

# Supporting Information

for

## Planar and Pyramidal Tetracoordinate Carbon in Organoboron Compounds

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**16** RB3LYP/6-311+G\*\* $E_{\text{total}} = -166.294792704$  a.u. $\omega_f = 119.8$  cm<sup>-1</sup>

C	0.000000	0.000000	0.089261
B	0.000000	0.743220	1.478175
B	0.000000	-0.743220	1.478175
H	0.000000	1.917522	1.556900
H	0.000000	-1.917522	1.556900
C	0.000000	0.642131	-1.250283
C	0.000000	-0.642131	-1.250283
H	0.000000	1.612217	-1.713863
H	0.000000	-1.612217	-1.713863

**16** MP2(full)/6-311+G\*\* $E_{\text{total}} = -165.8265047$  a.u. $\omega_f = 62.2$  cm<sup>-1</sup>

C	0.000000	0.000000	0.091355
B	0.000000	0.751207	1.476934
B	0.000000	-0.751207	1.476934
H	0.000000	1.928617	1.550679
H	0.000000	-1.928617	1.550679
C	0.000000	0.648905	-1.250383
C	0.000000	-0.648905	-1.250383
H	0.000000	1.624194	-1.707113
H	0.000000	-1.624194	-1.707113

**17** RB3LYP/6-311+G\*\* $E_{\text{total}} = -166.363579840$  a.u. $\omega_f = 194.9$  cm<sup>-1</sup>

C	0.000000	0.000000	0.282785
B	0.000000	1.200021	-0.799176
C	0.000000	1.367086	0.593312
H	0.000000	1.444325	-1.946689
H	0.000000	1.886715	1.534343
B	0.000000	-1.200021	-0.799176
C	0.000000	-1.367086	0.593312
H	0.000000	-1.444325	-1.946689
H	0.000000	-1.886715	1.534343

**17** MP2(full)/6-311+G\*\* $E_{\text{total}} = -165.8951845$  a.u. $\omega_f = 171.5$  cm<sup>-1</sup>

C	0.000000	0.000000	0.314782
B	0.000000	1.157946	-0.809756
C	0.000000	1.378347	0.590823
H	0.000000	1.402137	-1.960571
H	0.000000	1.921352	1.520067
B	0.000000	-1.157946	-0.809756
C	0.000000	-1.378347	0.590823
H	0.000000	-1.402137	-1.960571
H	0.000000	-1.921352	1.520067

**22** RB3LYP/6-311+G\*\* $E_{\text{total}} = -165.079657325$  a.u. $\omega_I = 455.2$  cm<sup>-1</sup>

C	0.000000	0.000000	0.446475
C	0.000000	1.407733	0.365769
C	0.000000	-1.407733	0.365769
B	0.000001	0.802748	-0.921923
B	-0.000001	-0.802748	-0.921923
H	0.000002	-2.213632	1.075573
H	-0.000002	2.213632	1.075573

**22** MP2(full)/6-311+G\*\* $E_{\text{total}} = -164.6349617$  a.u. $\omega_I = 420.1$  cm<sup>-1</sup>

C	0.000000	0.000000	0.445470
C	0.000000	1.413630	0.371844
C	0.000000	-1.413630	0.371844
B	0.000000	0.811841	-0.931502
B	0.000000	-0.811841	-0.931502
H	0.000000	-2.215236	1.090036
H	0.000000	2.215236	1.090036

**24** RB3LYP/6-311+G\*\* $E_{\text{total}} = -243.829957446$  a.u. $\omega_I = 105.5$  cm<sup>-1</sup>

B	0.000000	1.251058	0.000000
C	-1.247982	0.251016	0.000000
C	-0.871725	-1.123905	0.000000
C	0.431224	-1.564719	0.000000
C	1.545007	-0.683907	0.000000
C	1.382719	0.678886	0.000000
H	-2.331046	0.354595	0.000000
H	-1.665139	-1.865394	0.000000
H	0.613022	-2.634213	0.000000
H	2.538831	-1.123457	0.000000
H	2.266949	1.308901	0.000000
B	-1.302527	1.970271	0.000000
H	-2.345441	2.508692	0.000000

**24** MP2(full)/6-311+G\*\* $E_{\text{total}} = -243.1612612$  a.u. $\omega_I = 80.9$  cm<sup>-1</sup>

B	0.000000	1.254749	0.000000
C	-1.241777	0.250977	0.000000
C	-0.875994	-1.127234	0.000000
C	0.435697	-1.568012	0.000000
C	1.549292	-0.687597	0.000000
C	1.385463	0.684471	0.000000
H	-2.327794	0.370616	0.000000
H	-1.671182	-1.870103	0.000000
H	0.614529	-2.640426	0.000000
H	2.545907	-1.125833	0.000000
H	2.274190	1.311293	0.000000
B	-1.316586	1.972720	0.000000
H	-2.368812	2.501475	0.000000

