

Electronic Supporting Information

The Norbornene Mystery Revealed

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Figure S1: Molecules for $^1J_{CC}$ -coupling comparison between experiment and computation.

Table S2: $^1J_{CC}$ -coupling comparison between experiment and computation.

B3LYP/6-311+G(d,p) (BLW and canonical) optimized structures for all compounds considered in the article.

Computational Details

Standard geometries were optimized at the B3LYP¹, 2/6-311+G** level using Gaussian 09.³ The BLW-constrained B3LYP/6-311+G** geometries ('loc') were optimized using a modified version of GAMESS-US (release 2008)⁴ interfaced with the BLW-module.^{5, 6} Both the density and the J -coupling constants have been computed at the PBE⁷/IGLO-III level in Dalton 2.0.⁸ The BLW-eigenvalues and eigenvectors were optimized at the given DFT level with the SCF module of Dalton, SIRIUS, that has been interfaced with the BLW-module. The BLW-eigenvectors were normalized before being input into the property evaluation module, ABACUS, which computes the indirect spin-spin coupling constants (1J) using the linear-response formalism.⁹ Chemical shifts and nucleus-independent chemical shifts (NICS)^{10, 11} were computed at the (BLW)-IGLO level as previously reported:¹² (BLW)-PW91/IGLO-III orbitals are obtained with GAMESS, read into a modified version of deMon-MASTER¹³ and localized by the Pipek-Mezey algorithm.¹⁴ Isotropic

NMR ^{13}C chemical shifts are referenced to the experimental benzene ^{13}C chemical shift ($\delta=128.6$ ppm). ΔNICS corresponds to $[(\text{NICS})-(\text{BLW-NICS})]$ ¹²The graphical representations of the density are done with Molekel.¹⁵

Table S1: (BLW)-PBE/IGLO-III $^1J_{CC}$ -coupling isotropic coupling constants are given in Hz. The numbering corresponds to norbornene (see **1b'** in Figure 1) and localized geometries (BLW-optimized) are denoted 'loc'.

Compound	$^1J_{56}$	$^1J_{16}$	$^1J_{12}$	$^1J_{23}$	$^1J_{17}$
1a	28.5	29.8	29.8	28.5	28.2
1b	38.6	25.9	35.3	68.8	29.4
BLW-1b	34.0	26.1	37.1	71.4	26.8
1b_{loc}	36.9	27.6	31.7	72.3	30
BLW-1b_{loc}	32.6	27.5	32.8	74.6	27.6
1b'	38.2	26.1	35.6	68.8	29.5
BLW-1b'	33.3	25.5	36.8	70.8	27.3
2a	28.4	30.1	30.1	28.4	30.1
2b	34.3	28.6	36.3	66.1	28.6
BLW-2b	30.4	27.5	37.9	66.8	27.5
2b_{loc}	32.8	30.2	32.2	69.2	30.2
BLW-2b_{loc}	29.5	29.1	33.6	69.7	29.1
3b	44.7	25.2	35.7	75.2	35.7
BLW-3b	40.0	24.2	36.9	78.5	34.4
3b_{loc}	42.4	27.3	31.2	79.4	37.3
BLW-3b_{loc}	38.5	26.4	32.5	82.5	36.1
4a	29.4	28.9	28.9	29.4	37.3
4b	35.8	26.9	35.3	68.3	36.4
BLW-4b	32.5	25.8	36.4	70.0	34.7
4b_{loc}	34.3	28.6	31.5	71.5	37.9
BLW-4b_{loc}	31.5	27.4	32.4	73.0	36.1
5a	30.0	30.0	30.0	30.0	
5b	29.4	30.6	37.2	72.2	
BLW-5b	28.4	30.1	37.6	70.5	
5b_{loc}	29.4	30.7	33.3	75.0	
BLW-5b_{loc}	28.5	30.3	33.2	73.0	
5b'	35.1	29.0	37.5	69.3	
BLW-5b'	33.2	28.1	38.3	70.4	
5b'_{loc}	33.9	30.4	33.4	72.4	
BLW-5b'_{loc}	32.4	29.7	34.0	73.4	
6a	35.3	40.0	27.3	32.7	
6b	48.1	36.1	33.3	77.2	
BLW-6b	41.6	33.9	32.8	77.6	
6b_{loc}	45.8	38.7	28.4	81.5	
BLW-6b_{loc}	40.2	36.5	28.1	81.0	
7	34.7	27.6	36.3	66.0	42.0
BLW-7	30.3	27	37.6	68.7	39.4
8	39.4	26.4	35.5	70.1	24.3
BLW-8	35.3	25.8	35.8	72.9	21.0
9	34.0	26.6	39.4	49.0	29.0

