000	2.431689	0.646158
C	0.000000	-2.431689	0.646158
C	2.431689	0.000000	-0.646158
C	-2.431689	0.000000	-0.646158
C	0.000000	2.431689	-0.646158
C	0.000000	-2.431689	-0.646158
H	2.991556	0.000000	1.566775
H	-2.991556	0.000000	1.566775
H	0.000000	2.991556	1.566775
H	0.000000	-2.991556	1.566775
H	2.991556	0.000000	-1.566775
H	-2.991556	0.000000	-1.566775
H	0.000000	2.991556	-1.566775
H	0.000000	-2.991556	-1.566775

9d RB3LYP/6-311G(2df,p)

E_{Total}= -461.881503391 a.u. $\bar{\omega}_1 = 169.5 \text{ cm}^{-1}$

C	0.239984	1.093194	0.000000
C	1.086147	-0.270096	0.000000
C	-0.239984	-1.093194	0.000000
C	-1.086147	0.270096	0.000000
C	-0.243279	1.659174	1.323585
C	-1.378868	0.954340	1.323585
C	-0.243279	1.659174	-1.323585
C	-1.378868	0.954340	-1.323585
C	0.243279	-1.659174	1.323585
C	1.378868	-0.954340	1.323585
C	0.243279	-1.659174	-1.323585
C	1.378868	-0.954340	-1.323585
H	0.188770	2.379154	2.009922
H	-2.215804	0.886691	2.009922
H	0.188770	2.379154	-2.009922
H	-2.215804	0.886691	-2.009922
H	-0.188770	-2.379154	2.009922
H	2.215804	-0.886691	2.009922
H	-0.188770	-2.379154	-2.009922
H	2.215804	-0.886691	-2.009922

9e RB3LYP/6-311G(2df,p)

E_{Total}= -461.706387844 a.u. $\bar{\omega}_1 = 133.9 \text{ cm}^{-1}$

C	-0.771144	0.000000	-0.761662
C	-0.771144	0.000000	0.761662
C	0.771144	0.000000	0.761662
C	0.771144	0.000000	-0.761662

C	-0.785506	-0.772896	-2.061679
C	0.785506	-0.772896	-2.061679
C	-0.785506	0.772896	-2.061679
C	0.785506	0.772896	-2.061679
C	0.785506	-0.772896	2.061679
C	-0.785506	-0.772896	2.061679
C	0.785506	0.772896	2.061679
C	-0.785506	0.772896	2.061679
H	-1.527107	-1.423884	-2.507089
H	1.527107	-1.423884	-2.507089
H	-1.527107	1.423884	-2.507089
H	1.527107	1.423884	-2.507089
H	1.527107	-1.423884	2.507089
H	-1.527107	-1.423884	2.507089
H	1.527107	1.423884	2.507089
H	-1.527107	1.423884	2.507089

9f RB3LYP/6-311G(2df,p)

E_{Total}= -462.221060648 a.u. $\bar{\omega}_1$ = 162.5 cm⁻¹

C	0.000000	0.139933	0.000000
C	-1.157654	0.947567	0.000000
C	1.157659	0.947562	0.000000
C	-0.000003	-1.250774	0.000000
C	-0.678740	2.336998	0.000000
C	-2.380899	0.319868	0.000000
C	0.678751	2.336995	0.000000
C	2.380900	0.319857	0.000000
C	1.278376	-1.872909	0.000000
C	-1.278384	-1.872903	0.000000
C	-2.419592	-1.100253	0.000000
C	2.419587	-1.100265	0.000000
H	-1.313104	3.212019	0.000000
H	-3.311569	0.876401	0.000000
H	1.313119	3.212013	0.000000
H	3.311573	0.876385	0.000000
H	1.355488	-2.954414	0.000000
H	-1.355502	-2.954407	0.000000
H	-3.386775	-1.589017	0.000000
H	3.386768	-1.589032	0.000000

9g RB3LYP/6-311G(2df,p)

E_{Total}= -462.165012986 a.u. $\bar{\omega}_1$ = 105.7 cm⁻¹

C	1.908432	-1.439093	0.000000
C	0.752969	-0.709146	0.000000
C	0.752969	0.709146	0.000000
C	1.908432	1.439093	0.000000
C	3.110551	0.691436	0.000000
C	3.110551	-0.691436	0.000000