**25** RB3LYP/6-311+G\*\* $E_{\text{total}} = -243.819740167$  a.u. $\omega_l = 23.9$  cm<sup>-1</sup>

B	0.000000	0.000000	-1.142164
C	0.000000	1.301622	-0.345934
C	0.000000	1.232815	1.040225
C	0.000000	0.000000	1.711320
C	0.000000	-1.232815	1.040225
C	0.000000	-1.301622	-0.345934
B	0.000000	0.000000	-2.698142
H	0.000000	2.290500	-0.796631
H	0.000000	2.141034	1.637821
H	0.000000	0.000000	2.797233
H	0.000000	-2.141034	1.637821
H	0.000000	-2.290500	-0.796631
H	0.000000	0.000000	-3.877487

**25** MP2(full)/6-311+G\*\* $E_{\text{total}} = -243.1430632$  a.u. $i\omega = i100.2$  cm<sup>-1</sup>

B	0.032057	1.136087	0.000000
C	0.027873	0.353154	1.305500
C	0.027873	-1.039712	1.234962
C	0.033551	-1.713949	0.000000
C	0.027873	-1.039712	-1.234962
C	0.027873	0.353154	-1.305500
B	-0.164390	2.691353	0.000000
H	0.020915	0.802939	2.298278
H	0.029283	-1.639383	2.144665
H	0.034322	-2.802449	0.000000
H	0.029283	-1.639383	-2.144665
H	0.020915	0.802939	-2.298278
H	-0.343305	3.860541	0.000000

**26** RB3LYP/6-311+G\*\* $E_{\text{total}} = -255.351855042$  a.u. $\omega_I = 70.4$  cm<sup>-1</sup>

C	0.000000	0.726989	-1.048281
C	0.000000	-0.726989	-1.048281
B	0.000000	2.451073	-0.792594
B	0.000000	1.447704	0.323537
B	0.000000	-1.447704	0.323537
B	0.000000	-2.451073	-0.792594
C	0.000000	-0.680710	1.637508
C	0.000000	0.680710	1.637508
H	0.000000	-1.211629	2.587618
H	0.000000	1.211629	2.587618
H	0.000000	3.185623	-1.709768
H	0.000000	-3.185623	-1.709768
H	0.000000	1.119498	-2.067931
H	0.000000	-1.119498	-2.067931

**26** MP2(full)/6-311+G\*\* $E_{\text{total}} = -254.6280697$  a.u. $\omega_I = 79.9$  cm<sup>-1</sup>

C	0.006934	0.727674	-1.044028
C	-0.006934	-0.727674	-1.044028
B	0.079910	2.444920	-0.809534
B	0.001163	1.453198	0.329608
B	-0.001163	-1.453198	0.329608
B	-0.079910	-2.444920	-0.809534
C	0.001163	-0.686408	1.644338
C	-0.001163	0.686408	1.644338
H	0.002352	-1.212502	2.598800
H	-0.002352	1.212502	2.598800
H	0.121214	3.173745	-1.735430
H	-0.121214	-3.173745	-1.735430
H	0.009773	1.129760	-2.065602
H	-0.009773	-1.129760	-2.065602

**27** RB3LYP/6-311+G\*\* $E_{\text{total}} = -255.332460215$  a.u. $i\omega = i30.8$  cm<sup>-1</sup>

B	0.000000	0.000000	1.457973
B	0.000000	0.000000	-1.457973
C	0.000000	1.331601	0.689668
C	0.000000	1.331601	-0.689668
C	0.000000	-1.331601	-0.689668
C	0.000000	-1.331601	0.689668
H	0.000000	2.295290	1.198944
H	0.000000	2.295290	-1.198944
H	0.000000	-2.295290	-1.198944
H	0.000000	-2.295290	1.198944
B	0.000000	0.000000	3.024512
B	0.000000	0.000000	-3.024512
H	0.000000	0.000000	4.204090
H	0.000000	0.000000	-4.204090

**27** MP2(full)/6-311+G\*\* $E_{\text{total}} = -254.5931483$  a.u. $i\omega = i274.7; i87.4; i87.2$  cm<sup>-1</sup>

B	0.000000	0.000000	1.454449
B	0.000000	0.000000	-1.454449
C	0.000000	1.336619	0.693273
C	0.000000	1.336619	-0.693273
C	0.000000	-1.336619	-0.693273
C	0.000000	-1.336619	0.693273
H	0.000000	2.302959	1.204517
H	0.000000	2.302959	-1.204517
H	0.000000	-2.302959	-1.204517
H	0.000000	-2.302959	1.204517
B	0.000000	0.000000	3.028421
B	0.000000	0.000000	-3.028421
H	0.000000	0.000000	4.212122
H	0.000000	0.000000	-4.212122

**28** RB3LYP/6-311+G\*\* $E_{\text{total}} = -255.340223226$  a.u. $\omega_l = 62.6$  cm<sup>-1</sup>

B	-0.015047	1.384708	-0.420259
B	0.015047	-1.384708	0.420259
C	0.117414	1.044388	1.139844
C	0.123388	-0.319944	1.451774
C	-0.117414	-1.044388	-1.139844
C	-0.123388	0.319944	-1.451774
H	0.206628	1.679895	2.021647
H	0.213320	-0.585234	2.503218
H	-0.206628	-1.679895	-2.021647
H	-0.213320	0.585234	-2.503218
B	0.067062	2.681299	0.321323
B	-0.067062	-2.681299	-0.321323
H	0.140514	3.625292	1.014757
H	-0.140514	-3.625292	-1.014757

