

# Supporting Information

## Unveiling the Electronic and Structural Consequences of Removing Two Electrons from $B_{12}H_{12}^{2-}$

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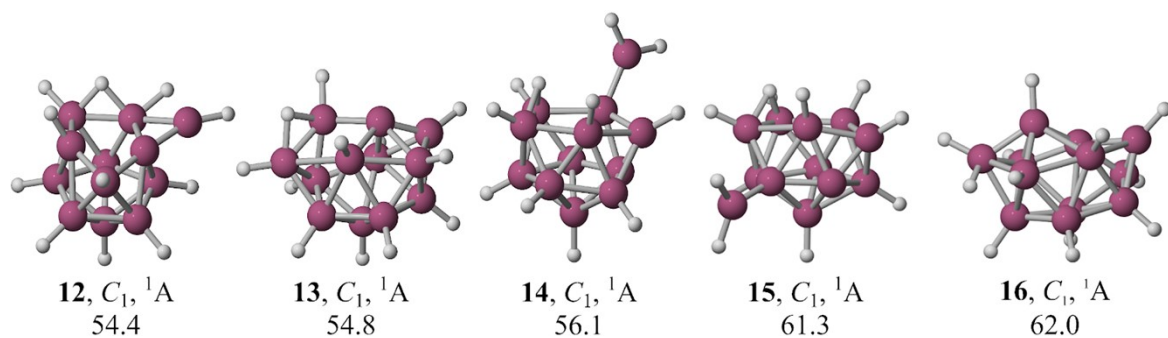
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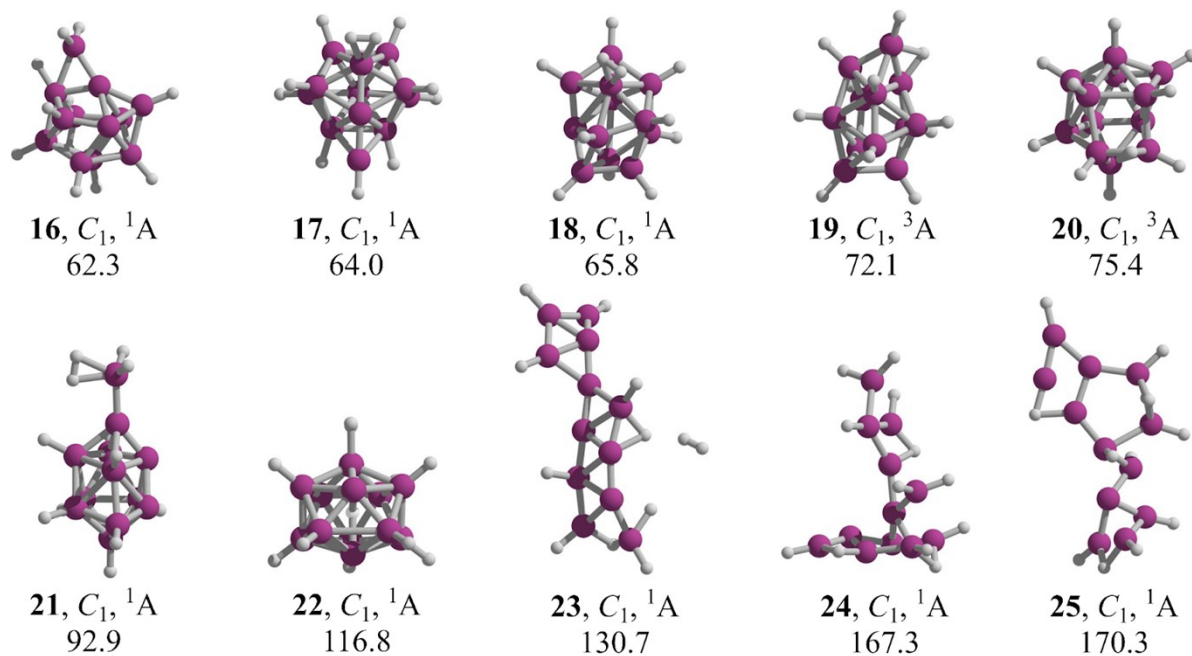
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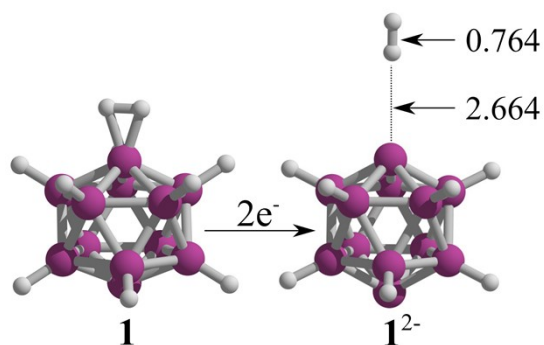
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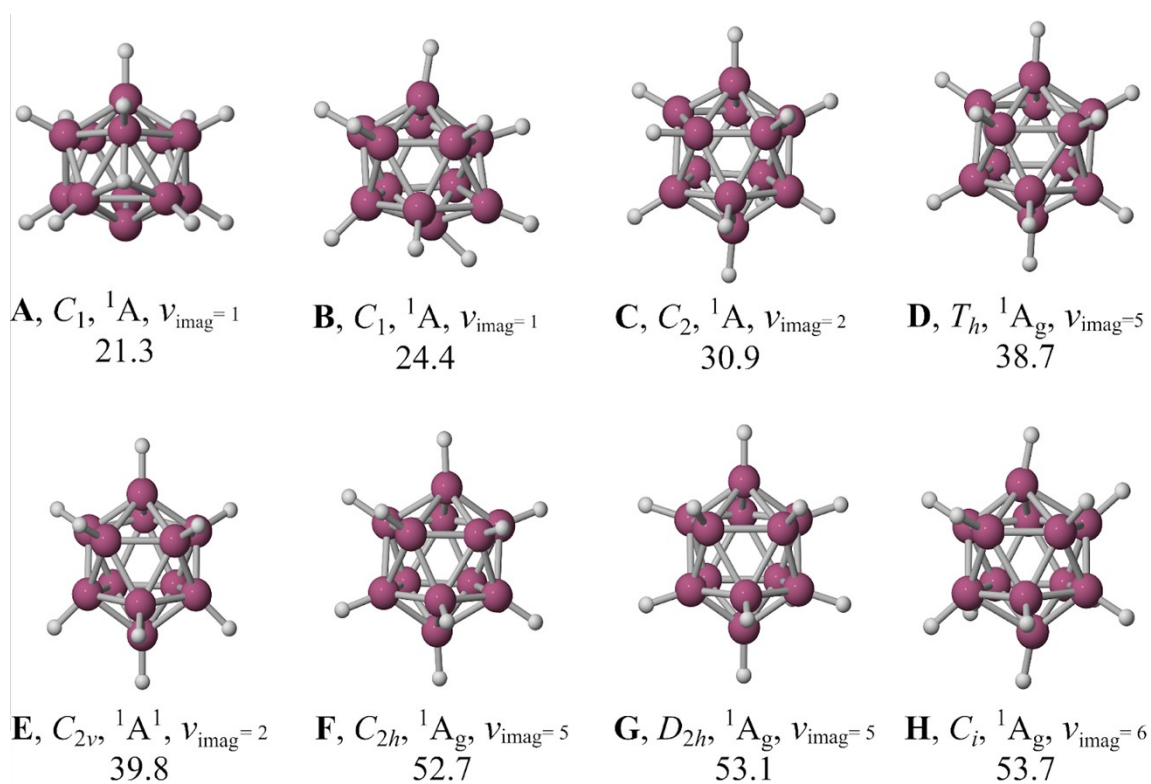
**Figure S1.** Higher-energy isomers of  $B_{12}H_{12}$ . Relative Gibbs free energies computed at the CCSD(T)/def2-TZVP//TPSS-D3/def2-TZVP level are in kcal/mol.