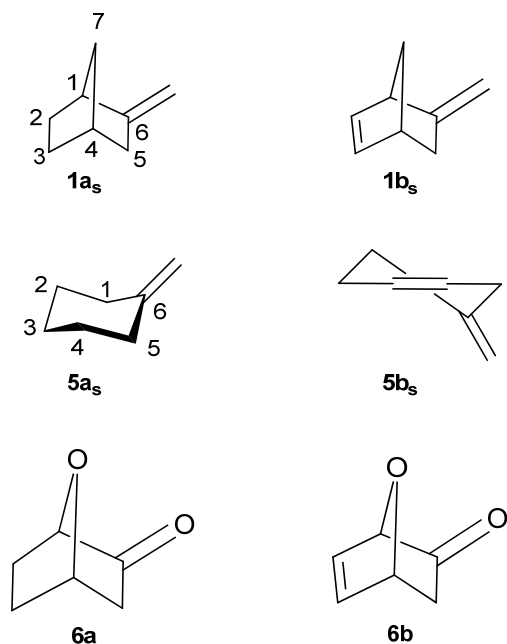


Table S2: (BLW)-PBE/IGLO-III $^1J_{CC}$ -coupling isotropic coupling constants (in Hz). The numbering corresponds to norbornene (see in Figure S1). Experimental values are taken from ref¹⁶.

Table S2: PBE/IGLO-III $^1J_{CC}$ -coupling and experimental (taken from ref¹⁶) isotropic coupling constants (in Hz). The numbering corresponds to norbornene (see in Figure S1).

	$^1J_{12}$	$^1J_{23}$	$^1J_{34}$	$^1J_{45}$	$^1J_{56}$	$^1J_{61}$	$^1J_{17}$	$^1J_{47}$	Others
1a_{s,exp}	30.7	32.5	31.0	32.5	37.3	39.6	31.1	29.6	74.2
1a_{s,calc}	28.1	29.2	29.5	29.9	35.3	37.4	28.4	27.7	77.8
1b_{s,exp}	40.0	67.3	42.6	31.1	47.3	36.1	31.0	30.4	75.4
1b_{s,calc}	33.7	70.3	35.1	26.7	46.3	33.7	29.4	28.7	79.3
5a_{s,exp}	31.9	33.3	33.3	31.9	39.7	39.7			72.3
5a_{s,calc}	28.9	30.2	30.2	28.9	37.0	37.0			75.0
5b_{s,exp}	40.0	60.0	40.5	33.3	40.0	40.0			73.0
5b_{s,calc}	36.7	72.9	37.7	29.2	37.3	37.8			76.1
6a,exp	30.5	33.5	33.5	35.6	38.1	42.8			
6a,calc	27.3	32.7	30.0	33.0	35.3	40.0			
6b,exp	36.2	71.7	38.9	32.9	48.2	39.8			
6b,calc	33.3	77.2	35.9	30.2	48.1	36.1			