**28** MP2(full)/6-311+G\*\* $E_{\text{total}} = -254.6154968$  a.u. $\omega_l = 11.8$  cm<sup>-1</sup>

B	-0.018439	1.387652	-0.434505
B	0.018439	-1.387652	0.434505
C	0.115779	1.059213	1.130046
C	0.125053	-0.311269	1.458500
C	-0.115779	-1.059213	-1.130046
C	-0.125053	0.311269	-1.458500
H	0.203636	1.698946	2.014166
H	0.215345	-0.563027	2.515826
H	-0.203636	-1.698946	-2.014166
H	-0.215345	0.563027	-2.515826
B	0.069691	2.669454	0.348560
B	-0.069691	-2.669454	-0.348560
H	0.144934	3.619846	1.040117
H	-0.144934	-3.619846	-1.040117

**29** RB3LYP/6-311+G\*\* $E_{\text{total}} = -293.444127142$  a.u. $\omega_I = 59.9$  cm<sup>-1</sup>

C	0.000000	1.006783	0.000000
C	1.333390	1.801024	0.000000
C	1.260866	0.342507	0.000000
B	-1.336391	1.894381	0.000000
B	-1.469916	0.400834	0.000000
B	0.619384	-1.741382	0.000000
B	1.970261	-0.966927	0.000000
C	-0.813258	-2.074022	0.000000
C	-1.768692	-1.082468	0.000000
H	-1.341406	3.069379	0.000000
H	3.142324	-1.117097	0.000000
H	-1.127063	-3.117242	0.000000
H	-2.811053	-1.398386	0.000000
H	1.573339	2.332934	0.917965
H	1.573339	2.332934	-0.917965

**30** RB3LYP/6-311+G\*\* $E_{\text{total}} = -293.442593811$  a.u. $\omega_I = 56.8$  cm<sup>-1</sup>

C	0.000000	0.725070	0.774021
C	0.000000	0.000000	2.081829
C	0.000000	-0.725070	0.774021
B	0.000000	2.285727	0.591875
B	0.000000	1.489679	-0.676204
B	0.000000	-1.489679	-0.676204
B	0.000000	-2.285727	0.591875
C	0.000000	-0.679933	-1.954750
C	0.000000	0.679933	-1.954750
H	0.000000	-1.206882	-2.907196
H	0.000000	1.206882	-2.907196
H	-0.919358	0.000000	2.661907
H	0.919358	0.000000	2.661907
H	0.000000	3.023471	1.505825
H	0.000000	-3.023471	1.505825

**30** MP2(full)/6-311+G\*\* $E_{\text{total}} = -292.6336983$  a.u. $\omega_I = 78.6$  cm<sup>-1</sup>

C	-1.050176	0.044179	0.000000
C	-1.431978	1.493486	0.000000
C	0.000000	1.051103	0.000000
B	-2.086107	-1.161317	0.000000
B	-0.615270	-1.516715	0.000000
B	1.541235	0.550978	0.000000
B	1.247971	2.035452	0.000000
C	1.846806	-0.934401	0.000000
C	0.855953	-1.884448	0.000000
H	-3.249752	-0.978905	0.000000
H	1.114635	3.205737	0.000000
H	2.885476	-1.265183	0.000000
H	1.142788	-2.936102	0.000000
H	-1.827960	1.906478	0.925610
H	-1.827960	1.906478	-0.925610



**31** RB3LYP/6-311+G\*\* $E_{\text{total}} = -495.586659702$  a.u. $\omega_l = 97.4$  cm<sup>-1</sup>

C	0.000000	0.000000	0.821927
C	0.000000	0.712010	-0.411297
C	0.000000	-0.712010	-0.411297
B	0.000000	0.758588	2.232665
B	0.000000	-0.758588	2.232665
B	0.000000	2.313106	-0.459359
B	0.000000	1.554555	-1.773335
B	0.000000	-2.313106	-0.459359
B	0.000000	-1.554555	-1.773335
C	0.000000	-2.965042	0.920194
C	0.000000	-2.279238	2.107762
C	0.000000	2.279238	2.107762
C	0.000000	2.965042	0.920194
C	0.000000	0.685664	-3.027666
C	0.000000	-0.685664	-3.027666
H	0.000000	-4.052698	0.973297
H	0.000000	-2.868900	3.023265
H	0.000000	2.868900	3.023265
H	0.000000	4.052698	0.973297
H	0.000000	1.183515	-3.996153
H	0.000000	-1.183515	-3.996153