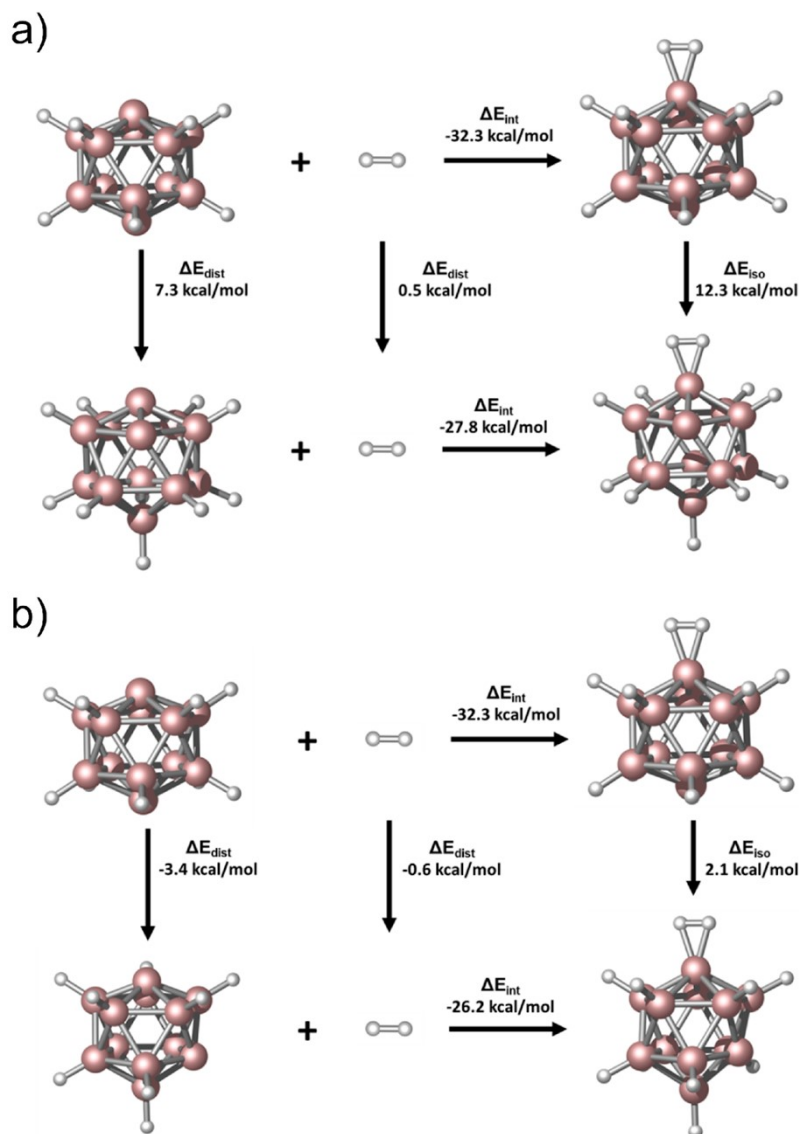
**Figure S2.** Higher-energy isomers of  $B_{12}H_{12}$  with relative Gibbs free energies above 60 kcal/mol computed at the TPSS-D3/def2-TZVP level.



**Figure S3.** Structure of  $1^{2-}$  optimized from the geometry of **1** at the CCSD(T)/def2-TZVP//TPSS-D3/def2-TZVP level.



**Figure S4.** Some stationary points of  $B_{12}H_{12}$ .  $\nu$  is the number of imaginary frequencies. Relative Gibbs free energies computed at the CCSD(T)/def2-TZVP//TPSS-D3/def2-TZVP level are in kcal/mol.



**Figure S5.** Energetic reaction cycle involving the isomerization between (a) the *para* and *ortho* and (b) the *para* and *meta* isomers.

**Table S1.** The HOMO-LUMO and energy gap ( $\Delta_{\text{H-L}}$ , eV) of the low-lying isomers of  $\text{B}_{12}\text{H}_{12}$  at the TPSS-D3/def2-TZVP level, in eV. The T1 diagnostic at the CCSD/cc-pVTZ level of theory is a measure of the significance of the multireference effects.

Isomer	$E_{\text{HOMO}}$	$E_{\text{LUMO}}$	$\Delta_{\text{H-L}}$	T1
1	-7.61	-3.86	3.75	0.01
2	-7.57	-4.02	3.55	0.01
3	-7.92	-4.19	3.73	0.01
4	-7.89	-4.11	3.78	0.01
5	-7.90	-4.39	3.51	0.01
6	-7.91	-4.34	3.57	0.01

<b>7</b>	-7.57	-4.42	3.15	0.01
<b>8</b>	-7.84	-5.36	2.48	0.01
<b>9</b>	-7.95	-5.14	2.81	0.02
<b>10</b>	-7.67	-5.03	2.65	0.02

**Table S2.** Gibbs free energies at the CCSD(T)/def2-TZVP//TPSS-D3/def2-TZVP and MP2/def2-TZVP level for the low-lying isomers of B<sub>12</sub>H<sub>12</sub>.

