Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Organic & Biomolecular Chemistry

Computational Investigation of Cycloadditions between Cyclopentadiene and Tropone-3,4-dimethylester.

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SUPPORTING INFORMATION

I. Computational Screening at the M06-2X/6-31G(d) level.

a. Cycloadditions between tropone and cyclopentadiene have been investigated previously at the DLPNO-CCSD(T)/cc-pVQZ//*w*B97X-D/def2-TZVP level.[S1] Given the greater number of potential pericyclic pathways that exist between tropone diester **1** and cyclopentadiene, an initial investigation of the many pericyclic reactions was carried out at the M06-2X/6-31G(d) level. Figure S1 provides a summary of the different reaction pathways along with the calculated relative free energy barriers for each pericyclic reaction.

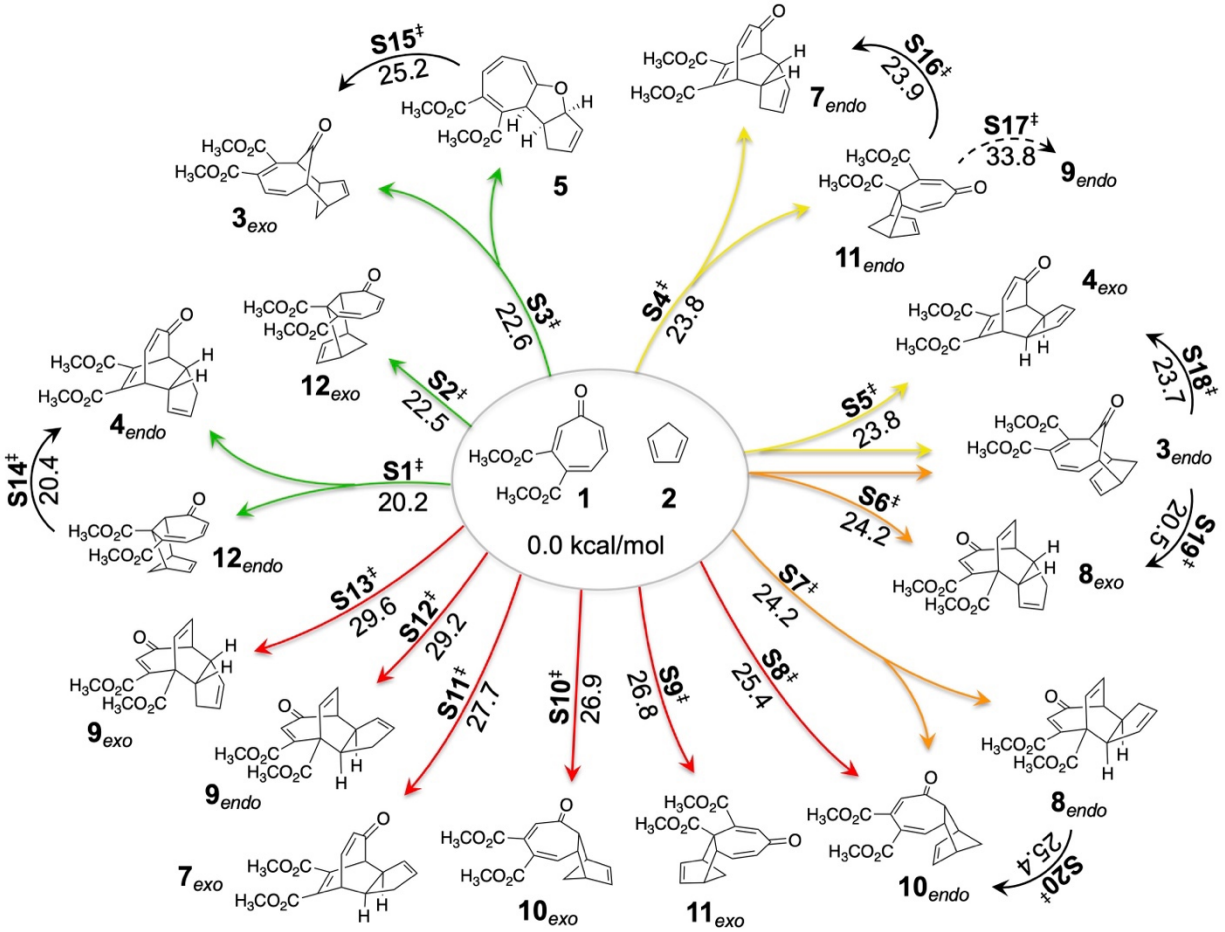


Figure S1. Summary of cycloaddition processes between tropone diester **1** and cyclopentadiene as modeled at the M06-2X/6-31G(d) level. Relative free energies are given in kcal/mol.

Molecules **1**-**12** shown in Figure S1 have the same labels as in Figure 2 of the main text. Transition states modeled using the M06-2X functional are identified as **S1**‡-**S13**‡ (cycloadditions) and **S14**‡-**S20**‡ (sigmatropic rearrangements). Ambimodal processes are indicated with branching arrows. Cycloadditions are positioned around the reactants in order of increasing transition state free energies (in kcal/mol) starting at roughly the 9 o'clock position, where **S1**‡ bifurcates to products **12**$_{endo}$ and **4**$_{endo}$, and progressing clockwise around the reactants until reaching the least favored cycloaddition transition state **S13**‡ leading to **9**$_{exo}$. Cycloaddition reaction arrows are grouped by color according to their relative probability: Boltzmann analysis predicts the pathways highlighted with green arrows will contribute to 99.4% of product formation, those highlighted in yellow contribute 0.4%, those in orange contribute 0.2%, and those highlighted in red are not predicted to contribute to product formation at all (see section **b** below).

b. Predicted cycloaddition probabilities. The relative free energy of each cycloaddition between **1** and **2** (in kcal/mol, ordered from lowest to highest) is given below along with its probability (given as a percentage) as calculated by a Boltzmann distribution at 298.15 K, the same temperature used for chemical calculations.

Table S1. Relative free energies of transition states **S1**‡- **S13**‡ and their relative probabilities.

S1‡	**S2**‡	**S3**‡	**S4**‡	**S5**‡	**S6**‡	**S7**‡	**S8**‡	**S9**‡	**S10**‡	**S11**‡	**S12**‡	**S13**‡
20.2	22.5	22.6	23.8	23.8	24.2	24.2	25.4	26.8	26.9	27.7	29.2	29.6
95.7%	2.0%	1.7%	0.2%	0.2%	0.1%	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%

c. Calculated absolute and relative enthalpies and free energies. Stationary points are listed to match the numbering system from Figure S1 of the Supporting Information. Enthalpy and free energy values are given in Hartrees and were calculated at the M06-2X/6-31G(d) level of theory in the gas phase at 298.15 K and 1.0 atm pressure as described in the text. With the exception of tropone-3,4-dimethyl ester (**1**) and cyclopentadiene (**2**) all structures share the same molecular formula and therefore enthalpy and free energy values relative to **1** + **2** are provided in kcal/mol for each structure.

Table S2. Summary of M06-2X/6-31G(d) computational results.

1	**2**	**3**$_{exo}$	**3**$_{endo}$	**4**$_{exo}$	**4**$_{endo}$	**5**	**6**
-800.73809	-193.90575	-994.68673	-994.67983	-994.69463	-994.69818	-994.67655	-994.68079
-800.7973	-193.9373	-994.75248	-994.7456	-994.76292	-994.765785	-994.74331	-994.74843
$\Delta H°$ relative to (**1**+**2**):		-26.9	-22.6	-31.9	-34.1	-20.5	-23.2
$\Delta G°$ relative to (**1**+**2**):		-11.2	-6.9	-17.8	-19.6	-5.5	-8.7

7$_{exo}$	**7**$_{endo}$	**8**$_{exo}$	**8**$_{endo}$	**9**$_{exo}$	**9**$_{endo}$	**10**$_{exo}$	**10**$_{endo}$
-994.69504	-994.69657	-994.69201	-994.691853	-994.69203	-994.69223	-994.67727	-994.67801
-994.76282	-994.7649	-994.75795	-994.758296	-994.75795	-994.75825	-994.7443	-994.7447
-32.1	-33.1	-30.2	-30.1	-30.2	-30.4	-21.0	-21.4
-17.7	-19.0	-14.7	-14.9	-14.7	-14.8	-6.1	-6.3

11$_{exo}$	**11**$_{endo}$	**12**$_{exo}$	**12**$_{endo}$	**S1**‡	**S2**‡	**S3**‡	**S4**‡
-994.66667	-994.67225	-994.67184	-994.67606	-994.63403	-994.63114	-994.63183	-994.62912
-994.73266	-994.73787	-994.73751	-994.74171	-994.70238	-994.69879	-994.69861	-994.69666
-14.3	-17.8	-17.6	-20.2	6.2	8.0	7.5	9.2
1.2	-2.1	-1.8	-4.5	20.2	22.5	22.6	23.8

S5‡	**S6**‡	**S7**‡	**S8**‡	**S9**‡	**S10**‡	**S11**‡	**S12**‡
-994.62794	-994.62797	-994.627565	-994.62581	-994.62469	-994.6237	-994.62145	-994.62097
-994.69668	-994.69606	-994.696061	-994.6942	-994.69194	-994.69176	-994.69041	-994.68805
10.0	10.0	10.2	11.3	12.0	12.6	14.1	14.4
23.8	24.2	24.2	25.4	26.8	26.8	27.7	29.2

S13‡	**S14**‡	**S15**‡	**S16**‡	**S17**‡	**S18**‡	**S19**‡	**S20**‡
-994.62074	-994.6352	-994.62776	-994.6305	-994.61524	-994.63036	-994.63723	-994.6271
-994.68746	-994.70211	-994.69451	-994.69647	-994.6807	-994.69686	-994.70196	-994.69407
14.5	5.4	10.1	8.4	17.9	8.5	4.2	10.5
29.6	20.4	25.2	23.9	33.8	23.7	20.5	25.4

d. Selection of cycloadditions to investigate further. Initial calculations at the M06-2X/6-31G(d) level provide valuable insight into the cycloaddition and sigmatropic processes that are possible between tropone diester **1** and cyclopentadiene. However, two significant issues were identified once all the pericyclic pathways summarized in Figure S1 were completed: (1) computations at this level incorrectly predict that product $\mathbf{4}_{endo}$ will be the major product and $\mathbf{3}_{exo}$ will be minor, which is opposite of experimental observations (note that $\mathbf{12}_{exo}$ is predicted to be reversible as described in the main text), and (2) despite extensive effort only a single *exo*-[6+4]/[8+2] transition state could be located using the M06-2X functional even though two should exist (one leading to [8+2] product **5** and another leading to [8+2] product **6**). Further computational investigations using the high accuracy CBS-QB3 compound method corrected both issues as detailed in the main text. CBS-QB3 calculations are, however, computationally intensive. Therefore, further computational investigations using the CBS-QB3 method were limited to those cycloaddition transition states highlighted in green and yellow in Figure S1 given that they were predicted to account for >99.4% of potential product formation. One additional cycloaddition transition state, $\mathbf{S6}^{\ddagger}$, was also included in the CBS-QB3 study so that both cycloaddition pathways leading to $\mathbf{3}_{endo}$ could be studied.

e. Impact of solvation on M06-2X reaction energetics. Upon selecting which cycloadditions are most likely to contribute to product formation but before investigating those pericyclic processes at the CBS-QB3 level, the impact of solvation on M06-2X/6-31G(d) reaction energetics was explored. Gleason et al.[S3] carried out thermal reactions between tropone diester **1** and cyclopentadiene **2** in toluene, therefore all stationary points involved in the pericyclic processes summarized in Figure S2 below were re-optimized in a CPCM implicit solvent model for toluene[S4] at 298.15 K and 1.0 atm pressure. Table S3 provides a summary of the absolute enthalpies and free energies of toluene solvated stationary points as well as a comparison of the pericyclic reaction energetics as calculated in the gas phase and in toluene.

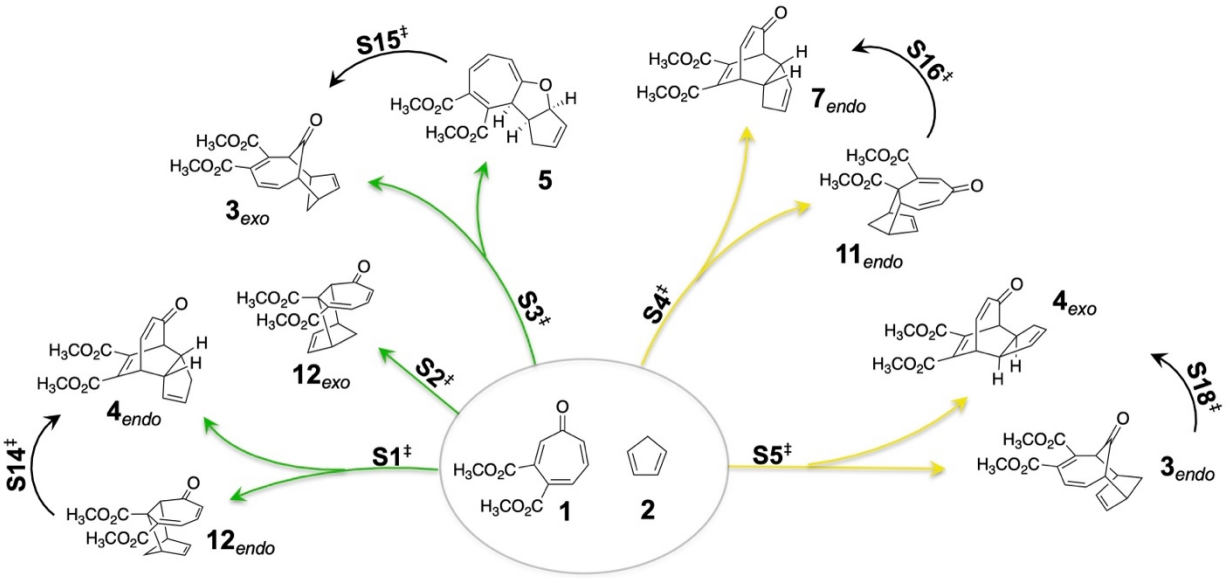


Figure S2. Summary of cycloaddition processes between tropone diester **1** and cyclopentadiene that were computationally modeled at the M06-2X/6-31G(d) level both in the gas phase and in a CPCM implicit solvent model for toluene, the solvent used during experimental investigations of the thermal reaction between **1** and **2**.

Table S3. (a) Calculated absolute enthalpy (top number) and free energy (bottom number) for stationary points optimized in a solvent model for toluene. (b) Comparison of reaction energetics calculated in the gas phase vs toluene at the M06-2X/6-31G(d) level.

(a)

1	**2**	**3**$_{exo}$	**3**$_{endo}$	**4**$_{exo}$	**4**$_{endo}$	**5**	**7**$_{endo}$
-800.74600	-193.90714	-994.69445	-994.687726	-994.70269	-994.70590	-994.68401	-994.70475
-800.80523	-193.9388	-994.76042	-994.75308	-994.77106	-994.77381	-994.75069	-994.77297

11$_{endo}$	**12**$_{exo}$	**12**$_{endo}$	**S1**‡	**S2**‡	**S3**‡	**S4**‡	**S5**‡
-994.68003	-994.67958	-994.68360	-994.64213	-994.63905	-994.64055	-994.63870	-994.63692
-994.774560	-994.74528	-994.74934	-994.71066	-994.70682	-994.70753	-994.70639	-994.70576

S14‡	**S15**‡	**S16**‡	**S18**‡
-994.64406	-994.63640	-994.64034	-994.63986
-994.71097	-994.70333	-994.70635	-994.70642

(b)

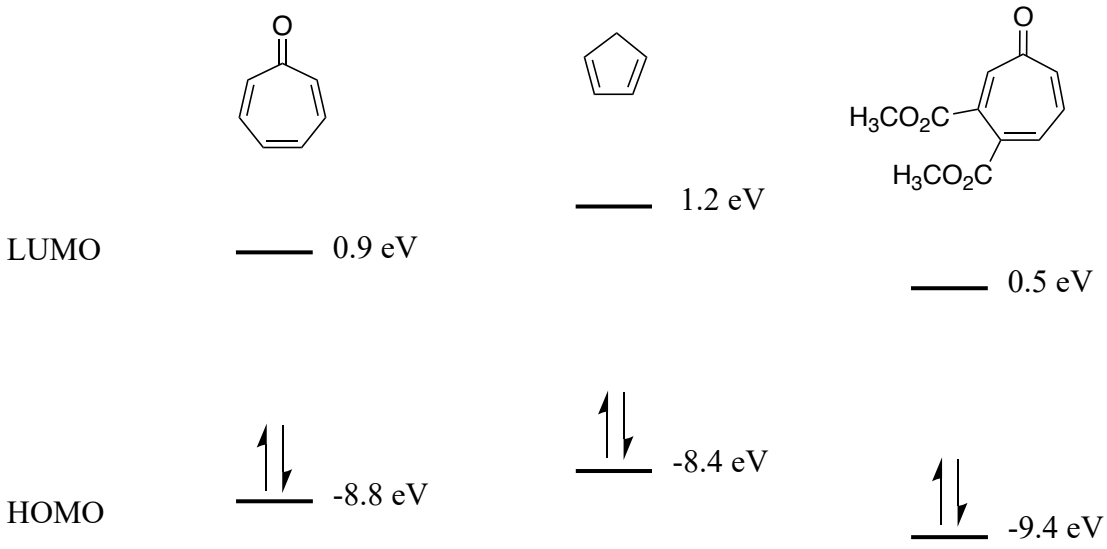
	$\Delta H°_{gas}$	$\Delta H°_{toluene}$	$\Delta G°_{gas}$	$\Delta G°_{toluene}$
3$_{exo}$	-26.9	-25.9	-11.2	-10.3
3$_{endo}$	-22.6	-21.4	-6.9	-5.7
4$_{exo}$	-31.9	-31.1	-17.8	-17.0
4$_{endo}$	-34.1	-33.1	-19.6	-18.7
5	-20.5	-19.4	-5.5	-4.2
7$_{endo}$	-33.1	-32.4	-19.0	-18.2
11$_{endo}$	-17.8	-16.9	-2.1	-1.0
12$_{exo}$	-17.6	-16.6	-1.8	-0.8
12$_{endo}$	-20.2	-19.1	-4.5	-3.4

	$\Delta H^{‡}_{gas}$	$\Delta H^{‡}_{toluene}$	$\Delta G^{‡}_{gas}$	$\Delta G^{‡}_{toluene}$
S1‡	6.2	6.9	20.2	20.9
S2‡	8.0	8.8	22.5	23.4
S3‡	7.5	7.9	22.6	22.9
S4‡	9.2	9.1	23.8	23.6
S5‡	10.0	10.2	23.8	24.0
S14‡	5.4	5.7	20.4	20.7
S15‡	10.1	10.5	25.2	25.5
S16‡	8.4	8.0	23.9	23.6
S18‡	8.5	8.3	23.7	23.6

Values are in kcal/mol relative to reactants **1** + **2**.