**32** RB3LYP/6-311+G\*\* $E_{\text{total}} = -281.045083210$  a.u. $\omega_I = 170.5$  cm<sup>-1</sup>

C	0.000000	0.000000	-1.000988
C	0.000000	1.231384	-0.247583
C	0.000000	1.221985	1.144482
C	0.000000	0.000000	1.825867
C	0.000000	-1.221985	1.144482
C	0.000000	-1.231384	-0.247583
H	0.000000	2.157536	1.692578
H	0.000000	0.000000	2.909200
H	0.000000	-2.157536	1.692578
B	0.000000	1.457600	-1.655792
H	0.000000	1.930484	-2.724253
B	0.000000	-1.457600	-1.655792
H	0.000000	-1.930484	-2.724253

**32** MP2(full)/6-311+G\*\* $E_{\text{total}} = -280.3044924$  a.u. $\omega_I = 165.6$  cm<sup>-1</sup>

C	0.000000	0.000000	-0.997160
C	0.000000	1.241014	-0.242732
C	0.000000	1.230930	1.150479
C	0.000000	0.000000	1.828999
C	0.000000	-1.230930	1.150479
C	0.000000	-1.241014	-0.242732
H	0.000000	2.166722	1.702902
H	0.000000	0.000000	2.914998
H	0.000000	-2.166722	1.702902
B	0.000000	1.441271	-1.671669
H	0.000000	1.914215	-2.744048
B	0.000000	-1.441271	-1.671669
H	0.000000	-1.914215	-2.744048

**33** RB3LYP/6-311+G\*\* $E_{\text{total}} = -330.309230553$  a.u. $\omega_l = 118.3$  cm<sup>-1</sup>

C	0.000000	0.000000	1.421887
C	0.000000	1.258107	0.719109
C	0.000000	1.258107	-0.719109
C	0.000000	0.000000	-1.421887
C	0.000000	-1.258107	-0.719109
C	0.000000	-1.258107	0.719109
B	0.000000	1.454129	2.097728
B	0.000000	1.454129	-2.097728
B	0.000000	-1.454129	-2.097728
B	0.000000	-1.454129	2.097728
H	0.000000	1.906894	3.177980
H	0.000000	1.906894	-3.177980
H	0.000000	-1.906894	-3.177980
H	0.000000	-1.906894	3.177980

**33** MP2(full)/6-311+G\*\* $E_{\text{total}} = -329.4274214$  a.u. $\omega_l = 109.4$  cm<sup>-1</sup>

C	0.000000	0.000000	1.419956
C	0.000000	1.266220	0.719141
C	0.000000	1.266220	-0.719141
C	0.000000	0.000000	-1.419956
C	0.000000	-1.266220	-0.719141
C	0.000000	-1.266220	0.719141
B	0.000000	1.436779	2.117652
B	0.000000	1.436779	-2.117652
B	0.000000	-1.436779	-2.117652
B	0.000000	-1.436779	2.117652
H	0.000000	1.886281	3.203270
H	0.000000	1.886281	-3.203270
H	0.000000	-1.886281	-3.203270
H	0.000000	-1.886281	3.203270

**34** RB3LYP/6-311+G\*\* $E_{\text{total}} = -407.773953047$  a.u. $\omega_I = 131.7$  cm<sup>-1</sup>

C	0.000000	1.563164	0.000000
C	0.000000	1.220462	1.387520
C	0.000000	-1.220462	1.387520
C	0.000000	-1.563164	0.000000
C	0.000000	-1.220462	-1.387520
C	0.000000	1.220462	-1.387520
B	0.000000	2.636370	1.145571
C	0.000000	0.000000	2.052114
B	0.000000	-2.636370	1.145571
B	0.000000	-2.636370	-1.145571
C	0.000000	0.000000	-2.052114
B	0.000000	2.636370	-1.145571
H	0.000000	3.784385	1.389316
H	0.000000	0.000000	3.136169
H	0.000000	-3.784385	1.389316
H	0.000000	-3.784385	-1.389316
H	0.000000	0.000000	-3.136169
H	0.000000	3.784385	-1.389316

**34** MP2(full)/6-311+G\*\* $E_{\text{total}} = -406.7029145$  a.u. $\omega_I = 110.4$  cm<sup>-1</sup>

C	0.000000	1.518518	0.000000
C	0.000000	1.216172	1.401659
C	0.000000	-1.216172	1.401659
C	0.000000	-1.518518	0.000000
C	0.000000	-1.216172	-1.401659
C	0.000000	1.216172	-1.401659
B	0.000000	2.638127	1.110915
C	0.000000	0.000000	2.082525
B	0.000000	-2.638127	1.110915
B	0.000000	-2.638127	-1.110915
C	0.000000	0.000000	-2.082525
B	0.000000	2.638127	-1.110915
H	0.000000	3.791177	1.351185
H	0.000000	0.000000	3.169474
H	0.000000	-3.791177	1.351185
H	0.000000	-3.791177	-1.351185
H	0.000000	0.000000	-3.169474
H	0.000000	3.791177	-1.351185