1a

C	0.000000	1.133216	0.339523
C	1.255384	0.782476	-0.493306
C	1.255384	-0.782476	-0.493306
C	0.000000	-1.133216	0.339523
C	0.000000	0.000000	1.388923
C	-1.255384	-0.782476	-0.493306
C	-1.255384	0.782476	-0.493306
H	0.889794	0.000000	2.025405
H	-0.889794	0.000000	2.025405
H	0.000000	2.152510	0.729862
H	-1.208094	1.204478	-1.500692
H	-2.158775	1.175953	-0.019056
H	-1.208094	-1.204478	-1.500692
H	-2.158775	-1.175953	-0.019056
H	0.000000	-2.152510	0.729862
H	2.158775	1.175953	-0.019056
H	1.208094	1.204478	-1.500692
H	2.158775	-1.175953	-0.019056
H	1.208094	-1.204478	-1.500692

1b

C	1.797490	1.440660	0.173910
C	1.449550	1.833770	1.652030
C	-0.111080	1.833770	1.652030
C	-0.459020	1.440660	0.173910
C	0.669230	2.180910	-0.583240
C	1.338470	0.000000	0.000000
C	0.000000	0.000000	0.000000
H	0.669230	3.262410	-0.415100
H	0.669230	1.972770	-1.655000
H	2.824200	1.658580	-0.119520
H	-1.485730	1.658580	-0.119520
H	1.846000	2.825930	1.884630
H	1.874480	1.130180	2.370050
H	-0.507530	2.825930	1.884630
H	-0.536010	1.130180	2.370050
H	1.993110	-0.863020	0.000000
H	-0.654650	-0.863020	0.000000

1b_{loc}

C	1.798682	1.463611	0.171458
C	1.454364	1.833930	1.642385
C	-0.115904	1.833960	1.642374
C	-0.460211	1.463594	0.171456
C	0.669226	2.192500	-0.586639
C	1.333260	-0.024727	0.016099
C	0.005251	-0.024739	0.016107
H	0.669210	3.273297	-0.416379
H	0.669235	1.990179	-1.659783
H	2.822781	1.672953	-0.134540
H	-1.484322	1.672914	-0.134528
H	1.848007	2.821077	1.897373
H	1.873199	1.117860	2.352792
H	-0.509507	2.821141	1.897287
H	-0.534779	1.117957	2.352826
H	1.999355	-0.878608	0.020297
H	-0.660878	-0.878606	0.020275

1b'

C	-0.458890	1.452340	-0.000020
C	-0.111410	2.027510	-1.416630
C	1.449480	2.027510	-1.416630
C	1.796950	1.452340	-0.000020
C	0.669030	2.093760	0.844840
C	1.338060	0.000000	0.000000
C	0.000000	0.000000	0.000000
H	0.669030	3.188250	0.814500
H	0.669030	1.753090	1.882200
H	-1.486320	1.629930	0.316980
H	2.824390	1.629930	0.316980
H	-0.508010	3.040780	-1.523590
H	-0.535380	1.418680	-2.216960
H	1.846070	3.040780	-1.523590
H	1.873440	1.418680	-2.216960
H	1.995910	-0.860250	0.000000
H	-0.657850	-0.860250	0.000000

2a

C	0.000000	0.000000	1.298791
C	0.000000	1.450879	0.779169
C	1.256498	-0.725440	0.779169
C	-1.256498	-0.725440	0.779169
C	0.000000	1.450879	-0.779169
C	1.256498	-0.725440	-0.779169
C	-1.256498	-0.725440	-0.779169
C	0.000000	0.000000	-1.298791
H	0.000000	0.000000	2.393497
H	0.877017	1.979498	1.166126
H	-0.877017	1.979498	1.166126
H	1.275787	-1.749269	1.166126
H	2.152805	-0.230230	1.166126
H	-2.152805	-0.230230	1.166126
H	-1.275787	-1.749269	1.166126
H	0.877017	1.979498	-1.166126
H	-0.877017	1.979498	-1.166126
H	1.275787	-1.749269	-1.166126
H	2.152805	-0.230230	-1.166126
H	-2.152805	-0.230230	-1.166126
H	-1.275787	-1.749269	-1.166126
H	0.000000	0.000000	-2.393497