The difference in calculated reaction free energies ($\Delta G°$) in the gas phase versus in toluene ranged from 0.8–1.3 kcal/mol. Differences in calculated transition state free energies ($\Delta G^{‡}$) in the gas phase versus toluene ranged from -0.3–0.9 kcal/mol. Overall, calculations in toluene predicted slightly less exergonic reactions with a mean absolute deviation (MAD) of 1.0 kcal/mol and slightly smaller differences in calculated free energy barriers, MAD = 0.37 kcal/mol. These results suggest that there is not a significant difference between gas phase versus toluene solvated calculations, as might be expected for concerted pericyclic reactions carried out in a nonpolar solvent. Subsequent CBS-QB3 calculations were, therefore, carried out in the gas phase.

II. Frontier Orbital Energy Comparisons. Comparison of HOMO and LUMO orbital energies of unsubstituted tropone, cyclopentadiene, and tropone-3,4-dimethyl ester calculated using the CBS-QB3 method and expressed in eV.



As may be expected, substitution of tropone with withdrawing methyl ester moieties at the 3- and 4-positions results in a more electrophilic derivative as indicated by a 0.4 eV lowering of its LUMO relative to unsubstituted tropone. Cyclopentadiene is the nucleophilic species in cycloaddition reactions with either unsubstituted tropone or tropone diester **1**.

III. Ambimodal Product Ratios. As noted in the main text, Houk et al. have shown that the ratio of products "A" and "B" from an ambimodal reaction can be related to partial bond lengths and bond orders in the transition structure according to the following relationships:[S2]

$$B/A = (n_{\text{bond B}}/n_{\text{bond A}})^{\lambda} \qquad \text{and} \qquad n_{\text{bond } x} = n_0 \exp((r_o - r_{\text{bond } x})/c)$$

Where n_o and r_o are the reference bond order and bond length, respectively, λ was determined previously to be -9.4, and c is a constant set to 0.6 for bonds in transition structures.[2] In the current study n_o = 1 and r_o = 1.54 Å for C-C bonds and 1.48 Å for C-O bonds. The following table summarizes predicted product ratios based on bond lengths obtained from CBS-QB3 optimized transition state structures. Transition state labels are from the main text (e.g. see Scheme 2).

	TS-1	**TS-2**	**TS-3**	**TS-5**	**TS-6**	**TS-S7**
bond A	2.87 Å	2.75 Å	3.20 Å	3.02 Å	3.11 Å	2.71 Å
bond B	3.14 Å	2.89 Å	3.24 Å	3.25 Å	3.49 Å	3.21 Å
% A	76%	87%	59%	90%	97%	95%
% B	24%	13%	41%	10%	3%	5%

IV. Stationary Point Coordinates:

a. M06-2X/6-31G(d) structures. All minima and transition states in this section were optimized and subjected to frequency analysis at the M06-2X/6-31G(d) level of theory in the gas phase at 298.15 K and 1.0 atm as described in the text. The naming system is the same as in Figure S1. Atoms are listed by their atomic symbol. Absolute enthalpies and free energies are given in section **I**c above.

Tropone 1

C	1.0734390	-1.0732760	-0.7746680
H	1.2439740	-2.1403470	-0.6499540
C	2.2036020	0.9647390	-1.8486310
H	3.1134520	1.2187290	-2.3867980
C	-0.1753010	-0.6254850	-0.5252820
C	1.1997610	1.8657950	-1.8212730
H	1.3778630	2.8004370	-2.3479490
C	-0.0598500	1.8105440	-1.1223110
H	-0.5923090	2.7543410	-1.0571090
C	-0.6648360	0.7450860	-0.5418880
C	2.2941870	-0.3502000	-1.1844480
O	3.3800280	-0.8959460	-1.0766420
C	-1.1718770	-1.7220960	-0.2268710
C	-1.9040920	1.0003460	0.2706680
O	-0.9390650	-2.7041400	0.4266710
O	-2.2480030	0.3038020	1.1951090
O	-2.3239610	-1.5014720	-0.8771060
O	-2.5579070	2.1081550	-0.1001780
C	-3.3677320	-2.4205780	-0.5546690
H	-3.0607720	-3.4420210	-0.7863340
H	-3.6047230	-2.3449150	0.5092690
H	-4.2209550	-2.1257020	-1.1632210
C	-3.6971890	2.4229030	0.7027210
H	-4.4246130	1.6101680	0.6562760
H	-3.3985180	2.5742200	1.7419400
H	-4.1110940	3.3368630	0.2809040

Cyclopentadiene

C	-0.7351430	-0.9875240	-0.0000030
C	-1.1772540	0.2814320	-0.0000010
C	1.1772540	0.2814330	-0.0000010
C	0.7351430	-0.9875230	-0.0000030
H	-1.3489260	-1.8810640	-0.0000040
H	1.3489270	-1.8810640	-0.0000040
H	-2.2091410	0.6102480	0.0000000
H	2.2091410	0.6102480	0.0000000
C	-0.0000000	1.2151510	0.0000040
H	-0.0000000	1.8745590	-0.8789360
H	-0.0000000	1.8745290	0.8789680

$\mathbf{3}_{exo}$

C	-2.3396560	0.9601990	-0.2187900
C	-2.4453160	-0.3480600	-0.3874790
H	-3.2572910	-0.9663130	-0.0505890
H	-3.0504520	1.5941020	0.2793240
C	-0.1604380	-1.2324390	0.1015810
H	-0.5488040	-2.0594220	0.6843720
C	0.0544080	1.3097910	0.4271730
H	-0.1744890	2.0323820	1.2018540
C	1.2116250	-1.6380550	-0.4141120
C	1.4794010	1.5251730	-0.0182550
H	1.8061530	2.5512400	-0.0109890
C	2.3776580	0.6256500	-0.4013990
H	3.3452770	1.0116250	-0.6541080
C	2.2727900	-0.8466900	-0.5946740
C	-0.0583720	-0.0605990	1.0668820
O	-0.0573220	-0.2191530	2.2461290
C	-0.9875030	1.4363940	-0.7323170
H	-0.9870380	2.4479650	-1.1213230
C	-1.1794110	-0.8899890	-1.0378350
H	-1.3261990	-1.7565320	-1.6656670
C	-0.7086880	0.3608230	-1.7905190
H	-1.3421020	0.5232380	-2.6553010
H	0.3166900	0.3201830	-2.1261530
C	1.2420400	-3.1152740	-0.7183770
C	3.5222680	-1.4965320	-1.1305340
O	3.5285180	-2.4531630	-1.8384970
O	0.5522880	-3.6081230	-1.5503570
O	1.9957410	-3.7895310	0.1236240
O	4.6250430	-0.8889220	-0.7342910
C	2.1176880	-5.1843240	-0.1070860
H	1.1511360	-5.6628520	-0.0512800
H	2.5559160	-5.3595330	-1.0783660
H	2.7654960	-5.5530720	0.6722880
C	5.8560640	-1.4336490	-1.1825500
H	5.9667700	-2.4484460	-0.8305420
H	5.9038370	-1.4204530	-2.2614510
H	6.6237410	-0.8036440	-0.7623830

$\mathbf{3}_{endo}$

C	1.8974550	-0.9060620	-1.9463840
C	2.4467180	-2.1184490	-1.8778840
H	2.1336570	-2.9964620	-2.4321840
H	1.0502130	-0.6043140	-2.5528200
C	1.8168020	-0.1373490	0.4839480
H	1.9096710	0.8040300	1.0346800
C	2.9153550	-2.4686800	0.6194120
H	3.6870450	-2.9316490	1.2419080

C	0.3519660	-0.4626220	0.3239650
C	1.7080330	-3.3670820	0.5949080
H	1.9123260	-4.4325880	0.6733750
C	0.4176340	-3.0121440	0.4956020
H	-0.3015590	-3.8242420	0.5063470
C	-0.2138290	-1.6882230	0.3145660
C	2.5256130	-1.1830000	1.3305030
O	2.7777420	-0.9907050	2.4962160
C	2.5398740	0.0040000	-0.9183050
H	2.5499450	1.0554840	-1.2065610
C	3.5183720	-2.1406920	-0.8029200
H	4.3411600	-2.8277000	-1.0146580
C	3.9281010	-0.6537090	-0.7918110
H	4.5320430	-0.4213490	-1.6725780
H	4.4809840	-0.3556430	0.1066610
C	-0.4435720	0.7699210	-0.0000650
C	-1.6819350	-1.7424880	-0.0267570
O	-2.2403040	-0.9930840	-0.7925820
O	-0.1525660	1.5025590	-0.9148490
O	-1.4167610	1.0087900	0.8817080
O	-2.3139290	-2.7433240	0.6021130
C	-2.2833990	2.0866930	0.5262110
H	-1.7150940	3.0106960	0.4048150
H	-2.7941720	1.8463710	-0.4093650
H	-2.9959350	2.1752560	1.3445000
C	-3.7061540	-2.8516740	0.3049860
H	-4.2252650	-1.9366930	0.5970950
H	-3.8540520	-3.0178940	-0.7641000
H	-4.0658460	-3.7009870	0.8829930

4$_{exo}$

C	1.3937150	-1.0779620	-1.1417480
C	2.7147180	-1.8008760	-1.1132720
H	2.7814690	-2.8846570	-1.1488150
H	0.8491090	-1.2982050	-2.0679980
C	1.0473670	1.2111160	0.0230590
H	1.1489290	2.2836520	-0.1591890
C	1.6667420	-0.4104540	1.9560500
H	2.1581390	-0.5020420	2.9204710
C	-0.4130870	0.8219050	0.0181130
C	1.1292430	-1.4777240	1.3548290
H	1.2165030	-2.4426850	1.8497100
C	0.4230770	-1.4712480	0.0184280
H	0.0384500	-2.4739630	-0.1748790
C	-0.7252340	-0.4789830	-0.0002920
C	1.6759140	0.9617500	1.3973400
O	2.2165860	1.8691430	1.9965540
C	1.7875320	0.4263060	-1.0985890
H	1.4641160	0.8946950	-2.0314210
C	3.7506100	-0.9703640	-1.0288930
H	4.7910800	-1.2773640	-0.9865270
C	3.3362990	0.4781480	-0.9990020
H	3.7690140	1.0355560	-1.8373000
H	3.6850150	0.9802090	-0.0876490
C	-1.4154420	1.9329220	-0.0522480
C	-2.1413290	-0.9281580	-0.1055770
O	-2.2222600	1.9592810	1.0091200
O	-2.2835690	-2.2147160	0.2550930
C	-3.2867730	2.9064630	0.9180010
H	-3.8281540	2.8338100	1.8595370
H	-2.8914080	3.9137330	0.7738970
H	-3.9345130	2.6445690	0.0781950
C	-3.6194880	-2.7113690	0.1736840
H	-4.2750350	-2.1405720	0.8344820
H	-3.9917070	-2.6312240	-0.8498040
H	-3.5679990	-3.7527400	0.4866090
O	-1.4273640	2.7375110	-0.9500290
O	-3.0614450	-0.2406300	-0.4800620

4$_{endo}$

C	2.2751610	0.9318140	-0.3999160
C	0.8090890	0.7640130	-0.7079190
H	0.5810850	1.0736160	-1.7344420
H	2.7670930	1.8983120	-0.4663880
C	-0.5781490	-1.0547800	0.5021740
H	-0.5828100	-2.1233090	0.7318990
C	-2.3071310	0.6451030	-0.4397120
H	-3.3100080	0.7657400	-0.8395820
C	-0.3014570	-0.2586020	1.7557590
C	-1.4969200	1.6982970	-0.2838940
H	-1.8639550	2.6797190	-0.5772650
C	-0.0792800	1.6365260	0.2375610
H	0.3293280	2.6483150	0.2589120
C	-0.0195850	1.0431970	1.6313100
C	-1.9503830	-0.7547340	-0.1049840
O	-2.7217670	-1.6609130	-0.3443130
C	2.8547440	-0.2044750	-0.0236320
H	3.8964850	-0.3063360	0.2642440
C	0.5570690	-0.7612800	-0.5181510
H	0.2718960	-1.2126730	-1.4725800
C	1.9005040	-1.3671570	-0.0209750
H	2.2410620	-2.1749720	-0.6785360
H	1.8028830	-1.7963870	0.9851590
C	-0.2180620	-1.0181420	3.0436630
C	0.4273790	1.8461400	2.8036040
O	0.3644910	3.1657630	2.5594790
O	-1.1179260	-0.6109750	3.9374200
O	0.5473020	-1.9376130	3.2056960
O	0.8180770	1.3862300	3.8503650
C	0.7958960	3.9919560	3.6406350
H	0.6950420	5.0171460	3.2886890
H	0.1705660	3.8210140	4.5192480
H	1.8339800	3.7693010	3.8960890
C	-0.9760110	-1.1996450	5.2307660
H	-1.7899880	-0.7953920	5.8297850
H	-1.0441780	-2.2872110	5.1658180
H	-0.0083380	-0.9180990	5.6522710

5

C	-3.3863110	-0.3963300	-0.3914600

C	-4.3193840	0.3081130	0.5512520
H	-5.3478290	0.0049520	0.7080960
H	-3.8325130	-0.7103400	-1.3416880
C	-0.8926040	-2.8625470	0.1537040
H	-1.4855770	-3.6830710	0.5448170
C	-1.0071810	-0.4449450	-0.7438000
H	-0.9222420	-0.6591180	-1.8207560
C	0.4771660	-3.1246160	-0.2053020
C	0.3577490	-0.0092110	-0.2454900
C	1.4471770	-0.8088530	-0.2092040
C	1.4877290	-2.2488980	-0.4058510
C	-1.5329550	-1.6982200	-0.0583110
O	-2.8400840	-1.5692280	0.2533280
C	-2.1782690	0.5413960	-0.5350500
H	-2.2912570	1.2074810	-1.3924710
C	-3.6693910	1.2746570	1.1953150
H	-4.0916250	1.9031390	1.9731930
C	-2.2253470	1.3740340	0.7724390
H	-1.5777930	0.9558490	1.5541500
H	-1.8996670	2.4068500	0.6177630
H	2.4644300	-2.6590000	-0.6378460
H	0.7302110	-4.1782980	-0.3027110
C	0.5345950	1.4500760	0.0815990
C	2.7859640	-0.1461230	-0.0037250
O	3.0710190	0.9659910	-0.3798270
O	0.8433900	1.8979510	1.1557040
O	0.2508350	2.2078480	-0.9909090
O	3.6587650	-0.9538190	0.6140060
C	4.9533230	-0.3876320	0.8148970
H	5.4066150	-0.1256130	-0.1436340
H	4.8792210	0.5117350	1.4294870
H	5.5357840	-1.1552830	1.3213700
C	0.4925290	3.6018210	-0.8025690
H	-0.1346400	3.9957640	0.0015050
H	1.5422120	3.7607620	-0.5467880
H	0.2474510	4.0771170	-1.7509790

6

C	-0.7166740	-2.7833510	-1.7041990
C	-0.1777570	-3.3590630	-2.9825350
H	-0.0155070	-4.4200230	-3.1321430
H	-0.2916020	-3.2131390	-0.7910600
C	-4.0027330	-1.8635060	-0.7084620
H	-4.4962390	-2.8290750	-0.6645740
C	-1.7644080	-0.6827380	-1.1299170
H	-1.5284120	-0.4632700	-0.0784170
C	-4.6987170	-0.7338950	-0.1559990
C	-2.3778790	0.5352390	-1.7718900
H	-1.8222330	1.0035130	-2.5799980
C	-3.5250210	1.1039830	-1.3789950
H	-3.8133630	2.0419340	-1.8438390
C	-4.4621110	0.5936090	-0.3864090
C	-2.7301740	-1.8465260	-1.1624650
O	-2.1522110	-2.9621490	-1.6405610
C	-0.5241200	-1.2625030	-1.8376350
H	0.4003810	-0.9477560	-1.3485280
C	-0.0004400	-2.3973930	-3.8859090
H	0.3396440	-2.5531460	-4.9049880
C	-0.4007170	-1.0392290	-3.3643280
H	-1.3593190	-0.7481570	-3.8133700
H	0.3188520	-0.2527490	-3.6128050
C	-5.8425250	-1.1563890	0.7387890
C	-5.2840870	1.5870140	0.3612770
O	-5.8952080	1.3646040	1.3823970
O	-5.7000230	-1.7981630	1.7467330
O	-5.2574290	2.8077110	-0.2069060
O	-7.0283560	-0.8274590	0.2104720
C	-6.0080220	3.8016190	0.4855130
H	-7.0627240	3.5212900	0.5277710
H	-5.6338780	3.9200530	1.5046780
H	-5.8769590	4.7210810	-0.0830410
C	-8.1366890	-1.0672020	1.0749160
H	-9.0212290	-0.7691010	0.5139540
H	-8.1900940	-2.1227400	1.3494090
H	-8.0284130	-0.4617850	1.9782380

***7**_{exo}*

C	1.6864190	-1.1588220	-0.9778440
C	3.0936700	-1.7728990	-0.7513910
H	3.1406590	-2.3777210	0.1633560
H	1.2421970	-1.5607390	-1.8922790
C	0.9891520	1.2314370	-0.2113180
H	0.9827590	2.2660740	-0.5621220
C	1.6575650	0.0087410	1.9799670
H	2.0782100	0.1255030	2.9747480
C	-0.4118200	0.6683080	-0.2323390
C	1.2785130	-1.1929430	1.5311670
H	1.4122860	-2.0500720	2.1879410
C	0.6823400	-1.4765440	0.1675620
H	0.4289070	-2.5370610	0.1193270
C	-0.5689730	-0.6501350	-0.0673070
C	1.5604460	1.2724420	1.2092510
O	1.9603290	2.3165040	1.6800090
C	1.8985430	0.3731470	-1.1436640
H	1.6324460	0.6791990	-2.1622590
C	4.0087620	-0.5784940	-0.6745800
H	5.0711610	-0.6716080	-0.4722220
C	3.3731270	0.5695350	-0.8934700
H	3.8307340	1.5543300	-0.8888660
C	-1.5281670	1.6236510	-0.5246900
C	-1.9124630	-1.2835020	-0.1756360
O	-2.4084990	1.6988260	0.4742510
O	-1.9315680	-2.5077060	0.3783280
C	-3.5656090	2.4831670	0.1836460
H	-4.1630270	2.4765710	1.0935470
H	-3.2796590	3.5016250	-0.0859580
H	-4.1150660	2.0270250	-0.6430690
C	-3.1920970	-3.1738350	0.3063120
H	-3.9549240	-2.5954830	0.8315160
H	-3.4963180	-3.2975500	-0.7351470