**35** RB3LYP/6-311+G\*\* $E_{\text{total}} = -405.198710195$  a.u. $\omega_l = 106.9$  cm<sup>-1</sup>

C	0.000000	1.255870	0.000000
C	0.000000	1.182990	1.416441
C	0.000000	-1.182990	1.416441
C	0.000000	-1.255870	0.000000
C	0.000000	-1.182990	-1.416441
C	0.000000	1.182990	-1.416441
B	0.000000	2.537689	0.803998
C	0.000000	0.000000	2.159891
B	0.000000	-2.537689	0.803998
B	0.000000	-2.537689	-0.803998
C	0.000000	0.000000	-2.159891
B	0.000000	2.537689	-0.803998
H	0.000000	0.000000	3.241799
H	0.000000	0.000000	-3.241799

**35** MP2(full)/6-311+G\*\* $E_{\text{total}} = -404.1831123$  a.u. $\omega_l = 90.3$  cm<sup>-1</sup>

C	0.000000	1.245377	0.000000
C	0.000000	1.181314	1.425685
C	0.000000	-1.181314	1.425685
C	0.000000	-1.245377	0.000000
C	0.000000	-1.181314	-1.425685
C	0.000000	1.181314	-1.425685
B	0.000000	2.548212	0.813554
C	0.000000	0.000000	2.178392
B	0.000000	-2.548212	0.813554
B	0.000000	-2.548212	-0.813554
C	0.000000	0.000000	-2.178392
B	0.000000	2.548212	-0.813554
H	0.000000	0.000000	3.263551
H	0.000000	0.000000	-3.263551

**36** RB3LYP/6-311+G\*\* $E_{\text{total}} = -328.971789981$  a.u. $\omega_I = 66.8$  cm<sup>-1</sup>

C	0.000000	0.705793	-0.650561
C	0.000000	-0.705793	-0.650561
C	0.000000	1.744056	0.318198
C	0.000000	-1.744056	0.318198
C	0.000000	2.867357	1.170631
C	0.000000	-2.867357	1.170631
H	0.000000	3.024668	2.232584
H	0.000000	-3.024668	2.232584
B	0.000000	2.008927	-1.243149
B	0.000000	-2.008927	-1.243149
B	0.000000	3.230266	-0.209289
B	0.000000	-3.230266	-0.209289

**36** MP2(full)/6-311+G\*\* $E_{\text{total}} = -328.1108013$  a.u. $\omega_I = 31.6$  cm<sup>-1</sup>

C	0.000000	0.707535	-0.672706
C	0.000000	-0.707535	-0.672706
C	0.000000	1.735929	0.311861
C	0.000000	-1.735929	0.311861
C	0.000000	2.845164	1.192044
C	0.000000	-2.845164	1.192044
H	0.000000	2.974731	2.260568
H	0.000000	-2.974731	2.260568
B	0.000000	2.028617	-1.259018
B	0.000000	-2.028617	-1.259018
B	0.000000	3.246483	-0.190534
B	0.000000	-3.246483	-0.190534

**36'** RB3LYP/6-311+G\*\* $E_{\text{total}} = -328.972211241$  a.u. $\omega_l = 62.4$  cm<sup>-1</sup>

C	0.005459	0.705440	-0.002494
C	-0.005459	-0.705440	0.002494
C	0.998150	1.720317	0.019119
C	-0.998150	-1.720317	-0.019119
C	1.878235	2.820468	0.037412
C	-1.878235	-2.820468	-0.037412
H	2.943529	2.950805	0.064100
H	-2.943529	-2.950805	-0.064100
B	-0.555781	2.022703	-0.021934
B	0.555781	-2.022703	0.021934
B	0.507796	3.218005	0.000755
B	-0.507796	-3.218005	-0.000755

**36'** MP2(full)/6-311+G\*\* $E_{\text{total}} = -328.1113265$  a.u. $i\omega = i64.0$  cm<sup>-1</sup>

C	0.000000	0.707232	0.000000
C	0.000000	-0.707232	0.000000
C	0.991910	1.727322	0.000000
C	-0.991910	-1.727322	0.000000
C	1.883404	2.826171	0.000000
C	-1.883404	-2.826171	0.000000
H	2.953259	2.944333	0.000000
H	-2.953259	-2.944333	0.000000
B	-0.575948	2.033925	0.000000
B	0.575948	-2.033925	0.000000
B	0.504509	3.241551	0.000000
B	-0.504509	-3.241551	0.000000

**38** RB3LYP/6-311+G\*\* $E_{\text{total}} = -90.1513958372$  a.u. $i\omega = i203.5$  cm<sup>-1</sup>

C	0.000000	0.000000	0.784360
B	0.000000	0.743004	-0.614787
B	0.000000	-0.743004	-0.614787
H	0.000000	0.881755	1.413628
H	0.000000	-0.881755	1.413628
H	0.000000	1.913519	-0.692774
H	0.000000	-1.913519	-0.692774

**38** MP2(full)/6-311+G\*\* $E_{\text{total}} = -89.864201$  a.u. $i\omega = i256.6$  cm<sup>-1</sup>

C	0.000000	0.000000	0.788641
B	0.000000	0.747749	-0.617456
B	0.000000	-0.747749	-0.617456
H	0.000000	0.893623	1.403346
H	0.000000	-0.893623	1.403346
H	0.000000	1.921186	-0.681989
H	0.000000	-1.921186	-0.681989