	MP2/def2-TZVP	CCSD(T)/def2-TZVP//TPSS-D3/def2-TZVP
<b>1</b>	0.0	0.0
<b>2</b>	2.8	3.2
<b>3</b>	5.2	5.7
<b>4</b>	6.7	7.3
<b>5</b>	8.0	8.4
<b>6</b>	8.7	8.5
<b>7</b>	12.9	13.9
<b>8</b>	21.2	20.4
<b>9</b>	20.3	21.3
<b>10</b>	19.0	23.5
<b>11</b>	48.2	40.3

### Cartesian Coordinates

**1**

CCSD(T)/def2-TZVP//TPSS/def2-TZVP

**G = -304.63101 a.u.**

H	-0.8078570	-1.4369990	2.4675540
B	-0.4837020	-0.8432910	1.4940160
B	0.4766740	0.6561280	1.4869360
H	0.8018220	1.2458030	2.4642520
B	-1.5692810	-0.8268790	-0.0000000

H	-2.6041520	-1.4050080	-0.0000000
B	-1.2527840	0.6645250	0.9252160
H	-2.0936090	1.2486430	-1.5252270
H	0.4300080	2.7258760	0.0000000
B	0.0020490	1.4530520	0.0000000
H	-0.4086070	2.7319080	-0.0000000
H	-2.0936090	1.2486430	1.5252270
B	-1.2527840	0.6645250	-0.9252160
H	2.1038220	-1.4238510	-1.5234330
B	-0.4837020	-0.8432910	-1.4940160
B	1.2645730	-0.8373920	-0.9259870
H	-0.8078570	-1.4369990	-2.4675540
B	-0.0026410	-1.4805800	-0.0000000
B	1.2645730	-0.8373920	0.9259870
H	2.1038220	-1.4238510	1.5234330
H	0.8018220	1.2458030	-2.4642520
B	0.4766740	0.6561280	-1.4869360
B	1.5564280	0.6627730	0.0000000
H	2.5940200	1.2385040	0.0000000

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**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.62582 a.u.**

H	-2.8030320	0.0043730	-0.0000000
B	-1.6160730	0.0470780	-0.0000000
B	-0.6281120	-1.3863360	-0.0000000
H	-1.6116990	-2.3255560	-0.0000000
B	-0.6898200	1.2653710	0.9074280
H	-1.2192800	2.1247680	1.5307250
B	-0.6898200	-0.4308650	1.4803430
H	1.4176640	0.8161660	2.4719210
H	1.3906290	-2.1024060	1.5303400
B	0.8363830	-1.2322640	0.9466970
H	-1.2366970	-0.8154890	2.4615020
B	0.8272500	0.5083190	1.4907450
H	1.4176640	0.8161660	-2.4719210
B	0.8268000	1.5765840	0.0000000
B	0.8272500	0.5083190	-1.4907450
H	1.4060330	2.6108390	0.0000000
B	-0.6898200	1.2653710	-0.9074280
B	-0.6898200	-0.4308650	-1.4803430
H	-1.2366970	-0.8154890	-2.4615020
B	1.4874960	0.0194740	0.0000000

B	0.8363830	-1.2322640	-0.9466970
H	-1.2192800	2.1247680	-1.5307250
H	1.3906290	-2.1024060	-1.5303400
H	-0.8864190	-2.7253460	-0.0000000

3

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.62200 a.u.**

B	1.4885530	0.0042310	0.0000000
H	1.3874360	-2.5929300	0.0000000
H	1.3982540	-0.8161030	2.4678390
B	-0.6668530	-1.2444730	-0.9749090
B	-0.6668530	-1.2444730	0.9749090
B	0.8422950	-0.4553450	1.4861010
H	-1.1844690	-2.1048400	-1.6078060
H	-1.1844690	-2.1048400	1.6078060
B	0.8148140	-1.5556660	0.0000000
H	1.3982540	-0.8161030	-2.4678390
B	0.8422950	-0.4553450	-1.4861010
B	0.8422950	1.2676920	0.9268660
H	1.4107760	2.0980540	1.5524330
B	-0.6816320	0.4916160	1.4674630
H	-1.2164370	0.8245570	2.4718540
H	-1.7097170	-1.2922450	0.0000000
H	-1.2133530	2.6032610	-0.0000000
B	0.8422950	1.2676920	-0.9268660
B	-0.6404450	1.5657860	-0.0000000
H	1.4107760	2.0980540	-1.5524330
B	-1.6284290	0.0883740	-0.0000000
H	-2.8141380	0.1700610	-0.0000000
H	-1.2164370	0.8245570	-2.4718540
B	-0.6816320	0.4916160	-1.4674630

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**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.61935 a.u.**

H	1.9379990	1.6219310	1.5011390
B	1.1245180	0.9570470	0.9549080
B	0.5071380	-0.5874640	1.5294730
H	0.9433310	-1.1331350	2.4870920

B	1.1245180	0.9570470	-0.9549080
H	1.9379990	1.6219310	-1.5011390
B	1.6153350	-0.4804590	-0.0000000
H	0.9433310	-1.1331350	-2.4870920
H	0.0976700	-2.7898680	-0.0000000
B	0.1572840	-1.5946780	-0.0000000
H	1.4537800	-1.8131910	-0.0000000
H	2.7823520	-0.7339590	-0.0000000
B	0.5071380	-0.5874640	-1.5294730
H	-2.7690620	1.0250630	0.0000000
B	-0.6017830	0.7933290	-1.4975510
B	-1.6536070	0.6254700	0.0000000
H	-1.0056870	1.3554350	-2.4595720
B	-0.1838240	1.4654770	0.0000000
B	-0.6017830	0.7933290	1.4975510
H	-1.0056870	1.3554350	2.4595720
H	-1.9324180	-1.4848210	-1.5119220
B	-1.1425880	-0.8115050	-0.9401670
B	-1.1425880	-0.8115050	0.9401670
H	-1.9324180	-1.4848210	1.5119220

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**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.61755 a.u.**

B	1.4735490	0.0383610	0.0000000
H	1.4962180	-2.5665810	-0.0000000
H	1.3930330	-0.8073650	2.4651170
B	-0.7542200	-1.1936300	-0.9717520
B	-0.7542200	-1.1936300	0.9717520
B	0.8264120	-0.4690860	1.4810700
H	-1.2877970	-2.0237490	-1.6313250
H	-1.2877970	-2.0237490	1.6313250
B	0.8909900	-1.5478950	-0.0000000
H	1.3930330	-0.8073650	-2.4651170
B	0.8264120	-0.4690860	-1.4810700
B	0.8264120	1.2815910	0.9256300
H	1.4159130	2.1059290	1.5395230
B	-0.6893230	0.5289980	1.4488060
H	-1.2175340	0.7868730	2.4788940
H	-0.4071030	-2.1431490	-0.0000000
H	-1.2286290	2.6229010	0.0000000
B	0.8264120	1.2815910	-0.9256300



B	-0.6994390	1.5617900	0.0000000
H	1.4159130	2.1059290	-1.5395230
B	-1.6164450	0.0372390	-0.0000000
H	-2.8038090	0.0372670	-0.0000000
H	-1.2175340	0.7868730	-2.4788940
B	-0.6893230	0.5289980	-1.4488060