2b

C	1.445520	2.137670	-1.254370
C	-0.108740	2.137670	-1.254380
C	1.958910	1.376770	0.000000
C	-0.622130	1.376770	0.000000
C	-0.108740	2.137670	1.254370
C	0.000000	0.000000	0.000000
C	1.445520	2.137670	1.254380
C	1.336780	0.000000	0.000000
H	1.836480	3.160220	-1.239960
H	1.834030	1.660310	-2.157220
H	-0.499700	3.160210	-1.239970
H	-0.497240	1.660310	-2.157220
H	3.050300	1.334800	0.000000
H	-1.713520	1.334800	0.000000
H	-0.497240	1.660310	2.157220
H	-0.499700	3.160220	1.239960
H	-0.604140	-0.901110	0.000000
H	1.834020	1.660310	2.157220
H	1.836480	3.160220	1.239970
H	1.940930	-0.901110	0.000000

2b_{loc}

C	1.448745	2.140698	-1.253589
C	-0.111933	2.140726	-1.253592
C	1.960214	1.399688	0.000017
C	-0.623426	1.399681	-0.000016
C	-0.111962	2.140702	1.253589
C	0.005005	-0.024000	0.000001
C	1.448716	2.140734	1.253598
C	1.331785	-0.024003	-0.000006
H	1.837490	3.164048	-1.255134
H	1.833056	1.654841	-2.154733
H	-0.500645	3.164088	-1.255060
H	-0.496265	1.654943	-2.154765
H	3.051476	1.348138	0.000034
H	-1.714687	1.348128	-0.000032
H	-0.496277	1.654857	2.154738
H	-0.500711	3.164050	1.255113
H	-0.611975	-0.916323	0.000011
H	1.833047	1.654950	2.154772
H	1.837420	3.164098	1.255073
H	1.948749	-0.916334	-0.000020

3b

C	1.333150	2.246890	-1.032360
C	1.947800	1.388450	0.060600
C	1.441130	2.012520	1.418860
C	-0.108040	2.012530	1.418830
C	-0.614660	1.388450	0.060560
C	0.000020	2.246870	-1.032390
C	1.333130	0.000000	0.000000
C	0.000000	0.000000	0.000000
H	1.834770	1.424990	2.251520
H	1.834790	3.027000	1.515460
H	-0.501720	1.425020	2.251480
H	-0.501700	3.027020	1.515400
H	3.036930	1.371040	0.022740
H	-1.703800	1.371040	0.022660
H	-0.616240	-0.891480	0.000000
H	-0.616210	2.827560	-1.708820
H	1.949370	-0.891480	0.000010
H	1.949400	2.827580	-1.708760

3b_{loc}

C	1.329430	2.278880	-1.030020
C	1.943620	1.438500	0.065120
C	1.439980	2.033130	1.421340
C	-0.117270	2.033150	1.421310
C	-0.620880	1.438520	0.065070
C	-0.006620	2.278890	-1.030060
C	1.322750	0.000000	0.000000
C	0.000000	0.000000	0.000000
H	1.828100	1.432470	2.248610
H	1.830590	3.045780	1.542080
H	-0.505440	1.432500	2.248560
H	-0.507870	3.045810	1.542040
H	3.032610	1.412300	0.022460
H	-1.709880	1.412340	0.022360
H	-0.630720	-0.881130	0.000000
H	-0.617220	2.847550	-1.722380
H	1.953460	-0.881130	0.000000
H	1.940070	2.847530	-1.722310