H	-3.0439790	-4.1407800	0.7839210
O	-1.5674730	2.2853190	-1.5317270
O	-2.8760870	-0.7818240	-0.7041070
H	3.3774770	-2.4365750	-1.5765210

7$_{endo}$

C	-1.2101520	-2.2887520	1.5983890
C	-1.7703390	-1.5799050	0.3351810
H	-2.6279730	-2.1313820	-0.0584260
H	-0.1630050	-2.5936240	1.4623120
C	-1.4713080	0.9929220	0.0532400
H	-1.6457870	1.9308300	0.5866880
C	-1.9221750	0.0954030	-2.3375520
H	-2.3626020	0.3141600	-3.3062530
C	0.0035820	0.6775990	0.0357550
C	-1.3325920	-1.0820650	-2.1005810
H	-1.3181750	-1.8185030	-2.9015970
C	-0.7017740	-1.5055540	-0.7930500
H	-0.2727530	-2.5000840	-0.9242830
C	0.3866620	-0.5462130	-0.3467030
C	-2.0461390	1.1936260	-1.3495350
O	-2.6339940	2.2169910	-1.6317830
C	-1.3462960	-1.2638160	2.6911930
H	-1.0152880	-1.4468720	3.7083630
C	-2.2230410	-0.1608100	0.7899080
H	-3.2957080	-0.0097380	0.6170880
C	-1.9000700	-0.1337590	2.2629720
H	-2.0771660	0.7499180	2.8682540
C	0.9251710	1.7245500	0.5825880
C	1.8080970	-0.9743480	-0.2291620
O	2.0380800	-2.1317830	-0.8737200
O	1.7962120	2.1616690	-0.3273330
O	0.8208700	2.1551200	1.7038160
O	2.6634710	-0.3825650	0.3856810
C	3.3815830	-2.6055490	-0.7840980
H	3.4033460	-3.5415640	-1.3395020
H	4.0682460	-1.8789160	-1.2230950
H	3.6575370	-2.7669200	0.2600750
C	2.7854730	3.0547950	0.1842390
H	3.3917620	3.3458070	-0.6716990
H	2.3143000	3.9271820	0.6411550
H	3.3925260	2.5353420	0.9292770
H	-1.7691820	-3.2037890	1.8267560

8$_{exo}$

C	1.1019300	-0.1715230	2.0811910
C	0.8191690	0.9190770	1.0785430
H	0.3948060	1.8002880	1.5781500
H	0.3023290	-0.7196380	2.5687390
C	1.0780830	-1.4460740	-0.8810900
H	1.1278760	-2.4961680	-1.1563120
C	2.3322200	0.8412280	-0.9784210
H	3.3056810	1.1540600	-1.3644890
C	-0.0810380	-0.9254220	-0.4615180
C	1.2000180	1.5048820	-1.7283950
H	1.4237130	2.0804480	-2.6212600
C	-0.0389420	1.4017580	-1.2551070
H	-0.8994880	1.8673790	-1.7217300
C	-0.2456430	0.5248990	-0.0333990
C	2.3433920	-0.6862100	-1.0562890
O	3.3836270	-1.2817840	-1.2552160
C	2.4075660	-0.3561150	2.2636090
H	2.8410600	-1.0832840	2.9425970
C	2.2178680	1.2742210	0.5100010
H	2.3538930	2.3581800	0.5132440
C	3.2475810	0.5814250	1.4354490
H	3.7582170	1.3145840	2.0714040
H	4.0259310	0.0570890	0.8682420
C	-1.2766950	-1.8285640	-0.5253440
C	-1.5777950	0.7112250	0.6785640
O	-1.2826020	-3.0014900	-0.2581880
O	-1.9811660	-0.0358030	1.5385690
O	-2.3407870	-1.1628930	-1.0124000
O	-2.2038290	1.8385840	0.3288660
C	-3.5597460	-1.9056270	-1.0076040
H	-3.4517100	-2.8182180	-1.5963590
H	-3.8268250	-2.1666740	0.0193150
H	-4.3092000	-1.2490710	-1.4470120
C	-3.4269570	2.0820630	1.0262750
H	-4.1313140	1.2683370	0.8405200
H	-3.2427520	2.1541920	2.0998790
H	-3.8092360	3.0225380	0.6338000

8$_{endo}$

C	0.7505580	1.1402180	1.1279360
C	1.1294170	-1.3242920	-0.6750420
H	1.1636840	-2.3965040	-0.8494560
C	2.4597320	0.9036950	-0.7966190
H	3.4727510	1.1883390	-1.0926730
C	-0.0375060	-0.7509680	-0.3513260
C	1.4229850	1.5982360	-1.6507860
H	1.7436120	2.1403780	-2.5349620
C	0.1424910	1.5455660	-1.2940350
H	-0.6485380	2.0328300	-1.8519280
C	-0.2129640	0.7370310	-0.0624190
C	2.4159240	-0.6155990	-0.9089460
O	3.4140020	-1.2539610	-1.1722480
C	2.2322930	1.3013430	0.6837960
C	-1.2325390	-1.6616320	-0.3627730
C	-1.6101010	0.9852550	0.4948240
O	-1.2488680	-2.7946570	0.0405520
O	-2.0453620	0.3859030	1.4492070
O	-2.2742880	-1.0637410	-0.9686500
O	-2.2624870	1.9770820	-0.1150580
C	-3.4906750	-1.8108240	-0.9355170
H	-3.3509470	-2.7857430	-1.4056120
H	-3.8075570	-1.9502750	0.1009030
H	-4.2183470	-1.2169420	-1.4864430

C	-3.5554400	2.2568880	0.4226420
H	-4.1904890	1.3712400	0.3498020
H	-3.4744930	2.5492520	1.4718220
H	-3.9557500	3.0722630	-0.1769280
C	2.6029650	2.7908930	0.9222410
H	3.5022960	2.8838460	1.5412100
H	2.8145960	3.3122430	-0.0204200
C	1.3918420	3.3699600	1.5978000
H	1.3521200	4.3969470	1.9474430
C	0.4026190	2.4892980	1.7106370
H	-0.5593340	2.6833440	2.1764240
H	2.8636270	0.6654740	1.3114800
H	0.6352930	0.3530910	1.8799820

9$_{exo}$

C	1.1635520	-0.8161120	-0.8276080
C	0.6014720	2.1858790	-0.2355410
H	0.2825100	3.1828130	-0.5283260
C	2.5580090	0.7591390	0.7018130
H	3.5847480	0.9567550	1.0192220
C	-0.2864410	1.1831800	-0.2458790
C	1.7355530	0.1749430	1.8272900
H	2.1370950	0.1818710	2.8358020
C	0.5333790	-0.3262880	1.5591900
H	-0.1091670	-0.7593950	2.3170300
C	0.0378650	-0.2587920	0.1253510
C	2.0132450	2.1024060	0.2257180
O	2.7098680	3.0954520	0.2154050
C	2.5682670	-0.2418060	-0.4879210
C	-1.6988570	1.5601910	-0.5902980
C	-1.1462840	-1.1744140	-0.1645640
O	-2.0309400	2.2204210	-1.5395610
O	-1.8449380	-1.0878110	-1.1465170
O	-2.5413010	1.1173920	0.3581100
O	-1.2569690	-2.1641080	0.7279330
C	-3.9244370	1.2863580	0.0462710
H	-4.1525160	2.3409800	-0.1172850
H	-4.1662930	0.7175100	-0.8549050
H	-4.4718790	0.9019570	0.9054870
C	-2.2890490	-3.1116070	0.4460700
H	-3.2600130	-2.6127150	0.4217470
H	-2.1102420	-3.5886340	-0.5195020
H	-2.2485280	-3.8410710	1.2528140
C	3.0366180	0.3629280	-1.7887720
H	3.9922490	0.8715760	-1.8743610
C	2.1481630	0.2164820	-2.7681970
H	2.2755460	0.5844630	-3.7813380
C	0.9103870	-0.5201100	-2.3317940
H	0.0054680	0.0769050	-2.4939050
H	3.2293730	-1.0595350	-0.1773660
H	0.7679530	-1.4461950	-2.8999120
H	1.1798130	-1.8958810	-0.6518220

9$_{endo}$

C	1.0548390	-0.7586560	-0.8872990
C	0.4373550	2.1866490	-0.0599820
H	0.0677680	3.1851100	-0.2784900
C	2.4899870	0.7761510	0.6415320
H	3.5330640	0.9745470	0.9012120
C	-0.4108670	1.1503640	-0.1193850
C	1.7726860	0.0579440	1.7608260
H	2.2518510	-0.0128700	2.7321500
C	0.5623090	-0.4500870	1.5444640
H	-0.0066550	-0.9649270	2.3096220
C	-0.0271410	-0.3038040	0.1541300
C	1.8651550	2.1346020	0.3575350
O	2.5055110	3.1617000	0.4370870
C	2.4285660	-0.0668960	-0.6671520
C	-1.8402340	1.5123240	-0.4144000
C	-1.2250790	-1.2077840	-0.1360600
O	-2.1975980	2.3216360	-1.2293540
O	-1.7516910	-1.2570000	-1.2216290
O	-2.6752810	0.8655680	0.4181810
O	-1.5893970	-1.9733400	0.8961030
C	-4.0625090	1.0686260	0.1466110
H	-4.3049350	2.1320400	0.1817410
H	-4.3041660	0.6739550	-0.8433210
H	-4.5990330	0.5243320	0.9223300
C	-2.7023590	-2.8295700	0.6352610
H	-3.5752140	-2.2324740	0.3620270
H	-2.4697870	-3.5138800	-0.1831050
H	-2.8797720	-3.3754300	1.5600330
C	3.4046080	-1.2154070	-0.6215230
H	4.4735680	-1.0486660	-0.5251660
C	2.8108400	-2.4025300	-0.6897300
H	3.3236120	-3.3587260	-0.6574950
C	1.3155120	-2.2900290	-0.8009200
H	0.9201800	-2.8076450	-1.6818260
H	2.6633230	0.6018940	-1.5046450
H	0.6634420	-0.5098890	-1.8757030
H	0.8289070	-2.7413280	0.0748160

10$_{exo}$

C	-1.9771980	0.1749520	-1.6921460
C	-2.1111130	1.1766920	-0.8186420
H	-2.4318620	2.1919540	-1.0246210
H	-2.1683350	0.1984630	-2.7591840
C	2.1936380	0.3559160	1.5474100
H	2.7944340	1.1604970	1.9659170
C	-0.0361390	0.5866940	0.3391850
H	0.3735480	1.4900400	-0.1297700
C	2.7961530	-0.6918970	0.9790590
C	0.1357340	-0.6262030	-0.6569420
H	0.6325860	-0.2839060	-1.5723930
C	0.8842810	-1.8370160	-0.1626880
H	0.4319210	-2.7964170	-0.4059550
C	2.0553050	-1.8763010	0.4886600
C	0.7011080	0.4426710	1.6573030
O	0.1455750	0.4588050	2.7318610
C	-1.3594460	-0.9952320	-0.9499040

H	-1.4718730	-1.9761890	-1.4166970
C	-1.5784530	0.6902940	0.5171780
H	-1.8712320	1.2425700	1.4092200
C	-1.9669160	-0.7990040	0.4523180
H	-3.0477340	-0.9546540	0.4717270
H	-1.4831320	-1.3992990	1.2312430
C	4.2931180	-0.6653390	0.8941070
C	2.6459240	-3.1853320	0.9100830
O	4.7371950	-1.4493950	-0.0983130
O	2.0585620	-4.2449940	0.3330010
O	3.5491540	-3.2826700	1.7066400
O	5.0066830	0.0214120	1.5811960
C	6.1574070	-1.5418960	-0.1914150
H	6.5627970	-1.9613690	0.7320010
H	6.3571860	-2.2013040	-1.0343660
H	6.5935950	-0.5551500	-0.3595630
C	2.5664750	-5.5088020	0.7582600
H	3.6288960	-5.5890540	0.5193150
H	2.4359750	-5.6281310	1.8358370
H	1.9914260	-6.2564110	0.2144820

10_*endo*_

C	-2.1844810	-0.1574380	0.8199910
C	-2.1205530	-1.1724530	-0.0473370
H	-2.4264630	-2.1990990	0.1198020
H	-2.5431560	-0.1779460	1.8413240
C	2.0837630	0.2063930	1.5687560
H	2.7478400	0.8940940	2.0880140
C	0.0196260	0.7135450	0.1496560
H	0.5663950	1.5558070	-0.2976700
C	2.5918190	-0.9091300	1.0362490
C	0.1184260	-0.5026030	-0.8433650
H	0.7085340	-0.1936680	-1.7168010
C	0.6969540	-1.7978140	-0.3499790
H	0.1865990	-2.6956300	-0.6926060
C	1.7807260	-1.9822580	0.4166180
C	0.6271510	0.5470120	1.5271990
O	0.0085060	0.7776740	2.5423180
C	-1.5019260	1.0359180	0.1749380
H	-1.7316460	2.0128460	0.6005680
C	-1.3797190	-0.6721230	-1.2774730
H	-1.4968930	-1.2594170	-2.1906180
C	-1.8451740	0.7924860	-1.3069150
H	-2.9135210	0.8889640	-1.5123940
H	-1.2702810	1.4192030	-1.9981310
C	4.0802360	-1.0851480	1.1295210
C	2.1825600	-3.3634440	0.8304160
O	2.9717110	-3.5914250	1.7168560
O	4.7864740	-0.5447460	1.9427130
O	1.5614590	-4.3301400	0.1366500
O	4.5387120	-1.8614220	0.1369000
C	5.9330060	-2.1525990	0.2085520
H	6.1504530	-2.7782840	-0.6555180
H	6.5176160	-1.2310130	0.1765030
H	6.1520220	-2.6854790	1.1366190
C	1.8860450	-5.6570790	0.5484520
H	1.6196240	-5.8061420	1.5969110
H	1.3058200	-6.3163740	-0.0949890
H	2.9554850	-5.8401780	0.4257270

11_*exo*_

C	0.1635630	-1.3592980	-3.6422440
C	0.8089700	-2.5219200	-3.5219100
H	0.6183680	-3.4405530	-4.0650420
H	-0.6600290	-1.1258910	-4.3033240
C	1.4729700	0.2709710	0.7591560
H	1.5442620	1.2170790	1.2900350
C	2.3858800	-2.1424750	1.0207420
H	3.0115590	-2.7099780	1.7043490
C	0.4847130	0.1654930	-0.1375500
C	1.6353020	-2.7976500	0.1324050
H	1.7008660	-3.8851620	0.1741540
C	0.8299280	-2.3446570	-1.0430450
H	0.0405170	-3.0907020	-1.1751580
C	0.1538230	-0.9181550	-1.1494050
C	2.5141760	-0.6866550	1.2137920
O	3.4500280	-0.2456890	1.8587260
C	0.6887280	-0.4291080	-2.5638040
H	0.5201000	0.6348210	-2.7257940
C	1.7473260	-2.3923950	-2.3431500
H	2.5512520	-3.1259820	-2.2661200
C	2.1455680	-0.9153620	-2.4581410
H	2.7187180	-0.7074420	-3.3639490
H	2.6813520	-0.5323270	-1.5840560
C	-0.3784620	1.4135400	-0.1907560
C	-1.3583180	-1.1606620	-1.1207730
O	-2.0695120	-1.3999120	-2.0612260
O	-0.2912800	2.3465420	0.5674580
O	-1.2744440	1.3782720	-1.1912050
O	-1.8010490	-1.1486170	0.1496150
C	-2.1528000	2.5013780	-1.2632330
H	-2.7039270	2.6081530	-0.3267030
H	-1.5821520	3.4141010	-1.4454500
H	-2.8274240	2.2918380	-2.0913960
C	-3.2045830	-1.3578280	0.2948220
H	-3.7562420	-0.5778090	-0.2358410
H	-3.4896450	-2.3306570	-0.1109620
H	-3.4026580	-1.3113120	1.3642170

11_*endo*_

C	2.1486450	-0.9985840	-1.2633790
C	1.5460430	0.1825660	-1.4409770
H	1.9956240	1.1650540	-1.3544600
H	3.1881950	-1.1728440	-1.0109000
C	0.8980660	0.7281940	1.6419370
H	0.9765560	1.6699730	2.1801950
C	1.8277470	-1.6614670	1.9502920
H	2.4632810	-2.1799590	2.6634440

C	-0.1534840	0.5833330	0.8279070
C	1.0078790	-2.3651050	1.1672080
H	1.0100010	-3.4453340	1.3111840
C	0.2071500	-1.9442310	-0.0218330
H	-0.5999570	-2.6784820	-0.1273210
C	-0.4551530	-0.5125640	-0.1747160
C	2.0192310	-0.1957230	1.9638000
O	3.0603030	0.2793170	2.3805300
C	1.0763480	-2.0649950	-1.3377560
H	1.4121840	-3.0869750	-1.5212470
C	0.0618530	-0.0840860	-1.6149720
H	-0.5445690	0.7086080	-2.0503580
C	0.1111510	-1.4347640	-2.3500420
H	0.5599660	-1.3349700	-3.3407630
H	-0.8577130	-1.9306640	-2.4171640
C	-1.0669290	1.7882360	0.8260060
C	-1.9651800	-0.7641360	-0.1986620
O	-2.6308170	-1.0116440	-1.1716880
O	-1.0471680	2.6737160	1.6436650
O	-1.9144460	1.7854210	-0.2184090
O	-2.4652040	-0.7472590	1.0488360
C	-2.8315180	2.8784370	-0.2602420
H	-3.4321220	2.9005050	0.6515770
H	-2.2891780	3.8216760	-0.3504280
H	-3.4562940	2.7034630	-1.1343270
C	-3.8749310	-0.9511760	1.1310440
H	-4.3986880	-0.1724790	0.5709800
H	-4.1444990	-1.9255090	0.7183300
H	-4.1213920	-0.8975600	2.1899800