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**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.61744 a.u.**

H	-1.4215220	2.0369590	1.6370990
B	-0.8260930	1.2301310	1.0045840
B	0.7200080	0.4390050	1.4629330
H	1.2423290	0.7790730	2.4720330
B	-0.8260930	1.2301310	-1.0045840
H	-1.4215220	2.0369590	-1.6370990
B	0.8099880	1.5070800	0.0000000
H	1.2423290	0.7790730	-2.4720330
H	2.8012700	-0.0277810	-0.0000000
B	1.6150560	-0.0700410	-0.0000000
H	1.3936660	2.5412950	0.0000000
H	-0.4128310	2.1728180	0.0000000
B	0.7200080	0.4390050	-1.4629330
H	-1.4556730	-2.5824150	-0.0000000
B	-0.8020790	-0.5266970	-1.4813640
B	-0.8414620	-1.5686140	-0.0000000
H	-1.4121520	-0.7668840	-2.4691600
B	-1.4697090	0.0007730	0.0000000
B	-0.8020790	-0.5266970	1.4813640
H	-1.4121520	-0.7668840	2.4691600
H	1.2126600	-2.1293150	-1.5395740
B	0.6943210	-1.2713960	-0.9057280
B	0.6943210	-1.2713960	0.9057280
H	1.2126600	-2.1293150	1.5395740

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**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.60893 a.u.**

B	0.1357420	0.0000750	1.6277370
H	0.2363360	0.0000920	2.8123470

B	-1.1656410	0.9043130	0.8370720
H	-2.0176180	-1.5387320	1.3669380
H	-2.6207410	0.4229320	-1.1830230
B	-1.4792320	0.0001530	-0.6228410
H	-2.6210490	-0.4230310	-1.1820060
H	-2.0173170	1.5392600	1.3668360
B	-1.1658160	-0.9039730	0.8371500
H	0.8741960	-2.4878670	1.1631370
B	0.5333220	-1.4576280	0.6826080
B	-0.4977750	-1.4840190	-0.7816110
H	-0.9005530	-2.4502770	-1.3415480
H	2.0389610	1.5486080	-1.5062420
B	-0.4975360	1.4840620	-0.7817220
B	1.2462340	0.9205400	-0.8872850
H	-0.9000140	2.4503690	-1.3417870
B	-0.0189190	-0.0000910	-1.4970850
B	1.2460970	-0.9208750	-0.8871670
H	2.0387300	-1.5491180	-1.5060670
B	1.5945120	-0.0001180	0.6149240
H	2.6914440	-0.0001790	1.0671140
B	0.5335940	1.4575880	0.6825000
H	0.8747080	2.4878050	1.1629060

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**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.59357 a.u.**

B	0.0000000	1.3980890	1.3966770
B	-0.0000000	-0.8880120	-1.4916130
B	-0.8916180	1.5452460	-0.1005560
B	0.8916180	1.5452460	-0.1005560
B	1.0260200	-0.0000000	0.9819360
B	-0.0000000	-1.3980890	1.3966770
B	-1.0260200	0.0000000	0.9819360
B	-1.3814860	0.0000000	-0.8024330
B	-0.8916180	-1.5452460	-0.1005560
B	0.8916180	-1.5452460	-0.1005560
B	1.3814860	-0.0000000	-0.8024330
B	0.0000000	0.8880120	-1.4916130
H	0.0000000	1.9436380	2.4408770
H	-0.0000000	-1.4945740	-2.5112160
H	-1.6872060	2.4269100	-0.0811820
H	1.6872060	2.4269100	-0.0811820

H	1.7177430	-0.0000000	1.9613360
H	-0.0000000	-1.9436380	2.4408770
H	-1.7177430	0.0000000	1.9613360
H	-2.5201040	0.0000000	-1.1459100
H	-1.6872060	-2.4269100	-0.0811820
H	1.6872060	-2.4269100	-0.0811820
H	2.5201040	-0.0000000	-1.1459100
H	0.0000000	1.4945740	-2.5112160

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**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.59710 a.u.**

H	-1.0695000	2.2444460	1.6453560
B	-0.6137240	1.3530780	1.0112760
B	0.7936380	0.3394630	1.4580240
H	1.2876020	0.6759980	2.4835570
B	-0.6137240	1.3530780	-1.0112760
H	-1.0695000	2.2444460	-1.6453560
B	0.8702500	1.4369960	0.0000000
H	1.2876020	0.6759980	-2.4835570
H	2.7965330	-0.2369650	-0.0000000
B	1.6063110	-0.1836740	-0.0000000
H	1.4835510	2.4531470	0.0000000
H	-1.6820420	1.4708210	0.0000000
B	0.7936380	0.3394630	-1.4580240
H	-1.6739580	-2.4306040	-0.0000000
B	-0.8449860	-0.4229370	-1.4833300
B	-0.9415130	-1.4974180	-0.0000000
H	-1.4691350	-0.6617040	-2.4628110
B	-1.4647060	0.1218020	0.0000000
B	-0.8449860	-0.4229370	1.4833300
H	-1.4691350	-0.6617040	2.4628110
H	1.0053860	-2.2422070	-1.5421110
B	0.5866220	-1.3374040	-0.8998250
B	0.5866220	-1.3374040	0.8998250
H	1.0053860	-2.2422070	1.5421110

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**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.59842 a.u.**

B	0.9262640	-1.4293060	0.0000000
B	1.4777690	0.0009060	0.9331500
H	1.5713030	-2.4248390	0.0000000
H	2.5230040	0.1007420	1.4859660
H	0.0328970	-1.5788560	2.4626080
B	0.0445830	-0.9270670	1.4721250
B	-0.8516800	-1.3533260	0.0000000
H	-1.6177790	-2.2689120	0.0000000
H	-2.4306730	0.1644540	1.4938440
B	-1.3805770	0.0311550	0.9567890
H	0.0762470	1.5760310	2.5132710
B	0.0445830	0.8377740	1.5881260
H	-2.4306730	0.1644540	-1.4938440
B	-1.3805770	0.0311550	-0.9567890
B	-0.9457620	1.5378090	-0.0000000
B	0.7509890	1.2313860	-0.0000000
B	0.0445830	0.8377740	-1.5881260
B	0.0445830	-0.9270670	-1.4721250
B	1.4777690	0.0009060	-0.9331500
H	0.0328970	-1.5788560	-2.4626080
H	-1.7353200	2.4210830	-0.0000000
H	0.0762470	1.5760310	-2.5132710
H	0.1161990	2.3874290	-0.0000000
H	2.5230040	0.1007420	-1.4859660

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**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**  
**G = -304.56681 a.u.**