**39** RB3LYP/6-311+G\*\* $E_{\text{total}} = -90.2017475802$  a.u. $\omega_I = 540.6$  cm<sup>-1</sup>

C	0.000000	0.000000	0.790985
B	0.000000	0.860955	-0.356518
B	0.000000	-0.860955	-0.356518
H	0.000000	0.000000	1.864073
H	0.000000	0.000000	-1.371884
H	0.000000	1.939296	-0.836462
H	0.000000	-1.939296	-0.836462

**39** MP2(full)/6-311+G\*\* $E_{\text{total}} = -89.9156978$  a.u. $\omega_I = 533.8$  cm<sup>-1</sup>

C	0.000000	0.000000	0.798309
B	0.000000	0.863235	-0.360241
B	0.000000	-0.863235	-0.360241
H	0.000000	0.000000	1.872401
H	0.000000	0.000000	-1.372151
H	0.000000	1.941660	-0.843847
H	0.000000	-1.941660	-0.843847



**40** RB3LYP/6-311+G\*\* $E_{\text{total}} = -129.524649804$  a.u. $\omega_I = 216.1$  cm<sup>-1</sup>

B	-0.976486	0.000000	-0.220803
C	0.000000	1.173509	0.167381
B	0.976486	0.000000	-0.220803
H	0.000000	-2.179231	-0.243372
H	0.000000	-1.210976	1.267497
H	0.000000	1.210976	1.267497
C	0.000000	-1.173509	0.167381
H	0.000000	2.179231	-0.243372
H	-1.936436	0.000000	-0.924393
H	1.936436	0.000000	-0.924393

**40** MP2(full)/6-311+G\*\* $E_{\text{total}} = -129.1277588$  a.u. $\omega_I = 90.5$  cm<sup>-1</sup>

B	-0.974290	0.000000	-0.230848
C	0.000000	1.174022	0.172974
B	0.974290	0.000000	-0.230848
H	0.000000	-2.189781	-0.209741
H	0.000000	-1.160999	1.274143
H	0.000000	1.160999	1.274143
C	0.000000	-1.174022	0.172974
H	0.000000	2.189781	-0.209741
H	-1.924780	0.000000	-0.948006
H	1.924780	0.000000	-0.948006

**41** RB3LYP/6-311+G\*\* $E_{\text{total}} = -129.481494286$  a.u. $i\omega = i630.3$  cm<sup>-1</sup>

B	0.135352	-0.060824	0.874377
C	-0.394552	-1.228256	0.000000
B	0.135352	-0.060824	-0.874377
H	0.202423	1.913790	-0.862991
H	0.202423	1.913790	0.862991
H	-1.481351	-1.312036	0.000000
C	0.135352	1.262049	0.000000
H	0.086351	-2.204127	0.000000
H	0.595916	0.047033	1.961305
H	0.595916	0.047033	-1.961305

**41** MP2(full)/6-311+G\*\* $E_{\text{total}} = -129.0864493$  a.u. $i\omega = i581.3$  cm<sup>-1</sup>

B	0.147295	-0.064901	0.874721
C	-0.432069	-1.219458	0.000000
B	0.147295	-0.064901	-0.874721
H	0.233027	1.898502	-0.873786
H	0.233027	1.898502	0.873786
H	-1.520870	-1.239896	0.000000
C	0.147295	1.260134	0.000000
H	0.009223	-2.213464	0.000000
H	0.640646	0.030657	1.949973
H	0.640646	0.030657	-1.949973

**42** RB3LYP/6-311+G\*\* $E_{\text{total}} = -218.552032159$  a.u. $\omega_f = 71.8$  cm<sup>-1</sup>

B	-0.933289	1.196639	0.276276
C	0.000000	2.049798	-0.657635
B	0.933289	1.196639	0.276276
B	0.933289	-1.196639	0.276276
C	0.000000	-2.049798	-0.657635
B	-0.933289	-1.196639	0.276276
H	0.000000	3.137993	-0.639414
H	0.000000	-3.137993	-0.639414
C	0.000000	0.000000	0.568726
H	0.000000	1.674066	-1.682854
H	0.000000	-1.674066	-1.682854
H	-1.915525	1.422955	0.899571
H	-1.915525	-1.422955	0.899571
H	1.915525	1.422955	0.899571
H	1.915525	-1.422955	0.899571

**42** MP2(full)/6-311+G\*\* $E_{\text{total}} = -217.9091682$  a.u. $\omega_f = 114.6$  cm<sup>-1</sup>

B	-0.942699	1.139095	0.301951
C	0.000000	1.845610	-0.749771
B	0.942699	1.139095	0.301951
B	0.942699	-1.139095	0.301951
C	0.000000	-1.845610	-0.749771
B	-0.942699	-1.139095	0.301951
H	0.000000	2.922410	-0.906440
H	0.000000	-2.922410	-0.906440
C	0.000000	0.000000	0.762940
H	0.000000	1.290639	-1.691606
H	0.000000	-1.290639	-1.691606
H	-1.921725	1.454968	0.894170
H	-1.921725	-1.454968	0.894170
H	1.921725	1.454968	0.894170
H	1.921725	-1.454968	0.894170