12*exo*

C	-2.3563900	1.9345300	1.6747720
C	-1.1529210	1.7491190	2.2240810
H	-0.5750950	2.4541190	2.8059250
H	-2.9657620	2.8305080	1.7047120
C	-1.6425860	0.8683330	-0.4161740
H	-1.6103340	1.9210470	-0.7060540
C	-2.3405410	-1.2893290	-1.7320570
H	-3.2251160	-1.6238970	-2.2672300
C	-0.2601020	0.4766180	0.2278440
C	-1.4211790	-2.1816810	-1.3435000
H	-1.6199060	-3.2290760	-1.5591360
C	-0.1078090	-1.9303360	-0.7564100
H	0.5671310	-2.7773370	-0.8279100
C	0.4001580	-0.8363820	-0.1606070
C	-2.2036020	0.1869200	-1.6469240
O	-2.6834200	0.8636990	-2.5352140
C	-2.6441100	0.7244310	0.8091620
H	-3.6814650	0.5715850	0.5054600
C	-0.6427810	0.3947690	1.7657280
H	0.1560120	-0.0445610	2.3628510
C	-1.9718120	-0.3738680	1.6470270
H	-2.4590090	-0.5052760	2.6155590
H	-1.8889080	-1.3367170	1.1377950
C	0.7039910	1.6242820	-0.0806840
C	1.8190410	-0.9267860	0.3309110
O	0.8710700	2.6131790	0.5822830
O	2.3458330	-0.0744990	1.0108750
O	1.2901850	1.4273910	-1.2754470
O	2.4617470	-2.0419170	-0.0452310
C	3.8059210	-2.1422130	0.4239710
H	3.8291590	-2.1340220	1.5156040
H	4.1829370	-3.0869200	0.0361600
H	4.3996040	-1.3054520	0.0506460
C	2.2262960	2.4372860	-1.6488470
H	3.0328600	2.4845920	-0.9133470
H	2.6079250	2.1421020	-2.6249410
H	1.7348930	3.4106570	-1.7042720

12*endo*

C	-1.0813550	-0.9392420	2.1753840
C	-2.3253190	-0.7758150	1.7125920
H	-3.1050390	-1.5260140	1.6461600
H	-0.6377710	-1.8527060	2.5546850
C	-1.5733800	0.7246620	-0.1568920
H	-1.6052530	1.7726150	-0.4704880
C	-2.2538400	-1.4701670	-1.4391530
H	-3.1457820	-1.8712130	-1.9132040
C	-0.1165850	0.4037920	0.3452230
C	-1.2257470	-2.2876480	-1.1752750
H	-1.3584340	-3.3364420	-1.4320200
C	0.1090860	-1.9681130	-0.6827770
H	0.8241320	-2.7731700	-0.8202120
C	0.5967700	-0.8549270	-0.1078660
C	-2.2875240	0.0018860	-1.2789300
O	-3.0289310	0.6436630	-1.9997640
C	-0.3291470	0.3552170	1.9187520
H	0.6018060	0.5167560	2.4601670
C	-2.4255210	0.6366640	1.1698740
H	-3.4280620	1.0457410	1.0363010
C	-1.4658080	1.3711580	2.1195580
H	-1.8276550	1.3687490	3.1504070
H	-1.2077590	2.3825370	1.8035160
C	0.7297830	1.6227330	-0.0331020
C	2.0482570	-0.8606540	0.2817460
O	0.8439910	2.6274230	0.6202430
O	2.5751080	0.0331610	0.9070670
O	1.2675230	1.4700320	-1.2546770
O	2.7221890	-1.9489830	-0.1175280
C	4.1003180	-1.9667290	0.2526960
H	4.2026430	-1.9316980	1.3392430
H	4.4991930	-2.8990070	-0.1432840
H	4.6190800	-1.1088410	-0.1797160
C	2.1043450	2.5480150	-1.6722640
H	2.9417390	2.6554630	-0.9788400
H	2.4565400	2.2820790	-2.6676220
H	1.5387870	3.4814960	-1.6986840

S1‡

C	-0.8843510	1.7640640	-0.2282750

C	-0.8157500	-0.7617960	-1.1269980
H	-1.2103260	-1.1214350	-2.0766250
C	-1.3514680	-1.2427790	1.3661830
H	-2.1383730	-1.5994430	2.0243480
C	0.6097610	-0.7726500	-1.1148280
C	-0.2228580	-0.7327420	1.9102950
H	-0.2039960	-0.6911540	2.9982850
C	0.9983560	-0.2782990	1.3004890
H	1.7330650	0.1110730	1.9985040
C	1.4178880	-0.4207260	0.0027830
C	-1.7153480	-1.3072230	-0.0464870
O	-2.7961470	-1.7641460	-0.3875250
C	-1.4618720	1.0127520	-1.2802900
C	1.2462040	-1.2189940	-2.3788480
C	2.8323380	0.0356800	-0.2705210
O	2.4504260	-1.7808190	-2.1684260
O	3.6835590	-0.3798740	0.6781760
C	3.1821120	-2.0945780	-3.3495180
H	2.6152680	-2.7839900	-3.9778390
H	3.3912830	-1.1822660	-3.9136420
H	4.1089000	-2.5549470	-3.0100080
C	5.0307590	0.0538590	0.4988090
H	5.4194740	-0.3121340	-0.4539390
H	5.0863740	1.1446760	0.5069340
H	5.5907160	-0.3679800	1.3316490
O	0.7405060	-1.1606750	-3.4810820
O	3.1715230	0.7353390	-1.1951650
C	-0.7238880	1.4352360	-2.5431590
H	-0.5775270	0.6582520	-3.2947270
H	-1.2978700	2.2557160	-3.0014140
C	0.5367940	1.9906610	-1.9790380
H	1.4336830	2.1854260	-2.5531550
C	0.3498250	2.2991510	-0.6554630
H	1.0737100	2.7875680	-0.0139310
H	-2.5279410	0.7986530	-1.3008940
H	-1.2884080	1.8402570	0.7747540

Imag. Freq. -328.02

S2‡

C	-2.1355690	-2.0924180	-0.8548050
C	-0.9154230	-2.2122820	-1.5357290
H	-0.3036380	-3.1053740	-1.5667850
H	-2.6218520	-2.8863720	-0.3004700
C	-1.6457300	-0.0234730	0.6786670
H	-1.9526720	-0.7789040	1.3964280
C	-2.0813290	2.5623120	0.6418800
H	-2.8586620	3.2827280	0.8805740
C	-0.2279170	-0.0418900	0.4563730
C	-0.9088480	3.0231900	0.1470790
H	-0.8574500	4.1010350	0.0038820
C	0.3011700	2.3360490	-0.2012440
H	1.0870450	2.9688050	-0.6022200
C	0.6120740	1.0173870	-0.0360570
C	-2.5098750	1.1920470	0.9183420
O	-3.6335910	0.9978860	1.3605430
C	-2.5344020	-0.7338830	-0.8356620
H	-3.5616190	-0.4582770	-0.6157510
C	-0.5582130	-0.9739640	-2.0274710
H	0.3672750	-0.7357870	-2.5352640
C	-1.7313580	-0.0554280	-1.9308060
H	-2.3004450	-0.1188310	-2.8704320
H	-1.4838830	0.9947970	-1.7611570
C	0.3922040	-1.2679920	1.0046270
C	2.0040490	0.6666450	-0.5191710
O	-0.2312210	-2.2670360	1.3074020
O	2.2607500	-0.1144670	-1.4036230
O	1.7243390	-1.1755010	1.1857010
O	2.9359480	1.3981800	0.1032930
C	4.2733620	1.1343380	-0.3169090
H	4.3931310	1.3564390	-1.3795380
H	4.9064740	1.7819320	0.2871720
H	4.5187340	0.0835710	-0.1459340
C	2.3540630	-2.3676520	1.6437520
H	2.2204380	-3.1720950	0.9166910
H	3.4095510	-2.1220420	1.7524230
H	1.9292270	-2.6786470	2.6002140

Imag. Freq. -357.06

S3‡

C	-3.9089100	0.3581480	0.8849290
C	-3.0883340	1.4961960	0.9822750
H	-3.4023800	2.5066160	0.7496830
H	-4.9446790	0.3687780	0.5675960
C	-0.9526930	0.8541260	-0.6854670
H	-0.9875120	1.9183890	-0.8979410
C	-2.3727480	-1.2470820	-0.9884430
H	-3.3554450	-1.5549890	-1.3337470
C	0.3469410	0.3313610	-0.4858530
C	-1.4087290	-2.2553630	-0.8464580
H	-1.7892520	-3.2726760	-0.9081340
C	-0.0491910	-2.1519160	-0.6060810
H	0.4978740	-3.0876550	-0.5336940
C	0.7413350	-1.0030680	-0.4131590
C	-2.1176640	0.1659200	-1.2723020
O	-2.9778670	0.8391090	-1.8274540
C	-3.1520850	-0.7828350	1.1360170
H	-3.5581370	-1.7762240	1.2843860
C	-1.7779190	1.1072690	1.2841240
H	-0.9909330	1.7840220	1.5984350
C	-1.8401620	-0.3358480	1.7214370
H	-1.9358040	-0.3499920	2.8182070
H	-0.9724710	-0.9477160	1.4692630
C	1.3657310	1.4163390	-0.2915260
C	2.1529950	-1.3379440	-0.0117500
O	2.8160950	-2.2171810	-0.5007660
O	1.1713830	2.4150690	0.3606560
O	2.4915520	1.1939490	-0.9858210
O	2.5624810	-0.5997770	1.0369120
C	3.5236830	2.1538540	-0.7661920
H	3.1879730	3.1486880	-1.0652350

H	3.7966430	2.1746480	0.2923960
H	4.3643510	1.8295010	-1.3773540
C	3.9201470	-0.8164900	1.4161920
H	4.0727370	-1.8571690	1.7089570
H	4.5847310	-0.5828730	0.5800030
H	4.1041690	-0.1476070	2.2556010

Imag. Freq. -432.36

S4‡

C	-2.0341590	-0.6877850	1.5765930
C	-0.8533790	-0.4032450	2.3042970
H	-0.6823850	0.4995350	2.8782870
H	-2.9433850	-0.0976320	1.5994570
C	-1.1760710	1.6957730	-0.0798850
H	-1.0219930	2.6684390	0.3816020
C	-2.9717690	0.4513120	-1.4282890
H	-3.8903480	0.6652790	-1.9677120
C	-0.0600900	0.9264650	-0.2796290
C	-2.3687930	-0.7308150	-1.5880810
H	-2.8252780	-1.4428170	-2.2735740
C	-1.1612920	-1.2410400	-0.9014480
H	-0.8792550	-2.2193560	-1.2869530
C	-0.0006360	-0.4324880	-0.6912050
C	-2.5763320	1.5218780	-0.4879650
O	-3.4205250	2.3255570	-0.1104500
C	-1.8210830	-1.8381560	0.7770600
H	-2.6665890	-2.4310660	0.4366750
C	0.0683050	-1.3850960	2.0632380
H	1.0921990	-1.3936960	2.4161730
C	-0.5753630	-2.5140510	1.3328230
H	-0.8989170	-3.2734450	2.0608500
H	0.0702080	-2.9981720	0.5978480
C	1.2038000	1.6161370	0.1841530
C	1.2860420	-1.0882660	-1.0217830
O	1.4700180	-2.2894120	-1.0495910
O	1.5322950	2.7254080	-0.1460660
O	1.8850420	0.8828500	1.0857550
O	2.2418980	-0.2102250	-1.3756300
C	3.1283630	1.4578240	1.4805990
H	3.7743010	1.5862130	0.6079050
H	2.9713590	2.4313290	1.9494560
H	3.5709360	0.7562870	2.1868390
C	3.5173640	-0.7827570	-1.6501710
H	3.9114330	-1.2759810	-0.7577500
H	3.4401350	-1.5158270	-2.4552930
H	4.1560120	0.0486300	-1.9448980

Imag. Freq. -350.05

S5‡

C	-0.8874390	1.6258660	-0.2559680
C	-1.9224260	1.8428820	0.7044860
H	-1.7863090	2.3480630	1.6536390
H	0.1016760	2.0642850	-0.2211990
C	-0.8050100	-1.0272730	-1.0376050
H	-1.2087100	-1.4059590	-1.9756640
C	-1.3367170	-1.2648050	1.4693750
H	-2.0944530	-1.6067680	2.1683230
C	0.6169950	-1.0087450	-1.0239890
C	-0.2547850	-0.5894140	1.9443150
H	-0.2655320	-0.3721170	3.0111590
C	0.9082800	-0.1217470	1.2733410
H	1.6045790	0.4301090	1.8979390
C	1.3810060	-0.4630460	0.0080590
C	-1.6603700	-1.5511260	0.0813290
O	-2.6657570	-2.1871190	-0.2171630
C	-1.3707590	0.8064520	-1.2984140
H	-0.9377290	0.8672430	-2.2934010
C	-3.0737950	1.2674520	0.2653100
H	-4.0096500	1.2119190	0.8085750
C	-2.8845580	0.7436380	-1.1199250
H	-3.3270610	1.4493960	-1.8380840
H	-3.3427840	-0.2337270	-1.2943840
C	1.2408520	-1.2991520	-2.3457630
C	2.7584230	0.0471700	-0.3296520
O	2.4115970	-1.9413110	-2.2284150
O	3.6209360	-0.1014230	0.6850200
C	3.1588690	-2.0381590	-3.4391360
H	4.0525540	-2.6090600	-3.1915910
H	2.5756120	-2.5464310	-4.2089990
H	3.4246550	-1.0359020	-3.7848640
C	4.9249880	0.4246360	0.4387330
H	5.3742450	-0.0729240	-0.4232130
H	4.8722190	1.4972720	0.2400010
H	5.4993500	0.2257450	1.3417870
O	0.7274510	-1.0238210	-3.4066370
O	3.0477270	0.5901590	-1.3694230

Imag. Freq. -372.70

S6‡

C	-1.1629760	-1.9052560	0.4547870
C	-0.3071770	-1.6964260	-0.6755340
H	0.4783940	-2.3729760	-0.9864430
H	-0.9820710	-2.6385650	1.2323290
C	0.3220040	0.6158920	1.6257690
H	-0.2234100	0.8903360	2.5239360
C	0.4651310	1.0470420	-0.8924150
H	0.0332150	1.7321110	-1.6210480
C	1.1532440	-0.4608970	1.6865890
C	1.8061810	0.6686210	-1.1451320
H	2.2496650	1.0256740	-2.0706590
C	2.4898640	-0.3093420	-0.4558470
H	3.4035130	-0.6917140	-0.9014600
C	2.0329190	-0.9849740	0.6844080
C	-0.0433260	1.4109920	0.4634670
O	-0.8236010	2.3523540	0.5611220
C	-2.1506920	-0.9737930	0.4406780
H	-2.9029980	-0.8317620	1.2072940
C	-0.7145280	-0.5488730	-1.3772220

H	-0.5073520	-0.4444750	-2.4371370
C	-2.0740960	-0.1588500	-0.8119680
H	-2.8389390	-0.5049050	-1.5225130
H	-2.2356960	0.9115020	-0.6550680
C	1.1104890	-1.1735360	3.0180760
C	2.5738800	-2.3523520	0.9380080
O	0.0939610	-1.4894070	3.5828010
O	1.9576430	-3.2190040	1.5212230
O	2.3384380	-1.3520180	3.5245490
O	3.7823760	-2.5637040	0.3951920
C	2.3800530	-2.1670650	4.6947230
H	1.7722370	-1.7288860	5.4884750
H	2.0026170	-3.1646930	4.4563870
H	3.4273700	-2.2098150	4.9896640
C	4.2898040	-3.8862210	0.5654360
H	4.3960280	-4.1157410	1.6277140
H	3.6149250	-4.6153400	0.1119410
H	5.2593750	-3.8965340	0.0704400

Imag. Freq. -403.20

S7‡

C	1.1454240	1.1229220	1.4842910
C	1.0568880	-1.2376980	-0.8869040
H	1.1791330	-2.3165710	-0.9024050
C	2.3129270	0.9982160	-1.0769630
H	3.3260680	1.3220330	-1.3125200
C	-0.1553640	-0.7369620	-0.5538920
C	1.2888940	1.8474180	-1.5561430
H	1.5931180	2.7742290	-2.0337390
C	-0.0521750	1.7037730	-1.2371710
H	-0.6997750	2.5580900	-1.4084190
C	-0.6054650	0.6419170	-0.5240980
C	2.2907790	-0.4992630	-1.1335500
O	3.3421380	-1.0844280	-1.3454940
C	2.4182310	1.2431700	0.8908650
C	-1.1877600	-1.8058870	-0.2656940
C	-1.8409860	0.8957360	0.2631340
O	-0.9841070	-2.7870970	0.4005200
O	-2.1977650	0.2061200	1.1951510
O	-2.3332550	-1.5659410	-0.9208560
O	-2.4850490	2.0220860	-0.0881270
C	-3.3964950	-2.4572240	-0.5896320
H	-3.1147030	-3.4882930	-0.8112070
H	-3.6312040	-2.3662230	0.4738260
H	-4.2435910	-2.1487950	-1.2003820
C	-3.6324120	2.3227280	0.7032580
H	-4.3663360	1.5176520	0.6289280
H	-3.3523700	2.4469110	1.7520690
H	-4.0355690	3.2499830	0.2994230
C	2.7911510	2.7194910	0.9675120
H	3.4624700	2.8528550	1.8289710
H	3.3076520	3.1223810	0.0930870
C	1.4757170	3.3691580	1.2645420
H	1.3087210	4.4392690	1.2300050
C	0.5823420	2.4308710	1.6634600
H	-0.4273000	2.6163580	2.0140930
H	3.1766900	0.4779690	1.0342860
H	0.6959620	0.2014520	1.8341940

Imag. Freq. -422.47

S8‡

C	-0.2581850	0.6447880	1.6174660
C	-0.9188260	-0.5839060	1.7187930
H	-0.5715530	-1.4329960	2.2961180
H	0.6718880	0.8952340	2.1143380
C	2.1877900	-0.0598700	-0.3139450
H	3.0687870	0.4813320	0.0233770
C	-0.1962050	0.4695450	-1.1628250
H	-0.7009590	1.2082590	-1.7808380
C	2.0837300	-1.3516580	0.0508210
C	-0.8027150	-0.8014560	-1.0939890
H	-1.7333300	-0.8978070	-1.6459710
C	-0.1548240	-2.0688150	-0.8477670
H	-0.7498300	-2.9480650	-1.0874950
C	1.0728270	-2.3343440	-0.3454340
C	1.2514510	0.7876030	-1.0855700
O	1.6592120	1.8339830	-1.5654450
C	-0.8762020	1.4177960	0.6262410
H	-0.6334250	2.4558010	0.4235790
C	-1.9810450	-0.5989810	0.8137250
H	-2.7197280	-1.3898100	0.7433300
C	-2.2505430	0.8294970	0.4262750
H	-2.9145040	1.2674610	1.1872750
H	-2.7034040	0.9863990	-0.5532320
C	3.1339500	-1.7947520	1.0368740
C	1.4243220	-3.7874040	-0.2995380
O	0.6280400	-4.6949110	-0.2540170
O	4.2811170	-1.4317680	1.0564320
O	2.7527070	-3.9855410	-0.3885060
O	2.5874430	-2.5901510	1.9761530
C	3.1627310	-5.3488890	-0.3217880
H	2.8403990	-5.7946910	0.6225760
H	2.7285990	-5.9167230	-1.1471270
H	4.2491810	-5.3343160	-0.3924930
C	3.5182250	-3.1068420	2.9248480
H	2.9394640	-3.7401490	3.5953060
H	4.2897700	-3.6877910	2.4128780
H	3.9952440	-2.2932480	3.4751040