B	0.4331140	1.5115830	0.7658430
B	0.0471630	-0.0326470	1.7472420
H	0.7901700	2.4912030	1.3252260
H	0.0229720	0.0109480	2.9294090
H	2.5417920	0.2673130	1.2887210
B	1.4994830	0.0247330	0.7528630
B	1.2075210	0.8730850	-0.7710450
H	2.0066040	1.3754280	-1.5070110
H	2.0953450	-1.6406350	-1.0506120
B	1.2155350	-0.8947800	-0.7303170
H	0.7853720	-2.4999650	1.3079090
B	0.4437540	-1.4762650	0.8227130
H	-0.0229720	0.0109480	-2.9294090
B	-0.0471630	-0.0326470	-1.7472420

B	-0.4437540	-1.4762650	-0.8227130
B	-1.2155350	-0.8947800	0.7303170
B	-1.4994830	0.0247340	-0.7528630
B	-0.4331140	1.5115830	-0.7658430
B	-1.2075210	0.8730850	0.7710450
H	-0.7901690	2.4912040	-1.3252260
H	-0.7853710	-2.4999650	-1.3079100
H	-2.5417930	0.2673120	-1.2887210
H	-2.0953450	-1.6406360	1.0506110
H	-2.0066040	1.3754290	1.5070110

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**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.54410 a.u.**

B	-2.3468310	-0.6658680	-0.3092650
B	-0.8311850	-0.9820860	-0.5816160
B	0.6615450	-1.6147370	-0.9559810
H	0.8843240	-2.4933220	-1.7162260
H	0.2317870	2.7822460	-1.4334090
B	-1.2791370	0.8093210	-0.3402760
B	0.0680260	1.7608930	-0.8574600
H	-2.5310690	0.8517120	-0.4560560
H	-0.9983390	1.3475810	-1.5072350
B	0.7804750	0.0749060	-1.3103570
H	0.8928570	0.1856560	-2.4919660
B	1.3533670	1.0679320	0.0799960
H	2.3032490	1.7777160	0.0392750
B	-0.1846120	1.4590830	0.9132530
H	1.2468540	0.1124680	2.5307980
H	-3.4437700	-0.8824210	0.0669930
B	-0.8925300	-0.1920280	1.0918090
H	-1.7977490	-0.3145770	1.8631250
H	-0.4162430	2.3530470	1.6568620
B	0.8164750	0.0637440	1.4267270
H	2.8675810	-0.9535370	0.1295360
B	1.7080060	-0.7104890	0.0612150
B	0.2670100	-1.5237780	0.7606950
H	0.1574680	-2.5010300	1.4246010

13

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**$G = -304.54368$  a.u.**

B	-1.2742920	-0.1946520	1.1589890
H	-1.9477120	-0.3317590	2.1270600
H	0.5916300	2.5309200	-0.9544490
H	2.8479770	-1.7273960	0.2589200
B	1.6524220	0.6139790	0.5966430
B	0.4854370	1.4453670	-0.4806270
H	2.5515790	1.1644850	1.1446640
B	1.9197430	-1.0170850	0.0828830
B	0.5229310	-1.1423630	-0.6376400
H	-3.3541060	0.0001330	-0.5383460
B	-2.1920580	-0.1815950	-0.3988050
H	-1.9082460	2.1493170	-0.1090270
B	-0.4274420	0.1274780	-1.4049880
H	-0.6992130	0.0712420	-2.5574400
B	-1.2052720	1.1965190	-0.0455060
B	0.4968280	-0.7543760	1.1879930
H	0.6446530	-1.4994120	2.1000150
B	1.5127100	0.2027580	-1.1556860
H	2.1841060	0.3824410	-2.1135640
H	-1.0210630	-2.6188780	-0.1686330
B	0.0024910	1.0074250	1.1959360
B	-1.0557380	-1.4164250	-0.1566590
H	-0.0032600	1.7408180	2.1284310
H	-2.0751460	-1.2970640	-1.0303010

**14**

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**$G = -304.54433$  a.u.**

H	-3.6957070	-0.1385230	-0.7269710
H	-2.0683130	2.1744650	0.2159070
B	-1.1557800	1.4487630	0.0048960
B	-2.8275120	-0.3947120	0.0537040
B	-0.0838910	0.8137810	1.2507740
H	-0.6233490	1.0324780	2.2891260
H	-0.5509260	-2.9016220	-0.0778470
H	0.9788800	-1.3679330	2.4323170
B	-1.2425800	-0.2455220	-0.3794280
B	0.6599380	-0.9490790	1.3691160
H	-3.1176480	-0.7224300	1.1651940
H	-0.5585490	-1.4351810	1.2549980

B	-0.1630570	-1.7903930	0.0466940
B	1.4843450	-1.1285940	-0.1959200
H	2.2767710	0.7551590	-1.8074370
B	0.1713420	-0.8004140	-1.3666100
H	2.4034380	-1.8550550	-0.3788700
H	-0.0297900	-1.3692820	-2.3907550
B	1.4372210	0.4467620	-1.0296670
B	-0.2151200	0.8417740	-1.1607960
B	0.6670400	1.7830000	-0.0161090
H	1.0768840	2.8921470	-0.0658740
B	1.5504240	0.4276420	0.7552160
H	2.4964610	0.6707450	1.4308610

15

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**$G = -304.53493$  a.u.**

B	-0.0197340	-1.3358100	0.3730130
H	0.3552110	-0.2054800	2.6578570
H	3.4647860	-0.6351860	1.3013450
B	-1.1823530	0.9922490	0.7945530
B	0.5947960	1.3564200	0.6235100
B	2.8890180	-0.7061810	0.2544090
H	-1.9113350	1.7561600	1.3381880
H	1.1773350	2.2201300	1.1902260
B	0.0599810	-0.0658210	1.5177860
H	-2.3223560	-1.1709010	1.7356410
B	-1.5422600	-0.7569860	0.9478540
B	1.2640770	-0.2654340	0.1608810
H	3.4973880	-1.0755050	-0.7066140
B	1.0174700	0.9350540	-1.0659540
H	1.9075840	1.2893150	-1.7642610
B	-0.5552330	1.6518180	-0.6971940
H	0.4644090	-1.1955970	-2.3171070
B	-1.2622070	-1.5977750	-0.6339680
B	0.1898870	-0.8138840	-1.2295250
H	-1.8364490	-2.4555820	-1.2063050
H	-0.0471190	1.1979000	-1.8184820
H	-1.0240220	2.6795880	-1.0621590
H	-2.5759120	0.2469220	-1.4032130
B	-1.6833450	0.0759970	-0.6343890

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**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**$G = -304.53102$  a.u.**