4a

C	-0.778470	1.256960	-1.184017
C	-1.296776	0.000000	-0.447006
C	-0.778470	-1.256870	-1.184168
C	0.778470	-1.256960	-1.184017
C	1.296776	0.000000	-0.447006
C	0.778470	1.256870	-1.184168
C	-0.744911	0.000000	0.967198
C	0.744911	0.000000	0.967198
C	-1.530639	-0.000323	2.050161
C	1.530639	0.000323	2.050161
H	-1.166426	-2.154207	-0.695453
H	-1.168207	-1.258386	-2.206981
H	1.166235	-2.154234	-0.695055
H	1.168389	-1.258725	-2.206768
H	-2.389335	0.000000	-0.422065
H	2.389335	0.000000	-0.422065
H	1.166426	2.154207	-0.695453
H	-1.166235	2.154234	-0.695055
H	-2.610940	-0.000422	1.954935
H	-1.132357	-0.000437	3.058433
H	2.610940	0.000422	1.954935
H	1.132357	0.000437	3.058433
H	-1.168389	1.258725	-2.206768
H	1.168207	1.258386	-2.206981

4b

C	0.000000	0.000000	0.000000
C	-0.620580	-1.382250	0.011290
C	-0.108470	-2.140890	-1.253710
C	1.443860	-2.140900	-1.253710
C	1.955970	-1.382250	0.011290
C	1.335390	0.000000	0.000000
C	-0.075920	-2.118590	1.233230
C	1.411310	-2.118580	1.233240
C	2.203950	-2.681960	2.150310
C	-0.868560	-2.682020	2.150270
H	-0.500750	-3.161030	-1.241990
H	-0.500450	-1.649600	-2.147460
H	1.836130	-3.161040	-1.241970
H	1.835850	-1.649620	-2.147460
H	-1.710440	-1.352480	0.032740
H	3.045830	-1.352480	0.032750
H	1.945910	0.895800	0.000000
H	-0.610520	0.895800	0.000000
H	-1.948230	-2.632380	2.063470
H	-0.473730	-3.205600	3.013620
H	3.283620	-2.632300	2.063520
H	1.809120	-3.205510	3.013680

4b_{loc}

C	0.000000	0.000000	0.000000
C	-0.626800	-1.428160	0.012500
C	-0.116980	-2.169420	-1.249870
C	1.442050	-2.169340	-1.249930
C	1.951880	-1.428160	0.012450
C	1.325090	0.000000	0.000000
C	-0.083460	-2.152440	1.233760
C	1.408550	-2.152450	1.233730
C	2.197760	-2.711530	2.156640
C	-0.872670	-2.711590	2.156630
H	-0.506990	-3.190310	-1.252580
H	-0.504320	-1.672180	-2.143290
H	1.832190	-3.190180	-1.252840
H	1.829280	-1.671950	-2.143300
H	-1.716570	-1.389930	0.036260
H	3.041660	-1.389960	0.036210
H	1.949160	0.886310	0.000020
H	-0.624080	0.886310	0.000000
H	-1.952790	-2.657860	2.074430
H	-0.476300	-3.235110	3.019370
H	3.277880	-2.657830	2.074420
H	1.801390	-3.234970	3.019430

5a

C	0.580751	-1.346761	-0.228258
C	-0.876420	-1.176246	0.228175
C	-1.456868	0.170699	-0.228344
C	-0.580751	1.346761	0.228257
C	1.456868	-0.170699	0.228344
C	0.876420	1.176246	-0.228175
H	0.609263	-1.413003	-1.324078
H	-0.987492	2.290594	-0.149990
H	-0.919513	-1.233472	1.324013
H	-1.490822	-2.000390	-0.149566
H	-2.477680	0.290755	0.149568
H	-1.527636	0.179092	-1.324187
H	1.527636	-0.179092	1.324187
H	1.490822	2.000390	0.149567
H	0.987492	-2.290594	0.149989
H	-0.609264	1.413004	1.324077
H	0.919514	1.233473	-1.324013
H	2.477680	-0.290755	-0.149568