Imag. Freq. -460.01

S9‡

C	0.1583650	-2.5589100	1.2641140
C	-0.9637740	-3.0601160	0.6037170
H	-1.0005520	-3.9960960	0.0586680
H	1.1284070	-3.0389890	1.2973000
C	-0.9678480	2.0672310	0.1425480
H	-0.6314120	3.0228750	0.5345130

C	-3.1007650	1.0004220	-0.8628000
H	-4.1122460	1.2756890	-1.1495550
C	-0.0248850	1.1104190	-0.0299070
C	-2.6532800	-0.2200400	-1.1921690
H	-3.3535090	-0.8505910	-1.7388100
C	-1.3798860	-0.8973680	-0.9175260
H	-1.1956220	-1.6940430	-1.6305640
C	-0.1613840	-0.2625040	-0.5030610
C	-2.4146680	2.0887460	-0.1402460
O	-3.0604050	3.0740270	0.1895850
C	-0.1256400	-1.2725320	1.7097500
H	0.5485760	-0.6347660	2.2645640
C	-1.9679180	-2.0661920	0.5799090
H	-3.0002760	-2.2920880	0.3300650
C	-1.6073300	-1.0802160	1.6650610
H	-2.0330710	-1.4321850	2.6161930
H	-1.9446720	-0.0541520	1.5081600
C	1.3473680	1.6063810	0.3882640
C	1.0169790	-0.9386510	-1.1149330
O	1.0304720	-2.1062940	-1.4459140
O	1.7934600	2.6828240	0.0889120
O	1.9904840	0.7487440	1.2027550
O	2.0601810	-0.1206430	-1.3441020
C	3.3217340	1.1418260	1.5282220
H	3.9158340	1.2306970	0.6149260
H	3.3235640	2.1023110	2.0469830
H	3.7164690	0.3550280	2.1696200
C	3.1966800	-0.7395750	-1.9407340
H	3.6083930	-1.5016000	-1.2744320
H	2.9202520	-1.2084690	-2.8869940
H	3.9163920	0.0615430	-2.1024890

Imag. Freq. -445.80

S10‡

C	-2.6529740	-0.6848730	-0.5238840
C	-2.4875030	0.6828690	-0.2953760
H	-3.0354260	1.4762220	-0.7907430
H	-3.3519850	-1.1266130	-1.2246770
C	2.2637840	0.6331370	0.7378050
H	2.9192520	1.3200170	1.2667200
C	0.1468520	0.6834010	-0.7907020
H	-0.2333020	1.3912190	-1.5206790
C	2.5849400	-0.6807740	0.7933750
C	0.1215110	-0.6784830	-1.1870300
H	-0.4481080	-0.8908390	-2.0851360
C	0.9276480	-1.7727960	-0.7478630
H	0.6568380	-2.7278230	-1.1897930
C	1.9445930	-1.8222450	0.1636580
C	1.1992890	1.3577010	0.0273490
O	1.1746910	2.5781300	0.1047300
C	-1.6770420	-1.3795980	0.1895060
H	-1.5959300	-2.4590730	0.2491700
C	-1.3611390	0.8764180	0.5324500
H	-1.1223630	1.8318200	0.9885980
C	-1.1135930	-0.4464320	1.2171770
H	-1.7587820	-0.4913770	2.1077630
H	-0.0875130	-0.6464590	1.5300980
C	3.8744580	-0.9320170	1.5450710
C	2.3953420	-3.1699150	0.6207740
O	2.1067770	-4.1539760	-0.2501590
O	4.7514450	-1.5871520	0.7700430
O	2.9261880	-3.3846460	1.6871910
O	4.1193950	-0.5186670	2.6475100
C	2.4662180	-5.4612370	0.1922370
H	3.5429170	-5.5197360	0.3639760
H	1.9470930	-5.7071320	1.1211390
H	2.1672600	-6.1364060	-0.6079960
C	5.9399850	-1.9937400	1.4458510
H	6.4661290	-1.1271270	1.8506260
H	5.6803210	-2.6747070	2.2601850
H	6.5485150	-2.4998150	0.6979370

S11‡

C	1.3282650	-1.1934940	-1.2973210
C	2.5807180	-2.0548890	-1.1899910
H	2.5485250	-2.8476810	-0.4363980
H	0.4800930	-1.5451450	-1.8753230
C	0.7998590	1.4373480	0.6099660
H	0.8682260	2.4972360	0.3693220
C	2.0679410	-0.3630550	1.9029480
H	2.8522650	-0.4926270	2.6435900
C	-0.4505250	0.8554940	0.4438880
C	1.3783400	-1.4288720	1.4685460
H	1.6452250	-2.3988330	1.8846610
C	0.3199910	-1.4737920	0.4579390
H	-0.0061800	-2.4881490	0.2491740
C	-0.7211230	-0.5140630	0.3749910
C	1.9841130	1.0008120	1.3533270
O	2.9171410	1.7768270	1.5267210
C	1.7619720	0.1413500	-1.3982460
H	1.1755110	0.9455110	-1.8241100
C	3.6666430	-1.0470710	-0.9609840
H	4.6827880	-1.3089900	-0.6907140
C	3.1913840	0.2009990	-1.1517690
H	3.7561350	1.1218670	-1.0737980
C	-1.5020900	1.8489150	0.0110810
C	-2.0422840	-0.9402230	-0.1515920
O	-2.3450290	2.1431110	1.0001370
O	-2.0847530	-2.2568140	-0.4470320
C	-3.4440810	2.9651650	0.6088130
H	-4.0398140	3.1105070	1.5083530
H	-3.0887120	3.9218600	0.2207530
H	-4.0237070	2.4508920	-0.1612030
C	-3.3322530	-2.7066110	-0.9727090
H	-4.1315500	-2.5384200	-0.2481100
H	-3.5726110	-2.1718490	-1.8938630
H	-3.2049960	-3.7707380	-1.1654300
O	-1.5024640	2.3697220	-1.0766710
O	-2.9952860	-0.2144170	-0.3282260
H	2.7313140	-2.5470100	-2.1613610

Imag. Freq. -471.03

S12‡

C	-1.1639630	0.8153830	-1.1689530
C	-0.4545540	-2.2330510	-0.1631940
H	-0.1139580	-3.1883890	-0.5527400
C	-2.4498270	-1.0569160	0.9133930
H	-3.5126400	-1.2209660	1.0877120
C	0.4371070	-1.2337670	-0.0543050
C	-1.7985700	-0.1977110	1.8024710
H	-2.3996460	0.2097610	2.6109110
C	-0.5782520	0.4058680	1.5692410
H	-0.2903170	1.2504970	2.1861570
C	0.1951420	0.1418370	0.4209660
C	-1.8984440	-2.1598530	0.1026760
O	-2.6462020	-3.0208020	-0.3410600
C	-2.4462480	0.2670510	-0.9678170
C	1.8537460	-1.6231990	-0.4014580
C	1.2957970	1.0983990	0.0550370
O	2.1658470	-2.3445250	-1.3120330
O	1.8872850	1.0573830	-0.9989820
O	2.7220550	-1.1329440	0.4991840
O	1.5043730	2.0524950	0.9725780
C	4.0945590	-1.3588690	0.1797880
H	4.2953400	-2.4284070	0.0959330
H	4.3363300	-0.8700390	-0.7671840
H	4.6651000	-0.9218810	0.9978550
C	2.4991460	3.0130460	0.6138730
H	3.4602260	2.5184030	0.4602450
H	2.2133330	3.5271940	-0.3065720
H	2.5509450	3.7101720	1.4480990
C	-3.3168560	1.3226120	-0.4443820
H	-4.3491120	1.1613880	-0.1539060
C	-2.6318100	2.4709980	-0.3325170
H	-3.0064580	3.4034160	0.0734580
C	-1.2531150	2.3110190	-0.9083050
H	-1.1828800	2.8343280	-1.8729730
H	-2.8187910	-0.6019760	-1.4978430
H	-0.4723870	0.4211630	-1.9045430
H	-0.4717540	2.7316920	-0.2679700

Imag. Freq. -462.46

S13‡

C	0.7846320	-0.1311730	2.2161790
C	0.9074750	1.0783430	1.3096130
H	0.3076130	1.9662470	1.4751490
H	-0.0389550	-0.8143400	1.9800120
C	1.1531350	-1.2670860	-1.0158770
H	1.2772010	-2.3450810	-1.0722760
C	2.3549640	0.9582080	-1.3830560
H	3.3539720	1.3361610	-1.5962630
C	-0.0365870	-0.7812420	-0.6157920
C	1.2819150	1.7688110	-1.7815020
H	1.5336200	2.6894290	-2.3021910
C	-0.0131210	1.6395900	-1.3322330
H	-0.6971080	2.4656080	-1.4932260
C	-0.4233070	0.6248550	-0.4429110
C	2.3842530	-0.5144580	-1.2912900
O	3.4448790	-1.1077820	-1.4269150
C	2.1408240	-0.7685050	2.1152550
H	2.3802670	-1.7290680	2.5556390
C	2.2450150	1.1697400	0.8762480
H	2.7239280	2.1184610	0.6690460
C	2.9750320	0.0054690	1.4041710
H	4.0113540	-0.2089430	1.1718560
C	-1.0805300	-1.8409560	-0.3534540
C	-1.6807500	0.8454900	0.3423820
O	-0.9178680	-2.7972100	0.3603010
O	-2.1686040	0.0327580	1.0965560
O	-2.1797890	-1.6200430	-1.0856640
O	-2.1643480	2.0904100	0.2149800
C	-3.2684850	-2.4941030	-0.7890560
H	-2.9846350	-3.5328620	-0.9675630
H	-3.5585690	-2.3710240	0.2572870
H	-4.0779910	-2.1958850	-1.4533240
C	-3.3206650	2.3662180	1.0060820
H	-4.1366370	1.6952300	0.7305970
H	-3.0944060	2.2330860	2.0659620
H	-3.5830630	3.4009490	0.7931270
H	0.6032810	0.2257690	3.2400950

Imag. Freq. -452.48

S14‡

C	-0.6057630	-0.7876820	2.4062810
C	-1.7990170	-0.9738040	1.7101060
H	-2.3082370	-1.9184060	1.5630390
H	0.0408750	-1.5794150	2.7652020
C	-1.6701170	0.6365380	-0.3445110
H	-1.9079070	1.6934960	-0.4708580
C	-2.4609720	-1.5122600	-1.5552560
H	-3.2873540	-1.9423870	-2.1130330
C	-0.2149530	0.4645720	-0.3873860
C	-1.4843810	-2.3229200	-1.0840800
H	-1.6283800	-3.3886170	-1.2574220
C	-0.2310680	-2.0131990	-0.4491650
H	0.3684300	-2.8842360	-0.1989050
C	0.4089160	-0.7920020	-0.3410530
C	-2.5693610	-0.0728440	-1.3502400
O	-3.4393310	0.5822490	-1.9002370
C	-0.3014660	0.5607050	2.4128010
H	0.6343910	0.9903620	2.7487820
C	-2.2634590	0.3078920	1.1786120
H	-3.3448770	0.4265540	1.0898990
C	-1.5099370	1.3422250	2.0401330
H	-2.1043130	1.5408650	2.9436540
H	-1.2964010	2.2882400	1.5414230
C	0.5775830	1.7084760	-0.5107760
C	1.8411140	-0.8632840	0.1310200

O	0.1940920	2.8142670	-0.1860610
O	2.2893060	-0.2626330	1.0793190
O	1.7820810	1.4992300	-1.0736250
O	2.5586180	-1.7388220	-0.5846490
C	3.9147700	-1.8813030	-0.1648430
H	3.9610400	-2.2372230	0.8667940
H	4.3603320	-2.6060190	-0.8440670
H	4.4310610	-0.9210690	-0.2303970
C	2.6491200	2.6291590	-1.0744110
H	2.8666500	2.9375350	-0.0488270
H	3.5590620	2.3037720	-1.5767130
H	2.1889860	3.4621400	-1.6091500

Imag. Freq. -124.19

S15‡

C	4.1323660	0.0834500	-0.7622570
C	3.3594170	1.2190750	-0.4546850
H	3.7456010	2.1590690	-0.0823560
H	5.1701730	-0.0448650	-0.4821140
C	1.1116560	0.7705800	0.4971840
H	1.1609550	1.7448420	0.9895320
C	2.0508400	-1.5234000	1.2275770
H	2.9360530	-1.9790860	1.6617590
C	-0.3157410	0.4196890	0.2857070
C	0.9989190	-2.3828250	0.8290920
H	1.2301270	-3.4433870	0.9075620
C	-0.2510600	-2.1004550	0.3466110
H	-0.8814420	-2.9523140	0.1145900
C	-0.8705440	-0.8194570	0.1495420
C	2.0674640	-0.1215130	1.2572880
O	3.0813080	0.5178490	1.6332640
C	3.3182040	-0.8744450	-1.3074760
H	3.6260670	-1.8806480	-1.5714590
C	1.9507470	1.0097470	-0.8728890
H	1.4831560	1.8644070	-1.3636470
C	1.9947060	-0.2917720	-1.6919690
H	1.9952030	-0.0680980	-2.7677220
H	1.1511580	-0.9624330	-1.5071930
C	-1.1597920	1.6393580	0.1003580
C	-2.2866200	-0.8960030	-0.3722920
O	-2.7055040	-0.2645260	-1.3119520
O	-0.7786450	2.6265770	-0.4875290
O	-2.3491480	1.5580910	0.7141030
O	-3.0186930	-1.8008490	0.2915070
C	-3.2644050	2.5995090	0.3801170
H	-2.8336510	3.5757010	0.6096270
H	-3.5038010	2.5472220	-0.6851000
H	-4.1530300	2.4177710	0.9827830
C	-4.3580260	-1.9422360	-0.1800530
H	-4.8890440	-0.9917570	-0.0928720
H	-4.3631600	-2.2553770	-1.2263110
H	-4.8165550	-2.6996020	0.4533360

Imag. Freq. -283.25

S16‡

C	2.0307440	-0.3770010	-1.5724220
C	0.8836850	-0.0408430	-2.2911180
H	0.7095120	0.9127270	-2.7747360
H	2.9539030	0.1906240	-1.5446420
C	1.2072540	1.5927330	0.2523200
H	1.1015710	2.6098310	-0.1195640
C	2.8727040	0.1992530	1.6131000
H	3.7147820	0.3562370	2.2815250
C	0.0491860	0.8531100	0.3690700
C	2.2512390	-0.9802710	1.5782410
H	2.5961210	-1.7623840	2.2519760
C	1.1566260	-1.3944920	0.6412990
H	0.8284570	-2.3949150	0.9259430
C	-0.0424860	-0.5387810	0.5530180
C	2.5718140	1.3578070	0.7426560
O	3.4522440	2.1757410	0.5032100
C	1.8007630	-1.6444610	-0.8679780
H	2.6864020	-2.2628330	-0.7139280
C	-0.0523000	-1.0450290	-2.1284530
H	-1.0807510	-1.0042570	-2.4667990
C	0.6222110	-2.2758440	-1.6283480
H	1.0075660	-2.8519290	-2.4813060
H	-0.0155420	-2.9220430	-1.0234020
C	-1.1865520	1.6463400	0.0134280
C	-1.3286210	-1.2160960	0.8279630
O	-1.5169370	-2.4122820	0.7189640
O	-1.4858500	2.6985120	0.5139800
O	-1.8786600	1.0897670	-1.0010570
O	-2.2847520	-0.3783210	1.2694500
C	-3.0966090	1.7634250	-1.3099970
H	-3.7524010	1.7678590	-0.4353250
H	-2.9014610	2.7950690	-1.6097110
H	-3.5494360	1.2031650	-2.1271950
C	-3.5617280	-0.9749220	1.4770830
H	-3.9529690	-1.3728810	0.5372020
H	-3.4884200	-1.7877860	2.2020440
H	-4.2012260	-0.1782120	1.8543100

Imag. Freq. -173.11

S17‡

C	3.0438510	-1.1178300	-0.9961760
C	2.0240790	-0.2553730	-1.4115320
H	2.1676770	0.7335040	-1.8309780
H	4.0857980	-0.8356320	-0.9052930
C	0.6027480	2.0509610	0.2236150
H	0.2270500	3.0583060	0.0627900
C	2.6760590	0.9280380	1.1742510
H	3.7077090	1.1441670	1.4432650
C	-0.2720250	1.0411920	0.1350990
C	2.0956610	-0.2054860	1.7207930
H	2.6855540	-0.7240930	2.4745600
C	0.9391570	-0.8581950	1.3301800
H	0.6504130	-1.7452720	1.8866910
C	0.0438820	-0.4411690	0.2315680
C	2.0756990	1.9988260	0.4068300

O	2.7417510	2.9314300	-0.0382980
C	2.4878880	-2.3119390	-0.5967240
H	3.0247340	-3.1371260	-0.1425620
C	0.7218400	-0.9087710	-1.2271680
H	-0.0471440	-0.6553870	-1.9594700
C	1.0861570	-2.3980080	-1.0934970
H	1.0799290	-2.8364990	-2.1023650
H	0.4083850	-2.9842400	-0.4801460
C	-1.6555990	1.4820470	-0.2562890
C	-1.2705890	-1.2259870	0.4052480
O	-1.6446160	-2.1792340	-0.2270510
O	-2.1650630	2.5318840	0.0388690
O	-2.2496820	0.5812240	-1.0656500
O	-1.9621070	-0.7115790	1.4340260
C	-3.5682850	0.9245570	-1.4905660
H	-4.2073970	1.1108590	-0.6244610
H	-3.5422690	1.8232170	-2.1102410
H	-3.9252060	0.0691600	-2.0619630
C	-3.2437610	-1.3026410	1.6471320
H	-3.8507220	-1.2124370	0.7425890
H	-3.1388980	-2.3597700	1.8994090
H	-3.6903930	-0.7494720	2.4711600