H	1.929698	-2.521810	0.000000
H	1.929698	2.521810	0.000000
H	4.057344	1.218221	0.000000
H	4.057344	-1.218221	0.000000
C	-1.908432	-1.439093	0.000000
C	-3.110551	-0.691436	0.000000
C	-3.110551	0.691436	0.000000
C	-1.908432	1.439093	0.000000
C	-0.752969	0.709146	0.000000
C	-0.752969	-0.709146	0.000000
H	-1.929698	-2.521810	0.000000
H	-4.057344	-1.218221	0.000000
H	-4.057344	1.218221	0.000000
H	-1.929698	2.521810	0.000000

10 RB3LYP/6-311G(2df,p)

$E_{\text{Total}} = -387.024740606$ a.u. $\bar{\omega}_1 = 565.8 \text{ cm}^{-1}$

C	-1.071288	0.784035	-0.778336
C	-1.071288	0.784035	0.778336
C	0.409196	0.784035	1.259375
C	1.324185	0.784035	0.000000
C	0.409196	0.784035	-1.259375
H	-1.807098	1.382763	-1.312934
H	-1.807098	1.382763	1.312934
H	0.690250	1.382763	2.124372
H	2.233696	1.382763	0.000000
H	0.690250	1.382763	-2.124372
C	-1.071288	-0.784035	-0.778336
C	-1.071288	-0.784035	0.778336
C	0.409196	-0.784035	1.259375
C	1.324185	-0.784035	0.000000
C	0.409196	-0.784035	-1.259375
H	-1.807098	-1.382763	-1.312934
H	-1.807098	-1.382763	1.312934
H	0.690250	-1.382763	2.124372
H	2.233696	-1.382763	0.000000
H	0.690250	-1.382763	-2.124372

10a RB3LYP/6-311G(2df,p)

$E_{\text{Total}} = -577.226259337$ a.u. $\bar{\omega}_1 = 385.2 \text{ cm}^{-1}$

C	-1.030384	0.000000	-0.748618
C	-1.030384	0.000000	0.748618
C	0.393572	0.000000	1.211289
C	1.273624	0.000000	0.000000
C	0.393572	0.000000	-1.211289
C	-1.101359	1.580521	-0.800184
C	-1.101359	1.580521	0.800184
C	0.420682	1.580521	1.294725

C	1.361354	1.580521	0.000000
C	0.420682	1.580521	-1.294725
H	-1.816432	2.219020	-1.319715
H	-1.816432	2.219020	1.319715
H	0.693815	2.219020	2.135344
H	2.245233	2.219020	0.000000
H	0.693815	2.219020	-2.135344
C	-1.101359	-1.580521	-0.800184
C	-1.101359	-1.580521	0.800184
C	0.420682	-1.580521	1.294725
C	1.361354	-1.580521	0.000000
C	0.420682	-1.580521	-1.294725
H	-1.816432	-2.219020	-1.319715
H	-1.816432	-2.219020	1.319715
H	0.693815	-2.219020	2.135344
H	2.245233	-2.219020	0.000000
H	0.693815	-2.219020	-2.135344

10b RB3LYP/6-311G(d,p)

E_{Total}= -767.432064838 a.u. $\bar{\omega}_1$ = 244.9 cm⁻¹

C	0.815873	0.402571	1.238986
C	0.815873	-1.053945	0.765736
C	0.815873	-1.053945	-0.765736
C	0.815873	0.402571	-1.238986
C	-0.815873	1.302747	0.000000
C	-0.815873	0.402571	1.238986
C	-0.815873	-1.053945	0.765736
C	-0.815873	-1.053945	-0.765736
C	-0.815873	0.402571	-1.238986
C	0.815873	1.302747	0.000000
C	2.406692	0.420191	1.293216
C	2.406692	-1.100075	0.799251
C	2.406692	-1.100075	-0.799251
C	2.406692	0.420191	-1.293216
C	-2.406692	1.359767	0.000000
C	-2.406692	0.420191	1.293216
C	-2.406692	-1.100075	0.799251
C	-2.406692	-1.100075	-0.799251
C	-2.406692	0.420191	-1.293216
C	2.406692	1.359767	0.000000
H	3.051323	0.691737	2.128947
H	3.051323	-1.810991	1.315762
H	3.051323	-1.810991	-1.315762
H	3.051323	0.691737	-2.128947
H	-3.051323	2.238507	0.000000
H	-3.051323	0.691737	2.128947
H	-3.051323	-1.810991	1.315762
H	-3.051323	-1.810991	-1.315762
H	-3.051323	0.691737	-2.128947
H	3.051323	2.238507	0.000000