**43** RB3LYP/6-311+G\*\* $E_{\text{total}} = -218.552458660$  a.u. $\omega_I = 127.5$  cm<sup>-1</sup>

B	-0.175259	1.462400	0.948847
C	0.000000	2.173845	-0.454216
B	0.770027	0.830966	-0.603261
B	0.175259	-1.462400	0.948847
C	0.000000	-2.173845	-0.454216
B	-0.770027	-0.830966	-0.603261
H	0.422202	3.162113	-0.611348
H	-0.422202	-3.162113	-0.611348
C	0.000000	0.000000	0.525033
H	-0.979950	2.078852	-0.942691
H	0.979950	-2.078852	-0.942691
H	-0.137524	1.899452	2.054041
H	-1.822151	-0.542776	-1.077734
H	1.822151	0.542776	-1.077734
H	0.137524	-1.899452	2.054041

**43** MP2(full)/6-311+G\*\* $E_{\text{total}} = -217.9042594$  a.u. $\omega_I = 137.3$  cm<sup>-1</sup>

B	-0.130701	1.481472	0.956224
C	0.000000	2.129631	-0.494254
B	0.756638	0.777287	-0.595710
B	0.130701	-1.481472	0.956224
C	0.000000	-2.129631	-0.494254
B	-0.756638	-0.777287	-0.595710
H	0.410398	3.109767	-0.717495
H	-0.410398	-3.109767	-0.717495
C	0.000000	0.000000	0.594357
H	-1.015273	1.997619	-0.896792
H	1.015273	-1.997619	-0.896792
H	-0.066792	1.972118	2.037636
H	-1.816748	-0.467823	-1.043462
H	1.816748	0.467823	-1.043462
H	0.066792	-1.972118	2.037636

**44** RB3LYP/6-311+G\*\* $E_{\text{total}} = -256.673481843$  a.u. $\omega_I = 142.8$  cm<sup>-1</sup>

B	0.942367	-0.782475	1.458990
B	0.942367	-0.782475	-1.458990
C	-0.388398	-0.363612	-2.218351
B	-0.388398	0.454821	-0.892139
C	-0.640076	1.720786	0.000000
B	-0.388398	0.454821	0.892139
C	-0.388398	-0.363612	2.218351
H	-0.379906	0.102139	-3.201533
H	0.169112	2.452555	0.000000
H	-0.379906	0.102139	3.201533
H	-1.106223	-1.188513	-2.183470
H	-1.612313	2.210449	0.000000
H	-1.106223	-1.188513	2.183470
C	0.550311	-0.525139	0.000000
H	2.037572	-1.012121	1.861242
H	2.037572	-1.012121	-1.861242

**44** MP2(full)/6-311+G\*\* $E_{\text{total}} = -255.9416386$  a.u. $\omega_I = 148.4$  cm<sup>-1</sup>

B	0.981591	-0.710398	1.476340
B	0.981591	-0.710398	-1.476340
C	-0.402342	-0.415239	-2.201854
B	-0.402342	0.433861	-0.886787
C	-0.685429	1.705133	0.000000
B	-0.402342	0.433861	0.886787
C	-0.402342	-0.415239	2.201854
H	-0.463707	0.023084	-3.195505
H	0.121766	2.439145	0.000000
H	-0.463707	0.023084	3.195505
H	-1.060490	-1.282073	-2.090368
H	-1.669130	2.171428	0.000000
H	-1.060490	-1.282073	2.090368
C	0.594204	-0.489852	0.000000
H	2.089356	-0.818025	1.897870
H	2.089356	-0.818025	-1.897870

**45** RB3LYP/6-311+G\*\* $E_{\text{total}} = -294.764395603$  a.u. $\omega_I = 127.3$  cm<sup>-1</sup>

B	0.000000	1.360164	0.157957
C	-1.512840	1.512840	-0.259228
B	-1.360164	0.000000	0.157957
C	-1.512840	-1.512840	-0.259228
B	0.000000	-1.360164	0.157957
C	1.512840	-1.512840	-0.259228
B	1.360164	0.000000	0.157957
C	1.512840	1.512840	-0.259228
H	-1.848853	1.848853	-1.238518
H	-1.848853	-1.848853	-1.238518
H	1.848853	-1.848853	-1.238518
H	1.848853	1.848853	-1.238518
C	0.000000	0.000000	0.978934
H	-2.044781	2.044781	0.535702
H	-2.044781	-2.044781	0.535702
H	2.044781	-2.044781	0.535702
H	2.044781	2.044781	0.535702