Imag. Freq. -169.84

S18‡

C	-1.6818930	0.8053280	-1.6212360
C	-2.8177150	1.5013080	-1.2571150
H	-2.9348440	2.5767110	-1.3259770
H	-0.8392540	1.2058450	-2.1717310
C	-1.0868640	-1.0897200	0.1096920
H	-1.1146550	-2.1802720	0.0756040
C	-2.2258170	0.6867640	1.5811720
H	-3.0327460	0.8547190	2.2883440
C	0.3253580	-0.6390400	0.1310410
C	-1.4002410	1.7467880	1.2344350
H	-1.7758840	2.7347530	1.4973650
C	-0.2251660	1.7566460	0.4942310
H	0.1849080	2.7423600	0.2949320
C	0.6753070	0.6722910	0.1965180
C	-1.9452590	-0.7191520	1.3171440
O	-2.4889830	-1.6133720	1.9484300
C	-1.8191230	-0.6323280	-1.2540820
H	-1.4169380	-1.3022470	-2.0172870
C	-3.6835810	0.6358900	-0.5923830
H	-4.6179290	0.9185020	-0.1213320
C	-3.3361960	-0.7661980	-0.9823050
H	-3.8471720	-1.0027160	-1.9250080
H	-3.5998510	-1.5333060	-0.2513460
C	1.3212610	-1.7107970	-0.1650770
C	2.0720760	1.0669620	-0.2062280
O	2.4161560	-1.6319250	0.6000950
O	2.5067470	2.1417920	0.4683440
C	3.4760950	-2.5015180	0.2073610
H	4.2688700	-2.3520550	0.9386330
H	3.1392340	-3.5397660	0.2075930
H	3.8186500	-2.2292600	-0.7941350
C	3.8130310	2.5856540	0.1033690
H	4.5439980	1.7956040	0.2872530
H	3.8422740	2.8548100	-0.9547430
H	4.0164640	3.4526800	0.7294230
O	1.1239490	-2.5835750	-0.9782420
O	2.7215240	0.5223570	-1.0665820

Imag. Freq. -234.28

S19‡

C	0.8403360	0.3047440	-1.9660430
C	1.0967050	-0.9806480	-1.5380580
H	0.4771580	-1.8490510	-1.7316870
H	-0.1094130	0.6512030	-2.3574830
C	1.1626570	1.1311930	0.8989910
H	1.2794490	2.1983690	1.0633060
C	2.4592670	-1.0785090	0.7162420
H	3.4689420	-1.3922220	0.9914880
C	-0.1091870	0.6420300	0.6296690
C	1.4513750	-2.0018830	1.3097150
H	1.8192010	-2.8754600	1.8397190
C	0.1289420	-1.8331120	1.1682040
H	-0.5449520	-2.6085580	1.5201920
C	-0.5085410	-0.6941910	0.5194750
C	2.3453040	0.3433940	1.2523570
O	3.2869460	0.8461720	1.8444540
C	1.8851470	1.1248810	-1.5363980
H	1.8967160	2.2051000	-1.6241380
C	2.4432170	-1.0619100	-0.8849170
H	2.9852880	-1.9577070	-1.1992750
C	3.0991560	0.2711600	-1.3240510
H	3.6040770	0.1326820	-2.2888670
H	3.8284190	0.6682190	-0.6147730
C	-1.0711990	1.7296130	0.2199550
C	-1.7950010	-0.9518210	-0.1857420
O	-0.8104420	2.5828080	-0.5945620
O	-2.2695170	-0.2301680	-1.0395830
O	-2.2089280	1.6837140	0.9201310
O	-2.3606160	-2.1220410	0.1557000
C	-3.2197710	2.5796600	0.4618770
H	-2.8653580	3.6113810	0.5021860
H	-3.4886530	2.3264190	-0.5667310
H	-4.0679110	2.4367020	1.1295690
C	-3.5644430	-2.4317760	-0.5426810
H	-4.3241370	-1.6727730	-0.3446520
H	-3.3808570	-2.4746270	-1.6184610
H	-3.8830750	-3.4024570	-0.1663030

Imag. Freq. -239.07

S20‡

C	-1.5485320	0.4022770	-1.5372980
C	-0.2882610	-2.1153720	0.1595160
H	0.0851050	-3.0955120	-0.1208240

C	-2.4587700	-0.7883020	0.6042980
H	-3.4554440	-1.0808110	0.9399280
C	0.5598450	-1.0609910	0.1022810
C	-1.9462860	0.3194480	1.4278130
H	-2.6113980	0.7374060	2.1776470
C	-0.6386810	0.7827470	1.3856900
H	-0.4304250	1.7052980	1.9198840
C	0.3791210	0.3045020	0.5636500
C	-1.6947950	-2.1014440	0.5433280
O	-2.3118090	-3.1364630	0.7306280
C	-2.7202540	-0.2607200	-0.9342300
C	1.9375190	-1.4424490	-0.3948510
C	1.4214730	1.2722450	0.1404770
O	2.1459590	-2.0449400	-1.4157720
O	2.1005070	1.1484320	-0.8578520
O	2.8865990	-1.1066700	0.4904340
O	1.4928890	2.3685870	0.9207060
C	4.2193580	-1.3038420	0.0229120
H	4.3853300	-2.3523080	-0.2319820
H	4.3905540	-0.6838490	-0.8606550
H	4.8695830	-0.9985210	0.8413560
C	2.4442610	3.3398490	0.4939510
H	3.4482480	2.9104270	0.4834070
H	2.2049290	3.6962480	-0.5107440
H	2.3817760	4.1525610	1.2160830
C	-3.6744080	0.9227160	-0.6711100
H	-4.2175790	1.1608130	-1.5956720
H	-4.4003870	0.7499880	0.1249330
C	-2.6665000	1.9897010	-0.3972500
H	-2.8828700	2.9211520	0.1133760
C	-1.5485180	1.7415910	-1.1926580
H	-0.7320880	2.4299610	-1.3804630
H	-3.1207920	-1.1109530	-1.4891210
H	-0.7899710	-0.1015230	-2.1256280

Imag. Freq. -195.46

b. CBS-QB3 structures. All minima and transition states in this section were optimized and subjected to frequency analysis were optimized using the CBS-QB3 compound method in the gas phase at standard temperature and pressure (298.15 K and 1.0 atm). The naming system is the same as in Scheme 2 of the main text. Atoms are listed by their atomic symbol. Absolute enthalpies and free energies are given in Hartrees.

1

C	-1.84823400	0.92897700	0.18782600
H	-2.05157900	1.98535300	0.33218500
C	-3.09731000	-1.20907700	-0.44865100
H	-4.10194400	-1.54744100	-0.68301900
C	-0.54227400	0.57642600	0.08846800
C	-2.06334300	-2.05174300	-0.68076900
H	-2.32099100	-3.02450500	-1.09035000
C	-0.66943700	-1.88469400	-0.39251000
H	-0.07522100	-2.78686700	-0.47244300
C	0.01360400	-0.76087800	-0.03332100
C	-3.08439100	0.12792000	0.16453400
O	-4.13040500	0.62144000	0.56796000
C	0.40321800	1.76125600	0.06486900
C	1.44510000	-0.92876900	0.39860500
O	0.27598200	2.75605000	0.72784900
O	1.98657200	-0.20799500	1.20143300
O	1.34375400	1.59626900	-0.88472200
O	2.03937200	-2.00082500	-0.15610600
C	2.32743100	2.64493300	-0.96791700
H	1.84521000	3.60735800	-1.14113900
H	2.90157600	2.68843100	-0.04129800
H	2.96722800	2.37683900	-1.80550000
C	3.38101000	-2.26910000	0.29547400
H	4.03368400	-1.42721100	0.06209900
H	3.39302400	-2.44318000	1.37214600
H	3.69457100	-3.15979500	-0.24363800

CBS-QB3 enthalpy: -800.06253
CBS-QB3 free energy: -800.12306

2

C	-0.73448900	-0.98928600	-0.00000500
C	-1.17944600	0.28096500	0.00000100
C	1.17944600	0.28096600	0.00000100
C	0.73449000	-0.98928500	-0.00000500
H	-1.34713500	-1.88179600	-0.00000800
H	1.34713700	-1.88179400	-0.00000800
H	-2.21024800	0.60776600	0.00000200
H	2.21024800	0.60776800	0.00000200
C	-0.00000100	1.21565500	0.00000600
H	-0.00000100	1.87699200	-0.87717000
H	-0.00000100	1.87697500	0.87719600

CBS-QB3 enthalpy: -193.70764
CBS-QB3 free energy: -193.73938

3$_{endo}$

C	1.61008600	0.28793300	-1.93199200
C	2.34034200	-0.81677300	-1.77972700
H	2.25719300	-1.72264500	-2.36634700
H	0.82059800	0.45456900	-2.65230000
C	1.09614300	1.02455100	0.48058500
H	0.98928500	1.96861600	1.02108200
C	2.51850100	-1.10507800	0.77850100
H	3.26760600	-1.46239900	1.48894100
C	-0.29163200	0.49466600	0.19210600
C	1.46335600	-2.16605500	0.61257800
H	1.81896800	-3.18931200	0.69554700
C	0.14858400	-2.00929100	0.38676600
H	-0.42326600	-2.92432000	0.31560400
C	-0.67798100	-0.80511400	0.17040400
C	1.87324200	0.11086400	1.42366000
O	1.98826400	0.36332500	2.59957500
C	1.95479300	1.28433800	-0.84061000
H	1.83053700	2.32373800	-1.14053000
C	3.24914300	-0.67394700	-0.57082500
H	4.18933500	-1.22051700	-0.65775000
C	3.41087000	0.86445900	-0.53205700
H	4.07055300	1.19497500	-1.33672100
H	3.79768900	1.24816500	0.41659400
C	-1.21090000	1.62948500	-0.18666300
C	-2.12542200	-1.05661200	-0.16447100
O	-2.88857500	-0.22774000	-0.60416400
O	-1.12811600	2.20203700	-1.24588100
O	-1.97650400	2.02160500	0.83949500
O	-2.50694000	-2.32657500	0.07847300
C	-2.89493800	3.09411700	0.55172200
H	-2.36045400	3.96952600	0.18106600
H	-3.61868600	2.76521200	-0.19515200
H	-3.38838100	3.31281500	1.49574800
C	-3.88255300	-2.62992600	-0.21594100
H	-4.54570500	-2.01466900	0.39348800
H	-4.09560800	-2.44763600	-1.27001900
H	-4.00449400	-3.68304000	0.02653100

CBS-QB3 enthalpy: -993.805512
CBS-QB3 free energy: -993.872931

3$_{exo}$

C	4.02434100	0.14902500	-0.42736300
C	3.37770700	1.31300300	-0.55481000
H	3.77668100	2.29239700	-0.31993800
H	5.03971200	0.01987700	-0.07233600
C	1.08606300	0.85982300	0.37035800
H	1.06245900	1.80714700	0.91528200
C	2.32894900	-1.38790700	0.61840400
H	3.04731500	-1.83448900	1.31013000
C	-0.34538800	0.44984800	0.09813300
C	1.18981300	-2.34960300	0.41623800
H	1.46750600	-3.39963600	0.44687600
C	-0.11188400	-2.08512900	0.21131900
H	-0.75286200	-2.95004900	0.10874700
C	-0.84230100	-0.81267200	0.05458800
C	1.80648200	-0.12585400	1.29111300
O	1.94795500	0.09205800	2.46962200
C	3.07231500	-1.00046400	-0.72410800
H	3.54551400	-1.88753000	-1.14946700
C	1.93315700	1.05747400	-0.95639100
H	1.46920600	1.83560000	-1.56050000
C	2.07446200	-0.30137200	-1.66502400
H	2.53415000	-0.15344900	-2.64529500
H	1.13605100	-0.83586800	-1.80134500
C	-1.18524000	1.66813600	-0.19935300
C	-2.31484600	-0.93561900	-0.24088600
O	-3.01682900	-0.03975400	-0.64901400
O	-1.08632000	2.29009700	-1.22821700
O	-1.89737800	2.05659100	0.86673700
O	-2.79422400	-2.17241000	0.00020900
C	-2.74189200	3.20586800	0.66029400
H	-2.15448100	4.05839300	0.31752400
H	-3.50708900	2.96883500	-0.08008000
H	-3.19296200	3.41036300	1.62839100
C	-4.19848600	-2.35590300	-0.25694600
H	-4.78980100	-1.69453700	0.37753900
H	-4.42499700	-2.14371500	-1.30257300
H	-4.40154700	-3.39791300	-0.02105500

CBS-QB3 enthalpy: -993.81194
CBS-QB3 free energy: -993.87946

4$_{endo}$

C	-1.50256000	-2.24866000	1.49087700
C	-1.86433900	-1.51283900	0.22389900
H	-2.71097100	-1.99667000	-0.27402400
H	-1.19935300	-3.29008700	1.48315400
C	-1.42105900	1.03320000	0.01118300
H	-1.59727500	1.98032200	0.52113100
C	-1.73798400	0.17716500	-2.42598900
H	-2.09379400	0.42522100	-3.42063800
C	0.04787000	0.67019200	0.07463000
C	-1.20309400	-1.02386400	-2.16763000
H	-1.14484400	-1.74721400	-2.97678100
C	-0.68943900	-1.48010400	-0.81941300
H	-0.29390300	-2.48825000	-0.92362700
C	0.41172400	-0.56349500	-0.30475500
C	-1.90417300	1.26016600	-1.43382000
O	-2.44220900	2.30742400	-1.73624100
C	-1.59264800	-1.48343300	2.57480100
H	-1.36980300	-1.80902300	3.58471000
C	-2.25532900	-0.08266700	0.71434000
H	-3.30758500	0.10955000	0.49688100
C	-2.03019400	-0.07840300	2.25953900
H	-2.94883700	0.19071600	2.79213200
H	-1.26867300	0.64875100	2.56208800
C	0.96244600	1.70058200	0.66708400
C	1.81843200	-1.02671800	-0.17908600
O	0.89229800	2.04307200	1.82245500

O	2.70085700	-0.42979400	0.39211000
O	1.76916900	2.24713400	-0.24755100
O	2.00997100	-2.22341800	-0.77918800
C	3.34551500	-2.75196100	-0.69284000
H	3.63514000	-2.88635300	0.35025400
H	3.31407100	-3.70789300	-1.21065700
H	4.05373900	-2.07604900	-1.17405900
C	2.71951800	3.20748400	0.25487900
H	3.42245500	2.71069600	0.92475300
H	3.23225000	3.59207100	-0.62340200
H	2.20856900	4.00900600	0.78920700

CBS-QB3 enthalpy: -993.82327
CBS-QB3 free energy: -993.89204

4*exo*

C	-1.70198600	1.15531900	-0.91137700
C	-3.11068300	1.64428700	-0.68639000
H	-3.33940100	2.68894700	-0.50510800
H	-1.27498900	1.62511300	-1.80442500
C	-0.94251400	-1.22445500	-0.20964600
H	-0.92100800	-2.25279700	-0.57051300
C	-1.58424800	-0.08247100	2.03683100
H	-1.97880600	-0.23366700	3.03616100
C	0.45264700	-0.63216200	-0.24059300
C	-1.25128800	1.14198700	1.60860200
H	-1.40461100	1.97959400	2.28346300
C	-0.68718300	1.47536100	0.24569500
H	-0.46069500	2.53903500	0.21878400
C	0.58762500	0.68614600	-0.03181800
C	-1.47802800	-1.31534900	1.23254900
O	-1.83941400	-2.38762200	1.67873300
C	-1.86764500	-0.37837700	-1.14290600
H	-1.53325500	-0.61576000	-2.15368800
C	-4.00950100	0.66496000	-0.74301900
H	-5.07764500	0.79639500	-0.61091300
C	-3.39099100	-0.68224800	-1.01750900
H	-3.78164500	-1.12057100	-1.94218400
H	-3.61864500	-1.40266800	-0.22438800
C	1.56417900	-1.57421600	-0.59643300
C	1.91552600	1.34819900	-0.11098400
O	2.33077400	-1.87074800	0.45874500
O	1.86129400	2.63656600	0.29734300
C	3.45214200	-2.73508900	0.18851300
H	3.90950800	-2.92525800	1.15644400
H	3.11727800	-3.66465500	-0.27281300
H	4.15332900	-2.22879200	-0.47613000
C	3.10718700	3.35486600	0.24570000
H	3.84564700	2.88195200	0.89455000
H	3.49262500	3.37644300	-0.77458000
H	2.87801600	4.35979800	0.59280500
O	1.67123000	-2.06259500	-1.69355200
O	2.93397400	0.82394300	-0.49761500

CBS-QB3 enthalpy: -993.81979
CBS-QB3 free energy: -993.889057

5

C	-3.43516100	0.11846500	-0.43937000
C	-4.26047000	0.15809100	0.81583800
H	-5.29804800	-0.14927300	0.84104200
H	-3.93435200	0.51602400	-1.32556500
C	-1.23178300	-2.69248700	-0.59041800
H	-1.96464600	-3.49199500	-0.58381400
C	-1.05378700	-0.09209800	-0.76877700
H	-1.07542200	0.20339100	-1.83148900
C	0.15601200	-3.06677200	-0.53922000
C	0.38010400	0.07943100	-0.30094600
C	1.35080300	-0.85832500	-0.16837200
C	1.25463900	-2.30231600	-0.35495600
C	-1.72929600	-1.44538800	-0.67505200
O	-3.07091200	-1.26667900	-0.75973600
C	-2.10919300	0.81400600	-0.06872500
H	-2.07770100	1.82648100	-0.47225500
C	-3.52767900	0.54832200	1.85693800
H	-3.88875100	0.61846600	2.87711700
C	-2.10072900	0.85873900	1.48502600
H	-1.41864700	0.11712400	1.91585800
H	-1.76140600	1.82614700	1.85869800
H	2.20284600	-2.81879900	-0.31772300
H	0.33683500	-4.13373000	-0.63434900
C	0.69409300	1.54555400	-0.08732500
C	2.72964000	-0.34160000	0.16778600
O	3.10916300	0.79370700	-0.00341200
O	0.69033600	2.10994400	0.97695400
O	0.82637800	2.16761000	-1.27443500
O	3.52569100	-1.29620000	0.68696800
C	4.85885800	-0.87547100	1.02724300
H	5.38204400	-0.51174600	0.14168800
H	4.82708900	-0.08071100	1.77359500
H	5.34782200	-1.76061800	1.42753200
C	1.17309700	3.56367900	-1.20565300
H	0.42128500	4.12177000	-0.64570700
H	2.14377000	3.67621400	-0.72139500
H	1.21713100	3.90321100	-2.23803500