10c RB3LYP/6-311G(2df,p) $E_{\text{Total}} = -577.292050427$ a.u. $\bar{\omega}_1 = 4.0$ cm⁻¹

C	0.964153	0.860892	0.036826
C	1.107616	-0.665768	0.042998
C	-0.294649	-1.251791	-0.122940
C	-1.275851	-0.121640	0.161921
C	-0.524733	1.174384	-0.116913
C	1.894439	1.753274	0.807285
C	2.177026	-1.363277	0.834188
C	-0.613307	-2.694895	0.116267
C	-2.327393	-0.224106	1.232235
C	-1.106895	2.530203	0.137873
C	2.036780	1.775513	-0.474170
C	2.338616	-1.368431	-0.445197
C	-0.595769	-2.334158	-1.122283
C	-2.758808	-0.261486	0.016640
C	-1.029928	2.189799	-1.104099
H	2.204356	2.107958	1.776302
H	2.534268	-1.645976	1.810562
H	-0.749771	-3.475890	0.845595
H	-2.540388	-0.246970	2.288129
H	-1.383434	3.265284	0.875270
H	2.552930	2.161493	-1.337512
H	2.930075	-1.657289	-1.298124
H	-0.708387	-2.595104	-2.161527
H	-3.591713	-0.338423	-0.662151
H	-1.195710	2.433831	-2.140328

11 RB3LYP/6-311G(2df,p) $E_{\text{Total}} = -464.417212796$ a.u. $\bar{\omega}_1 = 389.0$ cm⁻¹

C	-1.347866	0.781660	-0.778191
C	-1.347866	0.781660	0.778191
C	0.000000	0.781660	1.556382
C	1.347866	0.781660	0.778191
C	1.347866	0.781660	-0.778191
C	0.000000	0.781660	-1.556382
H	-2.151425	1.353256	-1.242126
H	-2.151425	1.353256	1.242126
H	0.000000	1.353256	2.484252
H	2.151425	1.353256	1.242126
H	2.151425	1.353256	-1.242126
H	0.000000	1.353256	-2.484252
C	-1.347866	-0.781660	-0.778191
C	-1.347866	-0.781660	0.778191
C	0.000000	-0.781660	1.556382
C	1.347866	-0.781660	0.778191
C	1.347866	-0.781660	-0.778191
C	0.000000	-0.781660	-1.556382
H	-2.151425	-1.353256	-1.242126

H	-2.151425	-1.353256	1.242126
H	0.000000	-1.353256	2.484252
H	2.151425	-1.353256	1.242126
H	2.151425	-1.353256	-1.242126
H	0.000000	-1.353256	-2.484252

11a RB3LYP/6-311G(2df,p)

$E_{\text{Total}} = -692.65369572$ a.u. $\bar{\omega}_1 = 393.8 \text{ cm}^{-1}$

C	-1.285111	0.000000	-0.741959
C	-1.285111	0.000000	0.741959
C	0.000000	0.000000	1.483919
C	1.285111	0.000000	0.741959
C	1.285111	0.000000	-0.741959
C	0.000000	0.000000	-1.483919
C	-1.398259	1.570430	-0.807285
C	-1.398259	1.570430	0.807285
C	0.000000	1.570430	1.614571
C	1.398259	1.570430	0.807285
C	1.398259	1.570430	-0.807285
C	0.000000	1.570430	-1.614571
H	-2.188928	2.168346	-1.263778
H	-2.188928	2.168346	1.263778
H	0.000000	2.168346	2.527556
H	2.188928	2.168346	1.263778
H	2.188928	2.168346	-1.263778
H	0.000000	2.168346	-2.527556
C	-1.398259	-1.570430	-0.807285
C	-1.398259	-1.570430	0.807285
C	0.000000	-1.570430	1.614571
C	1.398259	-1.570430	0.807285
C	1.398259	-1.570430	-0.807285
C	0.000000	-1.570430	-1.614571
H	-2.188928	-2.168346	-1.263778
H	-2.188928	-2.168346	1.263778
H	0.000000	-2.168346	2.527556
H	2.188928	-2.168346	1.263778
H	2.188928	-2.168346	-1.263778
H	0.000000	-2.168346	-2.527556

11b RB3LYP/6-311G(d,p)