**45** MP2(full)/6-311+G\*\* $E_{\text{total}} = -293.9512186$  a.u. $\omega_I = 127.3$  cm<sup>-1</sup>

B	0.000000	1.355663	0.157350
C	-1.511039	1.511039	-0.266445
B	-1.355663	0.000000	0.157350
C	-1.511039	-1.511039	-0.266445
B	0.000000	-1.355663	0.157350
C	1.511039	-1.511039	-0.266445
B	1.355663	0.000000	0.157350
C	1.511039	1.511039	-0.266445
H	-1.848345	1.848345	-1.244956
H	-1.848345	-1.848345	-1.244956
H	1.848345	-1.848345	-1.244956
H	1.848345	1.848345	-1.244956
C	0.000000	0.000000	1.007350
H	-2.030707	2.030707	0.545854
H	-2.030707	-2.030707	0.545854
H	2.030707	-2.030707	0.545854
H	2.030707	2.030707	0.545854

**46** RB3LYP/6-311+G\*\* $E_{\text{total}} = -294.672734043$  a.u. $i\omega = i524.3$  cm<sup>-1</sup>

B	0.000000	1.499925	0.000000
C	1.648315	1.648315	0.000000
B	1.499925	0.000000	0.000000
C	1.648315	-1.648315	0.000000
B	0.000000	-1.499925	0.000000
C	-1.648315	-1.648315	0.000000
B	-1.499925	0.000000	0.000000
C	-1.648315	1.648315	0.000000
H	2.114880	2.114880	0.875893
H	2.114880	-2.114880	0.875893
H	-2.114880	-2.114880	0.875893
H	-2.114880	2.114880	0.875893
C	0.000000	0.000000	0.000000
H	2.114880	2.114880	-0.875893
H	2.114880	-2.114880	-0.875893
H	-2.114880	-2.114880	-0.875893
H	-2.114880	2.114880	-0.875893

**46** MP2(full)/6-311+G\*\* $E_{\text{total}} = -293.8433338$  a.u. $i\omega = i547.3$  cm<sup>-1</sup>

B	1.061151	1.061151	0.000000
C	2.326065	0.000000	0.168667
B	1.061151	-1.061151	0.000000
C	0.000000	-2.326065	-0.168667
B	-1.061151	-1.061151	0.000000
C	-2.326065	0.000000	0.168667
B	-1.061151	1.061151	0.000000
C	0.000000	2.326065	-0.168667
H	2.795926	0.000000	1.161543
H	0.000000	-3.139381	0.566740
H	-2.795926	0.000000	1.161543
H	0.000000	3.139381	0.566740
C	0.000000	0.000000	0.000000
H	3.139381	0.000000	-0.566740
H	0.000000	-2.795926	-1.161543
H	-3.139381	0.000000	-0.566740
H	0.000000	2.795926	-1.161543

**47** RB3LYP/6-311+G\*\*E<sub>total</sub> = -358.720938546 a.u. $\omega_I = 78.1 \text{ cm}^{-1}$ 

B	-0.440103	1.364419	-0.296320
C	0.779704	2.346145	-0.314038
B	1.429118	0.951579	-0.003929
C	2.427059	0.000050	0.711893
B	1.429167	-0.951522	-0.003940
C	0.779805	-2.346110	-0.314059
B	-0.440043	-1.364435	-0.296324
C	-1.998673	-1.446868	0.232394
B	-2.252442	-0.000048	0.329890
C	-1.998750	1.446782	0.232362
H	0.899085	3.213488	0.330903
H	2.454500	0.000042	1.803640
H	0.899228	-3.213456	0.330870
H	-2.090914	-2.010030	1.168828
H	-2.091056	2.009968	1.168775
C	0.191479	0.000006	-0.557062
H	1.008856	2.612699	-1.354439
H	3.453141	0.000081	0.335365
H	1.008963	-2.612640	-1.354465
H	-2.626986	-1.954556	-0.512613
H	-2.627062	1.954410	-0.512686

**48** RB3LYP/6-311+G\*\*E<sub>total</sub> = -423.115546684 a.u. $\omega_I = 72.3 \text{ cm}^{-1}$ 

B	0.164619	1.469013	-0.521435
C	-1.308108	2.093081	-0.376422
B	-2.101035	0.819655	-0.094662
C	-2.741943	-0.011602	1.180090
B	-2.366452	-0.741665	-0.067970
C	-1.461592	-1.953205	-0.444346
B	0.045283	-1.473649	-0.509123
C	1.422117	-2.283929	-0.482469
B	1.745495	-0.948418	0.241279
C	2.429439	-0.071209	1.346799
B	1.800645	0.838981	0.237495
C	1.587561	2.187014	-0.516849
H	-1.286646	2.878647	0.387771
H	-2.565589	-0.224811	2.236494
H	-1.551839	-2.859933	0.167638
H	1.525052	-3.251983	0.004641
H	1.905300	-0.059298	2.303842
H	1.751951	3.152507	-0.041331
H	-1.527715	2.571569	-1.339347
H	-3.478226	0.818057	1.099935
H	-1.665016	-2.273198	-1.480074
H	1.834028	-2.314588	-1.496310
H	3.507944	-0.104423	1.492170
H	2.015946	2.168906	-1.522908
C	0.587866	-0.013656	-0.413544