H	-2.6880180	-1.6608020	-1.0443280
B	-2.0197450	-0.7916020	-0.6070690
B	0.8314230	-0.8609970	-1.1178650
H	0.9169860	-1.6187720	-2.0261440
H	0.9470590	1.8396570	-1.8115960
B	-2.0095880	0.8429730	-0.5330380
B	0.8331860	0.9880800	-0.9955970
H	-2.6635970	1.7593120	-0.8875300
B	-0.5983050	0.0416220	-1.0362170
B	2.2122450	0.0289890	-0.5484340
H	3.1625640	0.1311970	-1.2535210
B	-1.5836350	-0.0687790	0.9588520
H	-2.3009440	-0.1440560	1.9052070
B	-0.4751100	-1.3134720	0.2386400
H	0.1177350	-0.1567860	2.7075370
H	2.7293390	-0.2764780	0.5354190
B	1.3519570	-0.9857230	0.6305690
H	1.8517060	-1.8406760	1.2857080
H	-0.5610580	-2.4908680	0.3623390
B	0.1141470	-0.0737240	1.5241360
H	-0.6237150	2.4420970	0.6091460
B	-0.4812350	1.2833690	0.3843470
B	1.2656040	0.9725670	0.7410920
H	1.9072230	1.6996530	1.4206810

**TS<sub>8-6</sub>**

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**$G = -304.59697$  a.u.**

**$\nu = 504.0i$  cm<sup>-1</sup>**

H	-1.1674070	2.1482650	1.6740220
B	-0.6802530	1.3197460	0.9749130
B	0.7797110	0.3919530	1.4454570
H	1.2459270	0.7333320	2.4805400
B	-0.6802530	1.3197460	-0.9749130
H	-1.1674070	2.1482650	-1.6740220
B	0.8449080	1.4709130	-0.0000000
H	1.2459270	0.7333320	-2.4805400
H	2.8123100	-0.1797570	-0.0000000



B	1.6245940	-0.1205310	-0.0000000
H	1.4124070	2.5118910	-0.0000000
H	-1.6118410	1.6296480	-0.0000000
B	0.7797110	0.3919530	-1.4454570
H	-1.5336460	-2.5488420	0.0000000
B	-0.8470440	-0.4564260	-1.4731220
B	-0.8763120	-1.5631710	0.0000000
H	-1.4400300	-0.7044190	-2.4681940
B	-1.4745840	0.0250950	0.0000000
B	-0.8470440	-0.4564260	1.4731220
H	-1.4400300	-0.7044190	2.4681940
H	1.0859590	-2.1787700	-1.5628110
B	0.6354700	-1.3024020	-0.9029400
B	0.6354700	-1.3024020	0.9029400
H	1.0859590	-2.1787700	1.5628110

**TS<sub>6-5</sub>**

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.61178**

**v = 318.4i cm<sup>-1</sup>**

B	-0.0711340	0.1191790	-1.4527780
H	2.4592900	-0.1260250	-1.6343430
H	0.8570720	2.5437560	-1.2720660
B	1.1560640	-1.0868020	0.6588300
B	1.2643250	0.8186480	0.7565800
B	0.4410660	1.5592280	-0.7635710
H	2.0612070	-1.7180970	1.0892820
H	2.0594920	1.4249040	1.4110030
B	1.5237920	-0.0470280	-0.9004370
H	0.6846100	-2.3692770	-1.5833510
B	0.3826110	-1.4564670	-0.8892100
B	-1.2897980	1.0260580	-0.7181990
H	-2.1274880	1.6848880	-1.2359870
B	-0.4219990	1.4332430	0.7774360
H	-0.6113780	2.4152620	1.4144830
H	2.3107880	0.4907790	0.0357950
H	-2.5575580	0.0453720	1.3304240
B	-1.3322350	-0.8145500	-0.8441500
B	-1.5213230	0.0220210	0.7537450
H	-2.1989530	-1.3420350	-1.4564350
B	0.0334700	-0.1451570	1.6064540
H	0.0721380	-0.1668890	2.7923270

H	-0.9512960	-2.5253950	1.0831300
B	-0.5764230	-1.4998210	0.6204490

**TS<sub>5-3</sub>**

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.61410**

**v = 229.8i cm<sup>-1</sup>**

B	1.5105690	0.0376200	0.0000000
H	1.4084040	-2.6051450	0.0000000
H	1.3669820	-0.8184930	2.4685300
B	-0.7138390	-1.2055100	-0.9392090
B	-0.7138390	-1.2055100	0.9392090
B	0.8427030	-0.4860080	1.4599330
H	-1.2093300	-1.9941990	-1.6872200
H	-1.2093300	-1.9941990	1.6872200
B	0.9086280	-1.5328120	0.0000000
H	1.3669820	-0.8184930	-2.4685300
B	0.8427030	-0.4860080	-1.4599330
B	0.8245780	1.2705850	0.9238410
H	1.4015630	2.0803190	1.5697350
B	-0.7138390	0.5205430	1.4369740
H	-1.2198420	0.7800410	2.4767890
H	-1.0379830	-2.0916400	0.0000000
H	-1.1875690	2.6573820	-0.0000000
B	0.8245780	1.2705850	-0.9238410
B	-0.6820440	1.5848580	-0.0000000
H	1.4015630	2.0803190	-1.5697350
B	-1.6264080	0.0953960	-0.0000000
H	-2.8113620	0.0226560	-0.0000000
H	-1.2198420	0.7800410	-2.4767890
B	-0.7138390	0.5205430	-1.4369740

**TS<sub>3-1</sub>**

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.61682**

**v = 925.4i cm<sup>-1</sup>**

H	2.5331790	0.0541120	1.5086310
B	1.4946640	0.0368990	0.9387060
B	0.0369380	-0.7839260	1.5082830
H	0.0163840	-1.4769670	2.4708440

B	1.4946640	0.0368990	-0.9387060
H	2.5331790	0.0541120	-1.5086310
B	0.9372200	-1.3949280	-0.0000000
H	0.0163840	-1.4769670	-2.4708440
H	-1.5800090	-2.2540010	-0.0000000
B	-0.8339620	-1.2709560	-0.0000000
H	-0.3736350	-2.4325200	-0.0000000
H	1.5802210	-2.3963340	-0.0000000
B	0.0369380	-0.7839260	-1.5082830
H	-1.4927590	2.5473910	0.0000000
B	0.0369380	0.9857490	-1.4960210
B	-0.8960640	1.5233880	0.0000000
H	0.0762240	1.6713400	-2.4621220
B	0.7817910	1.2541940	0.0000000
B	0.0369380	0.9857490	1.4960210
H	0.0762240	1.6713400	2.4621220
H	-2.4426350	0.0691580	-1.5290070
B	-1.4130450	0.0954470	-0.9437730
B	-1.4130450	0.0954470	0.9437730
H	-2.4426350	0.0691580	1.5290070