CBS-QB3 enthalpy: -993.79459
CBS-QB3 free energy: -993.86378

6

C	3.76368800	-0.81365900	0.63369600
C	4.96728300	-0.84354600	-0.26039800
H	5.56205300	-1.73427400	-0.41541700
H	3.90559300	-1.30114300	1.60194700
C	0.29532700	-1.29442600	-0.11438200
H	0.28262500	-2.35127700	-0.35660300
C	1.80146200	0.62262100	0.69890200
H	1.42914600	0.65746900	1.73185800
C	-0.97099400	-0.63763900	0.02317900
C	1.09833300	1.67866700	-0.11876800
H	1.70573000	2.48996000	-0.50382100

C	-0.22085300	1.71615600	-0.36046700
H	-0.60472500	2.59304000	-0.86836600
C	-1.22452100	0.71347300	-0.03577800
C	1.51190400	-0.75519900	0.14370000
O	2.63047100	-1.48608000	-0.00897800
C	3.35153700	0.67266900	0.72098900
H	3.70462100	1.10620900	1.65736600
C	5.15116400	0.33728800	-0.84711300
H	5.93673500	0.56031500	-1.56037600
C	4.10064700	1.34874700	-0.46249900
H	3.44726300	1.54175000	-1.32013600
H	4.52960000	2.31361800	-0.17624400
C	-2.09423200	-1.63516700	0.23046700
C	-2.63258300	1.16614500	0.11365300
O	-3.57189000	0.46497600	0.42104900
O	-2.29601400	-2.20026500	1.27299800
O	-2.77595000	2.49390400	-0.12071700
O	-2.72432700	-1.90658200	-0.92499500
C	-4.11231100	3.00285600	0.01121400
H	-4.77793600	2.52716900	-0.71109800
H	-4.49428100	2.82073500	1.01681600
H	-4.03713300	4.07066600	-0.18366400
C	-3.84215700	-2.80615900	-0.81442400
H	-4.20234200	-2.94861800	-1.83096500
H	-3.53214400	-3.75604400	-0.37657000
H	-4.61528600	-2.35416200	-0.19141300
CBS-QB3 enthalpy:		-993.79994	
CBS-QB3 free energy:		-993.86929	

7*endo*

C	-1.55697000	-2.28338100	1.44942700
C	-1.91138700	-1.46141800	0.17321100
H	-2.77045600	-1.91259600	-0.32575200
H	-0.53126900	-2.66987400	1.42091200
C	-1.37409100	1.09087600	0.05550000
H	-1.52277500	2.01458100	0.61505300
C	-1.69706600	0.35182600	-2.41229300
H	-2.03389700	0.65010600	-3.39975000
C	0.07475900	0.66376500	0.12358900
C	-1.23285700	-0.88561700	-2.19100500
H	-1.21569100	-1.58376600	-3.02397000
C	-0.74186100	-1.41941900	-0.86139600
H	-0.38171000	-2.43456100	-1.01368800
C	0.39257500	-0.56707800	-0.30429300
C	-1.80779300	1.41106900	-1.38682800
O	-2.26813200	2.50207700	-1.65923600
C	-1.74812600	-1.31129200	2.58276400
H	-1.56931400	-1.57943500	3.61771500
C	-2.28838300	-0.02857100	0.66637300
H	-3.31937200	0.22380400	0.39535900
C	-2.14095800	-0.11152100	2.16675000
H	-2.32166000	0.74433600	2.80641300
C	1.02802400	1.64414300	0.74238700
C	1.78362300	-1.07917300	-0.20582600
O	1.91683300	-2.29415000	-0.78766200
O	1.80864200	2.22451800	-0.17712700
O	1.00510800	1.92791400	1.91325700
O	2.70206300	-0.50656000	0.33251400
C	3.23619400	-2.86580400	-0.73043900
H	3.15682000	-3.83052400	-1.22639300
H	3.95106900	-2.22424000	-1.24751000
H	3.55403700	-2.98847300	0.30583100
C	2.78646100	3.15119700	0.33450600
H	3.26982500	3.57432100	-0.54278000
H	2.30427800	3.92987200	0.92638400
H	3.50943000	2.61730500	0.95266400
H	-2.20829900	-3.15887100	1.55098400
CBS-QB3 enthalpy:		-993.82177	
CBS-QB3 free energy:		-993.89147	

8*exo*

C	1.08119200	-0.86300400	-1.92903300
C	0.90488300	-1.29780100	-0.49492800
H	0.57623400	-2.34241100	-0.45481900
H	0.23967800	-0.75467300	-2.60073300
C	0.96029300	1.73198600	0.17032200
H	0.93016200	2.78612700	-0.08230900
C	2.38981600	-0.14696300	1.27071700
H	3.37484400	-0.18246800	1.73817600
C	-0.15362600	0.99484300	0.03021300
C	1.30068100	-0.50036500	2.25953000
H	1.55442100	-0.59455900	3.30933600
C	0.06186400	-0.69963900	1.82089500
H	-0.76096500	-0.96523300	2.47006700
C	-0.21331100	-0.50021500	0.33570900
C	2.25965400	1.27438100	0.71253000
O	3.21443600	2.02968500	0.71460500
C	2.35779800	-0.64994600	-2.23804300
H	2.71204600	-0.34361500	-3.21565200
C	2.33583400	-1.19077700	0.11316900
H	2.59807900	-2.14400900	0.57413500
C	3.28992300	-0.89240400	-1.07944300
H	3.94757200	-1.74740200	-1.27432100
H	3.94752800	-0.03782400	-0.88905900
C	-1.38649400	1.75906600	-0.36710900
C	-1.52212600	-1.12036000	-0.15985600
O	-1.42593400	2.63573600	-1.19014400
O	-1.99762000	-0.90813200	-1.24875800
O	-2.43634400	1.39540100	0.40051400
O	-2.02575900	-2.01539300	0.70549800
C	-3.68407000	2.04513100	0.09268000
H	-3.57678600	3.12795400	0.16139100
H	-4.00485000	1.77646500	-0.91484300
H	-4.39258500	1.68009100	0.83276400
C	-3.20152800	-2.72115300	0.26204000
H	-4.02190100	-2.02199000	0.09657300
H	-2.99595100	-3.25709600	-0.66515800
H	-3.44245100	-3.41441900	1.06435700

CBS-QB3 enthalpy: -993.81754
CBS-QB3 free energy: -993.88495

11*endo*

C	2.36928800	-1.02387500	-1.60846400
C	1.25789100	-0.53279500	-2.16691300
H	1.19191300	0.26796900	-2.89143500
H	3.38788900	-0.70843800	-1.79055600
C	0.78820900	1.92348000	0.09493300
H	0.47240000	2.93332100	-0.14569900
C	2.73751400	0.79247900	1.38208800
H	3.61049200	1.08185600	1.95862900
C	-0.12086600	0.95968200	-0.11672400
C	2.33035200	-0.47901900	1.41966000
H	2.90950300	-1.14278300	2.06021300
C	1.29117700	-1.22209500	0.65019500
H	0.91749100	-1.99106000	1.33315500
C	0.00518000	-0.55336100	-0.01740800
C	2.17698700	1.91460100	0.61335700
O	2.84272500	2.93071100	0.46572100
C	1.93900200	-2.03061300	-0.55913500
H	2.69364300	-2.74166000	-0.22407200
C	0.06929700	-1.19466400	-1.48608200
H	-0.88574400	-1.14606300	-1.99876000
C	0.66147700	-2.59148400	-1.20750600
H	0.87115200	-3.12756100	-2.13444000
H	0.04859400	-3.20323800	-0.54840500
C	-1.43952100	1.51325400	-0.62738400
C	-1.19282700	-1.11055000	0.77744000
O	-1.77177500	-2.14455600	0.56352600
O	-1.69243800	2.68360900	-0.77065800
O	-2.32906900	0.53977400	-0.91587800
O	-1.46459200	-0.31632200	1.83277600
C	-3.61926800	0.97974500	-1.37854600
H	-4.09249200	1.61731000	-0.63090700
H	-3.51656800	1.53867300	-2.30945200
H	-4.19511000	0.07054000	-1.53417500
C	-2.53730600	-0.75277000	2.68780100
H	-3.47051500	-0.81149300	2.12585300
H	-2.31420800	-1.73324500	3.11091600
H	-2.60677300	-0.00194100	3.47135800

CBS-QB3 enthalpy: -993.79835
CBS-QB3 free energy: -993.86554

12*endo*

C	-2.18077600	-1.24578600	1.65644400
H	-2.83281000	-2.10517300	1.57113800
H	-0.32530500	-2.07583700	2.41438100
C	-1.72824600	0.46668900	-0.14703600
H	-1.93230400	1.51523500	-0.36942000
C	-2.03489600	-1.63512600	-1.71209800
H	-2.82519000	-2.11117100	-2.28363800
C	-0.21037400	0.35931900	0.30755100
C	-0.87081100	-2.28517800	-1.54276400
H	-0.81265300	-3.28056700	-1.97539100
C	0.37383500	-1.84181900	-0.94729100
H	1.20014000	-2.51706800	-1.13257300
C	0.68837400	-0.74500400	-0.22736500
C	-2.36367400	-0.25263600	-1.32390200
O	-3.26881700	0.31447700	-1.91510100
C	-0.38375200	0.18385200	1.89283200
H	0.51703900	0.45821100	2.43287500
C	-2.52228300	0.15955500	1.19481900
H	-3.57904200	0.40521000	1.10212100
C	-1.66797700	0.99028400	2.17207200
H	-1.99618500	0.87185700	3.20628400
H	-1.58662100	2.04538700	1.91831000
C	0.41165400	1.73071200	-0.02068700
C	2.11940400	-0.59365900	0.20638700
O	0.36802400	2.70980100	0.67715400
O	2.52358700	0.32864100	0.87982200
O	0.93306600	1.72814100	-1.26490500
O	2.93166400	-1.58353600	-0.21775900
C	4.31028000	-1.46803200	0.17663900
H	4.39794300	-1.46231600	1.26395700
H	4.80521600	-2.34008300	-0.24461900
H	4.74476500	-0.54940900	-0.21988500
C	1.52488000	2.96876900	-1.69349000
H	2.35794700	3.23212000	-1.04030900
H	1.87210900	2.78901600	-2.70849000
H	0.78608900	3.77094600	-1.67521500

CBS-QB3 enthalpy: -993.80229
CBS-QB3 free energy: -993.86973

12*exo*

C	-2.62438900	-1.56703600	-1.43469500
C	-1.39218400	-1.95227400	-1.78005100
H	-1.04585000	-2.95518300	-1.97695400
H	-3.49247900	-2.19474600	-1.27986500
C	-1.73704900	-0.03342400	0.28438100
H	-2.07141100	-0.87233300	0.89254000
C	-1.73329500	2.54577900	0.80478100
H	-2.44947300	3.29991000	1.11461400
C	-0.24764100	-0.32267100	-0.18452000
C	-0.53396300	2.93010500	0.33793100
H	-0.36123400	4.00046200	0.26419600
C	0.62791500	2.12624100	0.00875200
H	1.53221900	2.71070200	-0.10735400
C	0.78750200	0.79600800	-0.15895300
C	-2.16191800	1.16651300	1.11302300
O	-2.98251200	1.00169500	1.99996600
C	-2.55382700	-0.09121000	-1.09297900
H	-3.49940400	0.44780200	-1.05385200
C	-0.49104500	-0.73066500	-1.71678200
H	0.43908500	-0.80200600	-2.27318800
C	-1.49639400	0.37427500	-2.11040300
H	-1.84175700	0.26700500	-3.13961800

H	-1.13480300	1.39043700	-1.94985800
C	0.25198000	-1.49526300	0.67844300
C	2.17915100	0.30972800	-0.45961100
O	0.11999100	-2.66550000	0.44061200
O	2.45017600	-0.84504500	-0.70311000
O	0.78136500	-1.02603900	1.82945000
O	3.11725800	1.27867800	-0.43604500
C	4.46032500	0.84980200	-0.72225900
H	4.51790200	0.41258400	-1.72003400
H	5.06970200	1.74851900	-0.66034200
H	4.78844300	0.11050500	0.00952500
C	1.25459300	-2.02749800	2.74875800
H	2.05017100	-2.61461700	2.28778800
H	1.62925300	-1.47754000	3.60917700
H	0.44085100	-2.69227100	3.04134400

CBS-QB3 enthalpy: -993.79836
CBS-QB3 free energy: -993.86573

TS-1

C	3.98580	-0.40070	0.89263
C	3.05902	-1.46214	0.80343
H	3.30858	-2.48143	0.54425
H	5.04008	-0.48256	0.66688
C	1.01329	-0.82875	-0.71294
H	1.05234	-1.88437	-0.95845
C	2.19940	1.28256	-1.62718
H	3.13527	1.60156	-2.07334
C	-0.35853	-0.36806	-0.64289
C	1.23771	2.24339	-1.38085
H	1.54441	3.26597	-1.58497
C	-0.07410	2.11512	-0.91515
H	-0.63049	3.03968	-0.81627
C	-0.80450	0.95630	-0.61162
C	2.10908	-0.14805	-1.49110
O	3.00668	-0.88038	-1.91268
C	3.32856	0.74902	1.24876
H	3.77795	1.72496	1.37262
C	1.73202	-0.97303	0.99585
H	0.97827	-1.63181	1.41346
C	1.89965	0.43935	1.55929
H	1.76287	0.40344	2.65026
H	1.18739	1.17861	1.18907
C	-1.32011	-1.49827	-0.49893
C	-2.20796	1.28088	-0.15070
O	-1.04906	-2.56016	0.02070
O	-2.93519	2.08979	-0.66752
O	-2.51397	-1.25018	-1.07788
O	-2.50798	0.63654	0.99916
C	-3.49461	-2.29392	-0.95454
H	-4.37091	-1.93270	-1.48806
H	-3.12518	-3.21775	-1.40134
H	-3.72858	-2.47665	0.09586
C	-3.82045	0.89855	1.52566
H	-3.94382	1.96240	1.73321
H	-4.58529	0.58576	0.81288
H	-3.88764	0.31702	2.44242

Imag. Freq. -274.47
CBS-QB3 enthalpy: -993.76074
CBS-QB3 free energy: -993.83028

TS-2

C	-3.29481	-1.37701	1.03673
C	-3.96880	-0.22167	0.60053
H	-4.96624	-0.20897	0.18297
H	-3.68520	-2.38277	0.96612
C	-2.36961	1.04539	-1.14190
H	-3.30728	1.29052	-1.63143
C	-0.78555	-0.96723	-0.97248
H	-0.80617	-2.04733	-1.05803
C	-1.39781	2.09626	-1.21962
C	0.44115	-0.39263	-0.63831
C	0.78605	0.96991	-0.60924
C	-0.04826	2.05539	-0.97048
C	-2.02552	-0.37598	-1.43420
O	-2.89675	-1.08334	-1.94051
C	-2.03501	-1.03349	1.48163
H	-1.27836	-1.70884	1.85555
C	-3.09437	0.90006	0.65907
H	-3.49357	1.90334	0.75589
C	-1.92820	0.45817	1.53806
H	-2.13145	0.78779	2.56829
H	-0.95032	0.85876	1.27468
C	1.47426	-1.45025	-0.32037
C	2.14375	1.41594	-0.15790
O	1.32575	-2.31591	0.50618
O	2.71770	2.39928	-0.56146
O	2.53426	-1.37347	-1.14557
O	2.63407	0.63654	0.83327
C	3.55837	-2.36163	-0.93154
H	3.97220	-2.26779	0.07382
H	3.15159	-3.36595	-1.05646
H	4.31855	-2.15823	-1.68212
C	3.94261	0.99048	1.31292
H	4.67761	0.91047	0.51025
H	3.94427	2.01211	1.69481
H	4.16118	0.28186	2.10869
H	-1.79790	3.07808	-1.45764
H	0.47786	3.00213	-1.03018

Imag. Freq. -368.17
CBS-QB3 enthalpy: -993.7606
CBS-QB3 free energy: -993.82989

TS-3

C	-2.11234	-0.75162	1.60370
C	-1.69643	0.64925	-0.70828
H	-1.95910	1.69184	-0.86017
C	-2.43474	-1.58362	-1.78185

H	-3.23550	-2.05295	-2.34341
C	-0.27369	0.47317	-0.67160
C	-1.42650	-2.36190	-1.30530
H	-1.53068	-3.42847	-1.49202
C	-0.21161	-2.01628	-0.63939
H	0.39821	-2.86297	-0.34833
C	0.37338	-0.77221	-0.48535
C	-2.64757	-0.16481	-1.55741
O	-3.62866	0.40909	-2.01801
C	-2.46078	0.49884	1.03202
C	0.50337	1.73297	-0.79632
C	1.77217	-0.78437	0.09049
O	1.72720	1.52909	-1.32815
O	2.53988	-1.72770	-0.49028
C	2.57866	2.68431	-1.39929
H	2.08810	3.48763	-1.94955
H	2.82534	3.03328	-0.39487
H	3.47551	2.35293	-1.91823
C	3.86986	-1.85897	0.04256
H	4.42024	-0.92479	-0.07679
H	3.83578	-2.11766	1.10212
H	4.33575	-2.65503	-0.53374
O	0.08621	2.84110	-0.52301
O	2.15604	-0.08983	1.00006
C	-1.69436	1.54822	1.83737
H	-1.28524	2.37907	1.26074
H	-2.38764	1.97552	2.57782
C	-0.66534	0.72932	2.53757
H	0.19533	1.13839	3.04734
C	-0.99137	-0.59669	2.45426
H	-0.45023	-1.40869	2.92054
H	-3.48437	0.69379	0.72687
H	-2.60489	-1.68924	1.38788

Imag. Freq. -305.84
CBS-QB3 enthalpy: -993.75974
CBS-QB3 free energy: -993.829704

TS-4

C	-0.93876	-0.52822	2.32600
C	-2.15776	-0.71636	1.72241
H	-2.70423	-1.64876	1.67826
H	-0.33794	-1.29412	2.79599
C	-1.81186	0.55994	-0.50358
H	-2.03877	1.57487	-0.82211
C	-2.40260	-1.73107	-1.61787
H	-3.19535	-2.23728	-2.15849
C	-0.33269	0.44762	-0.38701
C	-1.34825	-2.45518	-1.17302
H	-1.40325	-3.52537	-1.35910
C	-0.11000	-2.04786	-0.56798
H	0.57023	-2.86760	-0.36918
C	0.38971	-0.79281	-0.33386
C	-2.63513	-0.30087	-1.46274
O	-3.56098	0.24155	-2.05022
C	-0.52293	0.79872	2.09204
H	0.44059	1.19943	2.36861
C	-2.53097	0.50710	0.99194
H	-3.59446	0.68286	0.83782
C	-1.72657	1.59843	1.73188
H	-2.26627	1.87450	2.64827
H	-1.52456	2.49630	1.15238
C	0.38695	1.70247	-0.72921
C	1.80790	-0.77135	0.19588
O	-0.09092	2.81849	-0.67259
O	2.17920	-0.16958	1.17600
O	1.64910	1.48453	-1.16574
O	2.61635	-1.57900	-0.51604
C	3.97050	-1.67664	-0.03991
H	3.99361	-2.07460	0.97594
H	4.47172	-2.35210	-0.72941
H	4.44696	-0.69544	-0.04702
C	2.42728	2.65961	-1.44364
H	2.58782	3.23615	-0.53087
H	3.37443	2.29473	-1.83526
H	1.92192	3.28692	-2.17855