5b

C	-0.833480	-1.257180	-0.003510
C	-0.001530	-2.501800	-0.347130
C	1.336200	-2.493190	0.404280
C	2.168250	-1.256800	0.032280
C	0.000000	0.000000	0.000000
C	1.334770	0.000000	0.000000
H	-1.308710	-1.380490	0.980110
H	2.994590	-1.130720	0.741410
H	0.194130	-2.517190	-1.426240
H	-0.567500	-3.409750	-0.117030
H	1.902150	-3.406200	0.195110
H	1.140510	-2.483800	1.483460
H	-0.533050	0.947560	0.000000
H	1.867820	0.947320	-0.021670
H	-1.659940	-1.147360	-0.715220
H	2.643590	-1.402580	-0.948200

5b_{loc}

C	-0.850870	-1.295450	0.007840
C	-0.004580	-2.529000	-0.337120
C	1.329230	-2.512680	0.422140
C	2.174790	-1.296860	0.019210
C	0.000000	0.000000	0.000000
C	1.326180	0.000000	0.000000
H	-1.299900	-1.414240	0.997590
H	3.008490	-1.169010	0.713990
H	0.198440	-2.542840	-1.415380
H	-0.565470	-3.441690	-0.111470
H	1.888590	-3.435500	0.237680
H	1.128030	-2.476080	1.500210
H	-0.543540	0.941350	0.000000
H	1.869840	0.941180	-0.012550
H	-1.672550	-1.189460	-0.704620
H	2.606600	-1.452300	-0.973070

5b'

C	2.067620	-1.316740	0.009770
C	1.444450	-2.317170	-0.994290
C	-0.109560	-2.317170	-0.994290
C	-0.732730	-1.316740	0.009770
C	1.334890	0.000000	0.000000
C	0.000000	0.000000	0.000000
H	3.129820	-1.181950	-0.210060
H	-1.794930	-1.181950	-0.210060
H	1.826690	-3.319940	-0.782260
H	1.801440	-2.057640	-1.994700
H	-0.491800	-3.319940	-0.782260
H	-0.466560	-2.057640	-1.994700
H	1.898510	0.927910	0.000000
H	-0.563620	0.927910	0.000000
H	2.018560	-1.746340	1.020480
H	-0.683670	-1.746340	1.020480

5b_{loc}

C	2.074850	-1.356500	0.004860
C	1.442370	-2.343770	-0.994940
C	-0.116730	-2.344320	-0.994400
C	-0.749420	-1.356460	0.004810
C	1.325520	0.000000	0.000000
C	0.000000	0.000000	0.000000
H	3.129320	-1.208770	-0.240520
H	-1.803770	-1.208680	-0.241070
H	1.821710	-3.349720	-0.792210
H	1.792790	-2.084780	-1.998650
H	-0.495230	-3.350300	-0.790260
H	-0.467970	-2.086830	-1.998220
H	1.899830	0.921300	-0.000020
H	-0.574290	0.921300	0.000000
H	2.043950	-1.766370	1.017220
H	-0.719010	-1.766050	1.017270

6a

C	0.128833	-0.827524	0.670944
C	1.224762	-0.020501	-0.036311
C	0.540072	1.316710	-0.355725
C	-0.888012	1.009665	0.132626
C	-1.575363	-0.005083	-0.808613
C	-0.840456	-1.327650	-0.430904
O	-0.624569	0.214034	1.313657
O	2.346066	-0.365331	-0.305190
H	-1.460694	0.262203	-1.860978
H	-2.641666	-0.067835	-0.588504
H	-1.527495	-2.062127	-0.008814
H	-0.317235	-1.791224	-1.269433
H	0.483509	-1.561516	1.388973
H	-1.485019	1.874810	0.411228
H	0.641521	1.570383	-1.412666
H	0.996080	2.111976	0.240348