$E_{\text{Total}} = -920.884476314$ a.u. $\bar{\omega}_1 = 269.8 \text{ cm}^{-1}$

C	-1.321443	0.816681	-0.762935
C	-1.321443	0.816681	0.762935
C	0.000000	0.816681	1.525870
C	1.321443	0.816681	0.762935
C	1.321443	0.816681	-0.762935
C	0.000000	0.816681	-1.525870
C	-1.321443	-0.816681	-0.762935

C	-1.321443	-0.816681	0.762935
C	0.000000	-0.816681	1.525870
C	1.321443	-0.816681	0.762935
C	1.321443	-0.816681	-0.762935
C	0.000000	-0.816681	-1.525870
C	-1.396594	2.398425	-0.806324
C	-1.396594	2.398425	0.806324
C	0.000000	2.398425	1.612648
C	1.396594	2.398425	0.806324
C	1.396594	2.398425	-0.806324
C	0.000000	2.398425	-1.612648
H	-2.176771	3.013847	-1.256759
H	-2.176771	3.013847	1.256759
H	0.000000	3.013847	2.513518
H	2.176771	3.013847	1.256759
H	2.176771	3.013847	-1.256759
H	0.000000	3.013847	-2.513518
C	-1.396594	-2.398425	-0.806324
C	-1.396594	-2.398425	0.806324
C	0.000000	-2.398425	1.612648
C	1.396594	-2.398425	0.806324
C	1.396594	-2.398425	-0.806324
C	0.000000	-2.398425	-1.612648
H	-2.176771	-3.013847	-1.256759
H	-2.176771	-3.013847	1.256759
H	0.000000	-3.013847	2.513518
H	2.176771	-3.013847	1.256759
H	2.176771	-3.013847	-1.256759
H	0.000000	-3.013847	-2.513518

11c RB3LYP/6-311G(2df,p)

$E_{\text{Total}} = -692.751697996$ a.u. $\bar{\omega}_1 = 53.8 \text{ cm}^{-1}$

C	0.000000	1.467986	0.205202
C	-1.271313	0.733993	-0.205202
C	-1.271313	-0.733993	0.205202
C	0.000000	-1.467986	-0.205202
C	1.271313	-0.733993	0.205202
C	1.271313	0.733993	-0.205202
C	0.000000	2.330560	1.441222
C	-2.568469	1.482906	-0.318176
C	-2.018324	-1.165280	1.441222
C	0.000000	-2.965812	-0.318176
C	2.018324	-1.165280	1.441222
C	2.568469	1.482906	-0.318176
C	0.000000	2.965812	0.318176
C	-2.018324	1.165280	-1.441222
C	-2.568469	-1.482906	0.318176
C	0.000000	-2.330560	-1.441222
C	2.568469	-1.482906	0.318176
C	2.018324	1.165280	-1.441222

H	0.000000	2.364497	2.518034
H	-3.379160	1.950959	0.213615
H	-2.047715	-1.182249	2.518034
H	0.000000	-3.901917	0.213615
H	2.047715	-1.182249	2.518034
H	3.379160	1.950959	0.213615
H	0.000000	3.901917	-0.213615
H	-2.047715	1.182249	-2.518034
H	-3.379160	-1.950959	-0.213615
H	0.000000	-2.364497	-2.518034
H	3.379160	-1.950959	-0.213615
H	2.047715	1.182249	-2.518034

11d RB3LYP/6-311G(2df,p)

$E_{\text{Total}} = -692.939557235$ a.u. $\bar{\omega}_1 = 94.9 \text{ cm}^{-1}$

C	-1.337573	0.000000	-0.809377
C	-1.337573	0.000000	0.809377
C	-0.032154	0.000000	1.563061
C	1.369728	0.000000	0.753684
C	1.369728	0.000000	-0.753684
C	-0.032154	0.000000	-1.563061
C	-2.147577	-1.290941	-0.664530
C	-2.147577	1.290941	0.664530
C	-2.147577	1.290941	-0.664530
C	-2.147577	-1.290941	0.664530
C	0.498289	-1.290941	2.192121
C	1.649288	1.290941	1.527591
C	0.498289	1.290941	2.192121
C	1.649288	-1.290941	1.527591
C	1.649288	-1.290941	-1.527591
C	0.498289	1.290941	-2.192121
C	1.649288	1.290941	-1.527591
C	0.498289	-1.290941	-2.192121
H	-2.603722	-1.933362	-1.407942
H	-2.603722	1.933362	1.407942
H	-2.603722	1.933362	-1.407942
H	-2.603722	-1.933362	1.407942
H	0.082547	-1.933362	2.958860
H	2.521175	1.933362	1.550918
H	0.082547	1.933362	2.958860
H	2.521175	-1.933362	1.550918
H	2.521175	-1.933362	-1.550918
H	0.082547	1.933362	-2.958860
H	2.521175	1.933362	-1.550918
H	0.082547	-1.933362	-2.958860