Imag. Freq. -116.86
CBS-QB3 enthalpy: -993.76146
CBS-QB3 free energy: -993.82928

TS-5

C	-2.09300	-0.66104	1.52146
C	-1.02470	-0.45208	2.43275
H	-0.92409	0.41210	3.07467
H	-2.98609	-0.05602	1.46213
C	-1.15756	1.67298	-0.14245
H	-1.03526	2.63539	0.34450
C	-2.86369	0.45346	-1.60766
H	-3.74832	0.66391	-2.19982
C	-0.01137	0.92014	-0.31414
C	-2.26939	-0.74230	-1.70610
H	-2.70208	-1.46716	-2.39162
C	-1.09922	-1.24287	-0.95619
H	-0.80700	-2.22749	-1.30745
C	0.06563	-0.42377	-0.74383
C	-2.51980	1.53097	-0.66048
O	-3.37626	2.36218	-0.36031
C	-1.81784	-1.80422	0.72196
H	-2.64689	-2.38565	0.33152
C	-0.12715	-1.47427	2.32380
H	0.81629	-1.54687	2.84695
C	-0.65412	-2.52427	1.40365
H	-1.06439	-3.35788	1.99289
H	0.09640	-2.94217	0.73051
C	1.22942	1.65355	0.15831
C	1.34956	-1.10988	-1.01418
O	1.49935	-2.31770	-1.03537
O	1.57381	2.73092	-0.25042
O	1.85130	1.00582	1.16802

O	2.34982	-0.25462	-1.31275
C	3.03297	1.65513	1.66937
H	3.77849	1.75000	0.87829
H	2.79327	2.64878	2.05040
H	3.40101	1.01526	2.46861
C	3.62835	-0.85124	-1.58497
H	4.00579	-1.36833	-0.70084
H	3.54887	-1.56392	-2.40655
H	4.28136	-0.02447	-1.85527

Imag. Freq. -338.46
CBS-QB3 enthalpy: -993.756353
CBS-QB3 free energy: -993.825482

TS-6

C	1.73580	-0.76306	-1.63888
C	2.96850	-1.43932	-1.43648
H	3.11022	-2.50705	-1.53896
H	0.83264	-1.21423	-2.02286
C	1.05587	0.99252	0.40537
H	1.18239	2.06902	0.34492
C	2.02417	-0.91153	1.84112
H	2.83945	-1.16798	2.50889
C	-0.32780	0.62004	0.33489
C	1.16882	-1.89679	1.43779
H	1.42637	-2.90274	1.76068
C	-0.03140	-1.82419	0.68877
H	-0.50750	-2.78018	0.50351
C	-0.78336	-0.70255	0.33280
C	2.00868	0.48460	1.45859
O	2.80341	1.29014	1.94235
C	1.86986	0.60663	-1.29158
H	1.27826	1.34835	-1.81730
C	3.92634	-0.54114	-1.06278
H	4.94547	-0.77465	-0.78503
C	3.37079	0.84289	-1.10730
H	3.74318	1.36532	-1.99985
H	3.64568	1.45590	-0.24500
C	-1.23664	1.75083	0.00035
C	-2.11187	-1.01308	-0.31474
O	-2.47951	1.57748	0.49354
O	-2.83545	-1.88612	0.40929
C	-3.44708	2.56717	0.10332
H	-4.35261	2.32191	0.65392
H	-3.09617	3.56673	0.36093
H	-3.62528	2.51185	-0.97207
C	-4.08442	-2.29498	-0.17908
H	-4.73841	-1.43290	-0.31625
H	-3.91494	-2.77029	-1.14641
H	-4.52022	-2.99874	0.52621
O	-0.89383	2.74133	-0.60813
O	-2.45537	-0.59264	-1.39308

Imag. Freq. -324.00
CBS-QB3 enthalpy: -993.754905
CBS-QB3 free energy: -993.825283

TS-7

C	-1.47469	0.26733	2.13849
C	-1.48899	-1.02053	1.53690
H	-0.72825	-1.77411	1.67589
H	-0.63480	0.68896	2.67280
C	-0.92539	1.19483	-0.97318
H	-1.01360	2.27471	-1.00725
C	-2.29737	-0.95779	-1.17189
H	-3.28972	-1.24638	-1.50865
C	0.26203	0.66817	-0.53607
C	-1.26276	-1.85912	-1.56468
H	-1.57716	-2.78010	-2.04589
C	0.06087	-1.75864	-1.21328
H	0.68639	-2.62380	-1.39726
C	0.68372	-0.70023	-0.51946
C	-2.15218	0.52343	-1.35275
O	-3.12103	1.15424	-1.77584
C	-2.64895	0.90551	1.86486
H	-2.89423	1.92443	2.13203
C	-2.66421	-1.18388	0.76250
H	-3.09148	-2.17282	0.64327
C	-3.57367	-0.01090	1.13245
H	-4.34999	-0.38339	1.81577
H	-4.08991	0.46692	0.29599
C	1.23318	1.73528	-0.06810
C	1.94483	-1.00956	0.21416
O	0.98196	2.55166	0.78123
O	2.38227	-0.34758	1.13084
O	2.36611	1.71904	-0.79243
O	2.53988	-2.14988	-0.20190
C	3.37997	2.64857	-0.36913
H	2.99695	3.66951	-0.38693
H	3.70752	2.40106	0.64181
H	4.19641	2.53068	-1.07814
C	3.72803	-2.52703	0.51380
H	4.50035	-1.76497	0.40002
H	3.51231	-2.65731	1.57536
H	4.04917	-3.46592	0.06815

Imag. Freq. -368.07
CBS-QB3 enthalpy: -993.754734
CBS-QB3 free energy: -993.824383

TS-8

C	-3.96312	0.07414	0.14429
C	-3.64360	1.09154	1.07058
H	-4.15791	2.04007	1.13597
H	-4.86427	0.03502	-0.44880
C	-0.68356	1.12066	-0.95729
H	-0.79599	2.19804	-1.01680
C	-2.10770	-1.04070	-1.11570
H	-2.84422	-1.31149	-1.87721
C	0.56813	0.64382	-0.51553
C	-0.98785	-2.00247	-1.18104

H	-1.27045	-2.99656	-1.51873
C	0.31865	-1.83643	-0.87524
H	0.93678	-2.72048	-0.96578
C	1.03804	-0.66341	-0.44337
C	-1.85958	0.44147	-1.30502
O	-2.92107	1.06383	-1.57953
C	-2.99012	-1.04319	0.25515
H	-3.46816	-2.02219	0.31094
C	-2.53268	0.73410	1.77916
H	-2.01784	1.35889	2.49810
C	-2.14116	-0.68129	1.49597
H	-2.41378	-1.31769	2.34897
H	-1.06608	-0.80500	1.35278
C	1.41404	1.78783	0.01412
C	2.42288	-0.86152	0.06299
O	2.21490	2.29287	-0.93524
O	2.81619	-2.15923	0.03538
O	1.26383	2.25882	1.11297
O	3.15457	0.01395	0.47454
C	3.08777	3.35140	-0.50120
H	3.63582	3.65823	-1.38929
H	2.51241	4.18434	-0.09464
H	3.76999	2.97336	0.26150
C	4.14926	-2.40965	0.50670
H	4.87978	-1.87985	-0.10690
H	4.25722	-2.08564	1.54295
H	4.28888	-3.48556	0.42424

Imag. Freq. -89.53
CBS-QB3 enthalpy: -993.75619
CBS-QB3 free energy: -993.82494

TS-9

C	-2.11234	-0.75162	1.60370
C	-1.69643	0.64925	-0.70828
H	-1.95910	1.69184	-0.86017
C	-2.43474	-1.58362	-1.78185
H	-3.23550	-2.05295	-2.34341
C	-0.27369	0.47317	-0.67160
C	-1.42650	-2.36190	-1.30530
H	-1.53068	-3.42847	-1.49202
C	-0.21161	-2.01628	-0.63939
H	0.39821	-2.86297	-0.34833
C	0.37338	-0.77221	-0.48535
C	-2.64757	-0.16481	-1.55741
O	-3.62866	0.40909	-2.01801
C	-2.46078	0.49884	1.03202
C	0.50337	1.73297	-0.79632
C	1.77217	-0.78437	0.09049
O	1.72720	1.52909	-1.32815
O	2.53988	-1.72770	-0.49028
C	2.57866	2.68431	-1.39929
H	2.08810	3.48763	-1.94955
H	2.82534	3.03328	-0.39487
H	3.47551	2.35293	-1.91823
C	3.86986	-1.85897	0.04256
H	4.42024	-0.92479	-0.07679
H	3.83578	-2.11766	1.10212
H	4.33575	-2.65503	-0.53374
O	0.08621	2.84110	-0.52301
O	2.15604	-0.08983	1.00006
C	-1.69436	1.54822	1.83737
H	-1.28524	2.37907	1.26074
H	-2.38764	1.97552	2.57782
C	-0.66534	0.72932	2.53757
H	0.19533	1.13839	3.04734
C	-0.99137	-0.59669	2.45426
H	-0.45023	-1.40869	2.92054
H	-3.48437	0.69379	0.72687
H	-2.60489	-1.68924	1.38788

Imag. Freq. -163.25
CBS-QB3 enthalpy: -993.75560
CBS-QB3 free energy: -993.82453

TS-10

C	-1.47469	0.26733	2.13849
C	-1.48899	-1.02053	1.53690
H	-0.72825	-1.77411	1.67589
H	-0.63480	0.68896	2.67280
C	-0.92539	1.19483	-0.97318
H	-1.01360	2.27471	-1.00725
C	-2.29737	-0.95779	-1.17189
H	-3.28972	-1.24638	-1.50865
C	0.26203	0.66817	-0.53607
C	-1.26276	-1.85912	-1.56468
H	-1.57716	-2.78010	-2.04589
C	0.06087	-1.75864	-1.21328
H	0.68639	-2.62380	-1.39726
C	0.68372	-0.70023	-0.51946
C	-2.15218	0.52343	-1.35275
O	-3.12103	1.15424	-1.77584
C	-2.64895	0.90551	1.86486
H	-2.89423	1.92443	2.13203
C	-2.66421	-1.18388	0.76250
H	-3.09148	-2.17282	0.64327
C	-3.57367	-0.01090	1.13245
H	-4.34999	-0.38339	1.81577
H	-4.08991	0.46692	0.29599
C	1.23318	1.73528	-0.06810
C	1.94483	-1.00956	0.21416
O	0.98196	2.55166	0.78123
O	2.38227	-0.34758	1.13084
O	2.36611	1.71904	-0.79243
O	2.53988	-2.14988	-0.20190
C	3.37997	2.64857	-0.36913
H	2.99695	3.66951	-0.38693
H	3.70752	2.40106	0.64181
H	4.19641	2.53068	-1.07814
C	3.72803	-2.52703	0.51380
H	4.50035	-1.76497	0.40002

H	3.51231	-2.65731	1.57536
H	4.04917	-3.46592	0.06815

Imag. Freq. -156.38
CBS-QB3 enthalpy: -993.76578
CBS-QB3 free energy: -993.83335

TS-11

C	-2.11831	-0.63209	1.65694
C	-0.95969	-0.27512	2.31322
H	-0.81082	0.63664	2.87417
H	-3.04976	-0.08284	1.67295
C	-1.07068	1.74479	-0.26093
H	-0.88358	2.76726	0.05037
C	-2.87969	0.42907	-1.52245
H	-3.74912	0.63113	-2.14002
C	0.00795	0.90077	-0.28150
C	-2.34877	-0.79567	-1.51043
H	-2.80818	-1.54644	-2.14934
C	-1.23334	-1.32329	-0.66097
H	-0.92402	-2.27463	-1.08880
C	0.00958	-0.51774	-0.48143
C	-2.45908	1.59203	-0.71450
O	-3.26103	2.49992	-0.50962
C	-1.84764	-1.80571	0.81202
H	-2.69668	-2.45613	0.60529
C	0.03921	-1.20746	1.99972
H	1.07411	-1.13222	2.29878
C	-0.61266	-2.44231	1.47888
H	-0.94029	-3.06631	2.32180
H	0.00869	-3.04223	0.81683
C	1.28930	1.62393	0.09301
C	1.23805	-1.22789	-0.91545
O	1.34211	-2.43691	-1.01418
O	1.66565	2.64367	-0.42153
O	1.91351	1.05772	1.15296
O	2.24924	-0.39605	-1.24878
C	3.12631	1.71386	1.56296
H	3.85838	1.69712	0.75409
H	2.92847	2.75013	1.84000
H	3.48951	1.14978	2.41968
C	3.47042	-1.02390	-1.67138
H	3.90343	-1.60898	-0.85789
H	3.28609	-1.68095	-2.52194
H	4.13213	-0.20775	-1.95282

Imag. Freq. -133.25
CBS-QB3 enthalpy: -993.757957
CBS-QB3 free energy: -993.825683

TS-12

C	1.74012	-0.46164	-1.80929
C	2.77603	-1.30205	-1.50189
H	2.83140	-2.34813	-1.77218
H	0.87890	-0.71463	-2.41252
C	1.12323	1.04867	0.26159
H	1.13745	2.12447	0.42259
C	2.26670	-0.94776	1.42209
H	3.07364	-1.21505	2.09549
C	-0.29872	0.60664	0.18119
C	1.37526	-1.95425	1.02633
H	1.71983	-2.97229	1.19093
C	0.14289	-1.85267	0.41386
H	-0.33643	-2.80179	0.19665
C	-0.68380	-0.70445	0.15638
C	1.95500	0.47756	1.41198
O	2.45105	1.24609	2.22466
C	1.92652	0.85920	-1.14561
H	1.60935	1.69908	-1.76378
C	3.66597	-0.64002	-0.63152
H	4.56769	-1.06893	-0.21638
C	3.43560	0.83198	-0.78824
H	4.00789	1.18247	-1.65727
H	3.71873	1.44630	0.06580
C	-1.25665	1.72074	-0.04653
C	-2.06895	-1.08358	-0.32047
O	-2.51457	1.42790	0.34481
O	-2.76165	-1.73016	0.63175
C	-3.50885	2.42091	0.04000
H	-4.42954	2.05951	0.49268
H	-3.22415	3.38569	0.46047
H	-3.62600	2.51864	-1.04067
C	-4.07156	-2.18629	0.24593
H	-4.70144	-1.33909	-0.02892
H	-4.00554	-2.87034	-0.60149
H	-4.47138	-2.69303	1.12112
O	-0.94314	2.79558	-0.51031
O	-2.46458	-0.91325	-1.44683

Imag. Freq. -193.85
CBS-QB3 enthalpy: -993.757273
CBS-QB3 free energy: -993.825459

TS-13

C	-1.14185	0.29773	2.04714
C	-1.46869	-0.98509	1.69896
H	-0.90307	-1.86936	1.95842
H	-0.23047	0.60635	2.53916
C	-1.07164	1.08735	-0.84118
H	-1.15502	2.14789	-1.05032
C	-2.45941	-1.07722	-0.74542
H	-3.42496	-1.37739	-1.15366
C	0.20097	0.59427	-0.50697
C	-1.41017	-2.03701	-1.18245
H	-1.75457	-2.95399	-1.64974
C	-0.08423	-1.87740	-1.01513
H	0.55902	-2.70358	-1.29297
C	0.61602	-0.73542	-0.45515
C	-2.23134	0.32814	-1.29831
O	-3.08351	0.84211	-2.01170
C	-2.08048	1.17665	1.47299

H	-2.03328	2.25440	1.53629
C	-2.70456	-1.00715	0.86210
H	-3.35691	-1.84870	1.10095
C	-3.31468	0.39025	1.15617
H	-3.93064	0.32757	2.06309
H	-3.93658	0.79706	0.35922
C	1.14532	1.70365	-0.09487
C	1.94715	-1.00924	0.16461
O	0.90525	2.49686	0.78341
O	2.48560	-0.29943	0.98725
O	2.21947	1.76808	-0.89641
O	2.49254	-2.17538	-0.24646
C	3.20968	2.74421	-0.52452
H	2.76937	3.74081	-0.47785
H	3.63139	2.48629	0.44819
H	3.97127	2.69445	-1.29944
C	3.75532	-2.51568	0.34957
H	4.51020	-1.76961	0.09687
H	3.66394	-2.57385	1.43518
H	4.02111	-3.48462	-0.06729

Imag. Freq. -159.18

CBS-QB3 enthalpy: -993.762571

CBS-QB3 free energy: -993.828373

V. Supporting References

S1. Jamieson, C. S.; Sengupta, A.; Houk, K. N. Cycloadditions of Cyclopentadiene and Cycloheptatriene with Tropones: All *Endo*-[6+4] Cycloadditions are Ambimodal. *J. Am. Chem. Soc.* **2021**, *143*, 3918-3926.

S2. Yang, Z.; Dong, X.; Yu, Y.; Yu, P.; Li, Y.; Jamieson, C.; Houk, K. N. Relationships Between Product Ratios in Ambimodal Pericyclic Reactions and Bond Lengths in Transition Structures. *J. Am. Chem. Soc.* **2018**, *140*, 3061-3067.

S3. Isakovic, L.; Ashenhurst, J. A.; Gleason, J. L. Application of Lewis Acid Catalyzed Tropone [6+4] Cycloadditions to the Synthesis of the Core of CP-225,917. *Org. Lett.* **2001**, *3*, 4189-4192.

S4. Cossi, M.; Rega, G.; Scalmani, G.; Barone, V. Energies, Structures, and Electronic Properties of Molecules in Solution with the C-PCM Solvation Model. *J. Comp. Chem.* **2003**, *24*, 669-681.

S5. Full author list for reference 29 of the manuscript: Zhang, B.; Wang, K. B.; Wang, W.; Wang, X.; Liu, F.; Zhu, J.; Shi, J.; Li, L. Y.; Han, H.; Xu, K.; Qiao, H. Y.; Zhang, X.; Jiao, R. H.; Houk, K. N.; Liang, Y.; Tan, R. X.; Ge, H. M. Enzyme-Catalyzed [6+4] Cycloadditions in the Biosynthesis of Natural Products. *Nature* **2019**, *568*, 122-126.

S6. Full author list for reference 46 of the manuscript: Gaussian 16, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.