6b

C	1.334300	0.000000	0.000000
C	1.736000	1.468160	-0.112900
C	-0.421010	1.465430	-0.125570
C	0.000000	0.000000	0.000000
C	-0.143440	1.907220	-1.588400
C	1.394350	1.831830	-1.584480
O	2.156400	2.014900	-2.495320
O	0.659110	2.134940	0.564200
H	-0.672390	-0.846670	0.000000
H	2.015020	-0.838870	-0.017320
H	2.711280	1.785490	0.242330
H	-1.378830	1.756540	0.297240
H	-0.581410	1.275860	-2.361730
H	-0.450360	2.942580	-1.755300

6b_{loc}
C 1.323930 0.000000 0.000000
C 1.730140 1.520130 -0.106580
C -0.425790 1.507700 -0.114270
C 0.000000 0.000000 0.000000
C -0.149690 1.941360 -1.571770
C 1.392160 1.862960 -1.573710
O 2.145210 1.989910 -2.500950
O 0.652360 2.164400 0.579040
H -0.682270 -0.838390 0.000000
H 2.018880 -0.826900 -0.005580
H 2.701150 1.828720 0.264830
H -1.380590 1.790800 0.317740
H -0.578410 1.304790 -2.347030
H -0.463870 2.973700 -1.742200

7
C -0.470290 1.440890 -0.089250
C -0.113440 1.944340 -1.527320
C 1.452270 1.944340 -1.527320
C 1.809120 1.440890 -0.089250
C 0.669420 2.112260 0.699010
C 0.000000 0.000000 0.000000
C 1.338830 0.000000 0.000000
H -1.480880 1.659870 0.250360
H 2.819710 1.659870 0.250360
H -0.504320 2.950190 -1.689210
H -0.537450 1.286280 -2.285920
H 1.843150 2.950190 -1.689210
H 1.876280 1.286280 -2.285920
H -0.656350 -0.860180 0.000000
H 1.995180 -0.860180 0.000000
F 0.669420 3.484770 0.597430
F 0.669420 1.853030 2.040690

8
C 1.796010 1.442590 0.188800
C 1.447420 1.780230 1.680400
C -0.109860 1.780200 1.680430
C -0.458500 1.442590 0.188830
C 0.668740 2.207990 -0.594540
C 1.337500 0.000000 0.000000
C 0.000000 0.000000 0.000000
Si 0.668740 4.110890 -0.463300
Si 0.668700 1.766980 -2.468150
H 2.826590 1.656710 -0.094080
H -1.489100 1.656700 -0.094000
H 1.847600 2.755910 1.965480
H 1.870270 1.040980 2.363290
H -0.510060 2.755870 1.965540
H -0.532660 1.040930 2.363320
H 1.994330 -0.861010 -0.000010
H -0.656830 -0.861010 0.000000
H -0.539290 4.646430 -1.145940
H 0.668760 4.629470 0.930470
H 1.876780 4.646430 -1.145910
H 0.668690 3.023110 -3.270700
H 1.881480 1.000170 -2.853260
H -0.544130 1.000260 -2.853230

9

C	1.406700	0.000000	0.000000
C	2.115850	1.191270	0.000000
C	1.400370	2.396550	-0.020800
C	0.006330	2.396550	-0.020800
C	-0.709150	1.191270	0.000000
C	0.000000	0.000000	0.000000
C	1.840250	-1.452230	0.058680
C	-0.433550	-1.452230	0.058680
C	1.484810	-1.969340	1.490680
C	-0.078110	-1.969340	1.490680
C	0.703350	-2.108460	-0.768940
H	3.201160	1.199080	0.004340
H	1.936510	3.339040	-0.041860
H	-0.529810	3.339040	-0.041860
H	-1.794460	1.199080	0.004340
H	1.907370	-1.331450	2.268670
H	1.880060	-2.978290	1.636130
H	-0.500670	-1.331450	2.268670
H	-0.473360	-2.978290	1.636130
H	2.864980	-1.655230	-0.252640
H	0.703350	-3.201010	-0.710400
H	0.703350	-1.798040	-1.815950
H	-1.458280	-1.655230	-0.252640

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