11e RB3LYP/6-311G(2df,p)

$E_{\text{Total}} = -692.757855129$ a.u. $\bar{\omega}_1 = 83.6 \text{ cm}^{-1}$

C	-1.299323	0.000000	-0.786216
C	-1.299323	0.000000	0.786216
C	-0.031222	0.000000	1.518354
C	1.330544	0.000000	0.732138
C	1.330544	0.000000	-0.732138
C	-0.031222	0.000000	-1.518354
C	-2.614016	-0.762807	-0.778206
C	-2.614016	0.762807	0.778206
C	-2.614016	0.762807	-0.778206
C	-2.614016	-0.762807	0.778206
C	0.633062	-0.762807	2.652907
C	1.980954	0.762807	1.874701
C	0.633062	0.762807	2.652907
C	1.980954	-0.762807	1.874701
C	1.980954	-0.762807	-1.874701
C	0.633062	0.762807	-2.652907
C	1.980954	0.762807	-1.874701
C	0.633062	-0.762807	-2.652907
H	-3.018517	-1.443678	-1.514893
H	-3.018517	1.443678	1.514893
H	-3.018517	1.443678	-1.514893
H	-3.018517	-1.443678	1.514893
H	0.197322	-1.443678	3.371559
H	2.821195	1.443678	1.856666
H	0.197322	1.443678	3.371559
H	2.821195	-1.443678	1.856666
H	2.821195	-1.443678	-1.856666
H	0.197322	1.443678	-3.371559
H	2.821195	1.443678	-1.856666
H	0.197322	-1.443678	-3.371559

11f RB3LYP/6-311G(2df,p)

E_{Total}= -693.364120979 a.u. $\bar{\omega}_1 = 57.2 \text{ cm}^{-1}$

C	0.000000	0.000000	0.723509
C	0.000000	0.000000	-0.723509
C	0.000000	1.230754	-1.401257
C	0.000000	-1.230754	-1.401257
C	0.000000	-1.230754	1.401257
C	0.000000	1.230754	1.401257
C	0.000000	2.440466	-0.723485
C	0.000000	-2.440466	-0.723485
C	0.000000	-2.440466	0.723485
C	0.000000	2.440466	0.723485
C	0.000000	3.697668	-1.403922
C	0.000000	-3.697668	-1.403922
C	0.000000	-3.697668	1.403922
C	0.000000	3.697668	1.403922
C	0.000000	4.868769	-0.713145
C	0.000000	-4.868769	-0.713145
C	0.000000	-4.868769	0.713144

C	0.000000	4.868769	0.713144
H	0.000000	1.230663	-2.486457
H	0.000000	-1.230663	-2.486457
H	0.000000	-1.230663	2.486458
H	0.000000	1.230663	2.486458
H	0.000000	3.696287	-2.488350
H	0.000000	-3.696287	-2.488350
H	0.000000	-3.696288	2.488350
H	0.000000	3.696288	2.488350
H	0.000000	5.814359	-1.242034
H	0.000000	-5.814359	-1.242034
H	0.000000	-5.814360	1.242032
H	0.000000	5.814360	1.242032

11g RB3LYP/6-311G(2df,p)