1-

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**  
**G = -304.65785 a.u.**

H	-1.5378740	2.1167020	1.3988040
B	-0.8911930	1.2266210	0.9136500
B	-0.0000000	1.5154050	-0.6522100
H	-0.0000000	2.6159960	-1.1364960
B	-1.4419800	-0.4685280	0.9136500
H	-2.4883320	-0.8085080	1.3988040
B	-1.4412360	0.4682860	-0.6522100
H	-1.5376440	-2.1163860	-1.1364960
H	0.0000000	0.0000000	-4.1856090
B	0.0000000	0.0000000	-1.5213440
H	0.0000000	0.0000000	-4.9497240
H	-2.4879600	0.8083870	-1.1364960
B	-0.8907330	-1.2259880	-0.6522100
H	2.4883320	-0.8085080	1.3988040
B	-0.0000000	-1.5161870	0.9136500
B	1.4419800	-0.4685280	0.9136500
H	-0.0000000	-2.6163870	1.3988040
B	0.0000000	0.0000000	1.7789070
B	0.8911930	1.2266210	0.9136500
H	1.5378740	2.1167020	1.3988040
H	1.5376440	-2.1163860	-1.1364960

B	0.8907330	-1.2259880	-0.6522100
B	1.4412360	0.4682860	-0.6522100
H	2.4879600	0.8083870	-1.1364960

**B<sub>12</sub>H<sub>12</sub><sup>2-</sup>, I<sub>h</sub>**

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.79964 a.u.**

B	0.000000000	0.000000000	1.700239000
B	-1.446309000	0.469934000	0.760370000
H	0.000000000	0.000000000	2.905667000
H	-2.471708000	0.803107000	1.299454000
H	-1.527600000	-2.102561000	1.299454000
B	-0.893868000	-1.230304000	0.760370000
B	0.893868000	-1.230304000	0.760370000
H	1.527600000	-2.102561000	1.299454000
H	-0.000000000	-2.598908000	-1.299454000
B	-0.000000000	-1.520740000	-0.760370000
H	-2.471708000	-0.803107000	-1.299454000
B	-1.446309000	-0.469934000	-0.760370000
H	2.471708000	-0.803107000	-1.299454000
B	1.446309000	-0.469934000	-0.760370000
B	0.000000000	-0.000000000	-1.700239000
B	-0.893868000	1.230304000	-0.760370000
B	0.893868000	1.230304000	-0.760370000
B	1.446309000	0.469934000	0.760370000
B	0.000000000	1.520740000	0.760370000
H	2.471708000	0.803107000	1.299454000
H	0.000000000	-0.000000000	-2.905667000
H	1.527600000	2.102561000	-1.299454000
H	-1.527600000	2.102561000	-1.299454000
H	0.000000000	2.598908000	1.299454000

**A**

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.59708 a.u.**

H	0.0476130	2.8711210	-0.8144250
B	0.0258160	1.7172440	-0.5454570
B	-0.9348010	1.1020040	0.8705640
H	-1.4770550	2.0031030	1.4207280
B	1.6400360	0.4537370	-0.6093590
H	2.6185310	0.8555400	-1.1394850
B	0.9345850	1.0654020	0.8860200
H	2.3954860	-1.1091340	1.2205090
H	-0.0614370	-0.2825010	2.7820240

B	-0.0609160	-0.2317260	1.5903960
H	1.5290010	1.8793620	1.5137960
H	0.5929790	1.3567330	-1.7716780
B	1.3999730	-0.6867330	0.7312030
H	-1.5136910	-1.8091260	-1.7503050
B	0.9037680	-1.1680290	-0.9348320
B	-0.9464490	-1.1070740	-0.9799030
H	1.4772050	-1.9254400	-1.6455230
B	0.0370540	0.2060680	-1.4443110
B	-1.4952840	0.5971550	-0.7467620
H	-2.4159870	1.0565390	-1.3349230
H	-0.1305010	-2.7685590	0.8364010
B	-0.0868830	-1.6343960	0.4922300
B	-1.5189540	-0.5555610	0.6131070
H	-2.5518730	-0.9180960	1.0684050

**B**

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**$G = -304.59217$  a.u.**

B	1.2650900	1.4309290	-0.2624600
B	-0.9164810	-1.4430220	0.1984840
B	1.5568270	-0.2806410	-0.8358350
B	1.5014540	0.0420670	0.8887350
B	-0.0407030	1.1349660	0.9948110
B	-1.2729110	1.4159800	-0.2767770
B	0.0207000	0.6836480	-1.1865150
B	0.0344490	-1.0762780	-1.2478810
B	-1.5280070	-0.1788360	-0.9360590
B	-1.5471700	0.0920410	0.8417340
B	-0.0398860	-0.5732870	1.4943140
B	0.8659650	-1.4905600	0.2668580
H	1.8395990	2.4610300	-0.2616940
H	-1.5510370	-2.4367650	0.3283180
H	2.4448710	-0.3680890	-1.6173780
H	2.4195110	0.2688800	1.6072450
H	0.0279680	2.1151140	1.6712310
H	-1.7303590	2.4909260	-0.4415160
H	0.4961650	1.7375460	-1.6378070
H	0.0348740	-1.6520960	-2.2875210
H	-2.3876070	-0.3432630	-1.7350210
H	-2.4877950	0.2409250	1.5511160
H	-0.0465810	-0.7918160	2.6640690

H 1.4437560 -2.5074250 0.4619200

C

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.58181 a.u.**

B	0.3690690	0.8147220	-1.4672610
B	-0.3690690	-0.8147220	-1.4672610
B	0.4595190	0.7631240	1.4858500
B	-0.4595190	-0.7631240	1.4858500
B	-1.3484530	0.5806140	-0.9388240
B	1.3484530	-0.5806140	-0.9388240
B	-1.4552350	0.5662280	0.8254670
B	1.4552350	-0.5662280	0.8254670
B	-0.2121900	1.5249060	0.0200420
B	1.4552350	0.9731790	-0.0702750
B	-1.4552350	-0.9731790	-0.0702750
B	0.2121900	-1.5249060	0.0200420
H	-2.2325900	1.0536270	-1.5720630
H	-0.3429630	2.5151400	0.7197570
H	0.5841090	1.4407190	-2.4523430
H	-0.5841090	-1.4407190	-2.4523430
H	-2.3948840	-1.6957520	-0.0461790
H	0.3429630	-2.5151400	0.7197570
H	-0.7082440	-1.2095180	2.5543840
H	2.3317040	-0.9539260	1.5214560
H	0.7082440	1.2095180	2.5543840
H	2.3948840	1.6957520	-0.0461790
H	-2.3317040	0.9539260	1.5214560
H	2.2325900	-1.0536270	-1.5720630