E_{Total}= -693.379120739 a.u. $\bar{\omega}_1$ = 53.3 cm⁻¹

C	1.331340	0.546615	0.000000
C	1.155698	-0.857680	0.000000
C	2.301166	-1.676812	0.000000
C	3.573025	-1.149980	0.000000
C	3.746192	0.234533	0.000000
C	2.643270	1.058390	0.000000
H	2.194962	-2.751752	0.000000
H	4.432296	-1.809706	0.000000
H	4.741481	0.662301	0.000000
H	2.805091	2.126373	0.000000
C	-0.192287	-1.426282	0.000000
C	-1.320622	-0.572024	0.000000
C	-2.602745	-1.154462	0.000000
C	-2.782424	-2.519340	0.000000
C	-1.669984	-3.361564	0.000000
C	-0.405043	-2.818334	0.000000
H	-3.480568	-0.525017	0.000000
H	-3.783400	-2.933628	0.000000
H	-1.797171	-4.437394	0.000000
H	0.438948	-3.492466	0.000000
C	0.164924	1.429704	0.000000
C	0.301579	2.831275	0.000000
C	-0.790601	3.669320	0.000000
C	-2.076207	3.127031	0.000000
C	-2.238227	1.759944	0.000000
C	-1.139053	0.879667	0.000000
H	1.285606	3.276769	0.000000
H	-0.648897	4.743334	0.000000
H	-2.944310	3.775093	0.000000
H	-3.244038	1.366093	0.000000

13a,b RB3LYP/6-311G(2df,p)

E_{Total}= -346.907606461 a.u. $\bar{\omega}_1$ = 243.5 cm⁻¹

C	-0.005928	0.070032	0.822222
C	-0.005928	0.070032	-0.822222
C	-0.512712	1.231256	0.000000
C	-1.370777	-0.669882	0.750422
C	-1.370777	-0.669882	-0.750422
C	-1.918699	0.529287	0.000000
H	-1.899338	-1.287074	1.474386
H	-1.899338	-1.287074	-1.474386
H	-2.927855	0.916074	0.000000
C	1.451847	-0.446482	0.746333
C	1.451847	-0.446482	-0.746333
C	2.284650	0.597821	0.000000
H	1.801976	-1.218116	1.428717
H	1.801976	-1.218116	-1.428717
H	3.325044	0.224059	0.000000
H	-0.223607	2.276045	0.000000

14 RB3LYP/6-311G(2df,p)

E_{Total}= -346.863983089 a.u. $\bar{\omega}_1$ = -606.6 cm⁻¹

C	-0.007117	0.826062	0.000000
C	-0.007117	-0.826062	0.000000
C	-1.257781	0.000000	0.000000
C	0.570378	0.751287	1.430167
C	0.570378	-0.751287	1.430167
C	-0.588125	0.000000	2.012572
H	1.225099	1.464591	1.924433
H	1.225099	-1.464591	1.924433
H	-0.780741	0.000000	3.084576
C	0.570378	0.751287	-1.430167
C	0.570378	-0.751287	-1.430167
C	-0.588125	0.000000	-2.012572
H	1.225099	1.464591	-1.924433
H	1.225099	-1.464591	-1.924433
H	-0.780741	0.000000	-3.084576
H	-2.338407	0.000000	0.000000

15a RB3LYP/6-311G(2df,p)

E_{Total}= -346.711455277 a.u. $\bar{\omega}_1$ = 271.3 cm⁻¹

C	-0.525358	0.000000	1.163603
C	-0.033549	0.878480	0.109654
C	-0.033549	-0.878480	0.109654
C	2.246807	0.000000	0.455952
C	1.346652	0.801515	-0.416353
C	1.346652	-0.801515	-0.416353
H	2.048124	0.000000	1.524868
H	1.677356	1.397068	-1.254367
H	1.677356	-1.397068	-1.254367

C	-1.945172	0.000000	0.532278
C	-1.373314	0.831724	-0.565295
C	-1.373314	-0.831724	-0.565295
H	-2.939871	0.000000	0.947191
H	-1.844389	1.482360	-1.292013
H	-1.844389	-1.482360	-1.292013
H	3.290685	0.000000	0.173635

15b RB3LYP/6-311G(2df,p)

E_{Total}= -346.676504216 a.u. $\bar{\omega}_1$ = 199.6 cm⁻¹

C	0.383155	0.914763	0.000000
C	0.642632	-0.566872	0.000000
C	-0.816424	-0.909759	0.000000
C	0.187216	1.031888	1.383469
C	0.662559	-0.419690	1.609452
C	-0.814513	-0.298719	1.428892
H	0.007785	1.851660	2.062781
H	1.270935	-0.813053	2.409504
H	-1.564540	-0.253543	2.209160
C	0.187216	1.031888	-1.383469
C	0.662559	-0.419690	-1.609452
C	-0.814513	-0.298719	-1.428892
H	0.007785	1.851660	-2.062781
H	1.270935	-0.813053	-2.409504
H	-1.564540	-0.253543	-2.209160
H	-1.107671	-1.960679	0.000000