D

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.56931 a.u.**

B	0.0000000	0.8439440	-1.5140700
B	-0.0000000	-0.8439440	-1.5140700
B	-0.0000000	0.8439440	1.5140700
B	0.0000000	-0.8439440	1.5140700
B	-1.5140700	0.0000000	-0.8439440
B	1.5140700	0.0000000	-0.8439440
B	-1.5140700	0.0000000	0.8439440
B	1.5140700	-0.0000000	0.8439440

B	-0.8439440	1.5140700	-0.0000000
B	0.8439440	1.5140700	0.0000000
B	-0.8439440	-1.5140700	-0.0000000
B	0.8439440	-1.5140700	0.0000000
H	-2.5134330	0.0000000	-1.4784110
H	-1.4784110	2.5134330	-0.0000000
H	-0.0000000	1.4784110	-2.5134330
H	-0.0000000	-1.4784110	-2.5134330
H	-1.4784110	-2.5134330	0.0000000
H	1.4784110	-2.5134330	-0.0000000
H	-0.0000000	-1.4784110	2.5134330
H	2.5134330	0.0000000	1.4784110
H	0.0000000	1.4784110	2.5134330
H	1.4784110	2.5134330	0.0000000
H	-2.5134330	0.0000000	1.4784110
H	2.5134330	-0.0000000	-1.4784110

## E

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.56750 a.u.**

B	-0.0000000	0.8937550	1.5001240
B	-0.0000000	-0.8937550	1.5001240
B	0.0000000	0.8373790	-1.5425060
B	-0.0000000	-0.8373790	-1.5425060
B	1.4480980	-0.0000000	0.9378860
B	-1.4480980	0.0000000	0.9378860
B	1.5600520	-0.0000000	-0.8443990
B	-1.5600520	0.0000000	-0.8443990
B	0.8340870	1.4156380	0.0349150
B	-0.8340870	1.4156380	0.0349150
B	0.8340870	-1.4156380	0.0349150
B	-0.8340870	-1.4156380	0.0349150
H	2.4731030	-0.0000000	1.5342930
H	1.5621820	2.2895530	-0.3613480
H	-0.0000000	1.5256600	2.5032970
H	-0.0000000	-1.5256600	2.5032970
H	1.5621820	-2.2895530	-0.3613480
H	-1.5621820	-2.2895530	-0.3613480
H	0.0000000	-1.5660570	-2.4748660
H	-2.5758830	0.0000000	-1.4446960
H	0.0000000	1.5660570	-2.4748660
H	-1.5621820	2.2895530	-0.3613480
H	2.5758830	-0.0000000	-1.4446960

H	-2.4731030	0.0000000	1.5342930
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**F**

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.54697 a.u.**

B	-0.6847040	1.5659780	0.0000000
B	0.7458170	1.1507240	0.9295540
B	0.6847040	-1.5659780	0.0000000
B	0.7458170	-0.4831450	1.5169900
B	0.7458170	1.1507240	-0.9295540
B	1.7090800	0.0143410	-0.0000000
B	-0.7458170	-1.1507240	-0.9295540
B	0.7458170	-0.4831450	-1.5169900
B	-1.7090800	-0.0143410	-0.0000000
B	-0.7458170	0.4831450	1.5169900
B	-0.7458170	-1.1507240	0.9295540
B	-0.7458170	0.4831450	-1.5169900
H	1.3582930	-0.8803420	-2.4511420
H	-1.3582930	0.8803420	-2.4511420
H	1.3649380	2.1054500	-1.3214930
H	2.8630610	-0.2701070	-0.0000000
H	1.4146460	-2.5038910	-0.0000000
H	1.3582930	-0.8803420	2.4511420
H	-1.3649380	-2.1054500	1.3214930
H	-1.3582930	0.8803420	2.4511420
H	-2.8630610	0.2701070	-0.0000000
H	-1.4146460	2.5038910	-0.0000000
H	-1.3649380	-2.1054500	-1.3214930
H	1.3649380	2.1054500	1.3214930

**G**

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.54638 a.u.**

B	0.0000000	1.4263050	0.9418260
B	-0.9296480	0.0000000	1.3711780
B	-0.0000000	-1.4263050	-0.9418260
B	-1.5169670	-0.8886890	0.0000000
B	0.9296480	-0.0000000	1.3711780
B	-0.0000000	-1.4263050	0.9418260
B	0.9296480	0.0000000	-1.3711780
B	1.5169670	-0.8886890	0.0000000
B	0.0000000	1.4263050	-0.9418260



B	-1.5169670	0.8886890	0.0000000
B	-0.9296480	0.0000000	-1.3711780
B	1.5169670	0.8886890	0.0000000
H	2.4511030	-1.6187010	0.0000000
H	2.4511030	1.6187010	0.0000000
H	1.3215700	-0.0000000	2.5090840
H	0.0000000	-2.5491410	1.3314220
H	0.0000000	-2.5491410	-1.3314220
H	-2.4511030	-1.6187010	-0.0000000
H	-1.3215700	-0.0000000	-2.5090840
H	-2.4511030	1.6187010	0.0000000
H	0.0000000	2.5491410	-1.3314220
H	0.0000000	2.5491410	1.3314220
H	1.3215700	0.0000000	-2.5090840
H	-1.3215700	0.0000000	2.5090840

**H**

**CCSD(T)/def2-TZVP//TPSS/def2-TZVP**

**G = -304.54549 a.u.**

B	-0.7671140	0.7198640	-1.3545340
B	1.1042730	0.3678870	-1.2602800
B	0.7671140	-0.7198640	1.3545340
B	1.5562960	0.5527300	0.4092710
B	-0.1359560	-1.0790980	-1.3260810
B	1.2817310	-1.0861270	-0.2659230
B	-1.1042730	-0.3678870	1.2602800
B	-0.3244770	-1.6411450	0.3087890
B	-1.2817310	1.0861270	0.2659230
B	0.3244770	1.6411450	-0.3087890
B	0.1359560	1.0790980	1.3260810
B	-1.5562960	-0.5527300	-0.4092710
H	-0.5502470	-2.8114100	0.4266750
H	-2.6712330	-0.9468240	-0.5986300
H	-0.1666220	-1.5353570	-2.4239360
H	2.1904730	-1.8613880	-0.3530290
H	1.0656820	-1.0260800	2.4642410
H	2.6712330	0.9468240	0.5986300
H	0.1666220	1.5353570	2.4239360
H	0.5502470	2.8114100	-0.4266750
H	-2.1904730	1.8613880	0.3530290
H	-1.0656820	1.0260800	-2.4642410
H	-1.5997150	-0.5248080	2.3299570
H	1.5997150	0.5248080	-2.3299570

