

Supporting Information for:

E pluribus unum: Isolation, structure determination, network analysis and DFT studies of a single metastable structure from a shapeshifting mixture of 852 bullvalene structural isomers

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I. General Procedures

^1H , ^{13}C and 2D-NMR spectra were measured on Bruker 500 or 600 MHz spectrometer. Chemical shifts are expressed in parts per million (ppm) downfield from residual solvent peaks and coupling constants are reported as Hertz (Hz). NMR splitting parameters are indicated as follows: s, singlet; d, doublet; t, triplet; q, quartet; dd, doublet of doublet; m, multiplet.

II. Isolation and Characterization of Fraction e

Bullvalene **6** (~ 4 mg) was injected onto an achiral preparative HPLC (Alltima Silica column, 250 × 22 mm ID, EtOAc:Hex 1:9, 10 mL/min flow rate, 286 nm detection) at rt, fraction e (Figure S1) was collected and kept at $-20\text{ }^\circ\text{C}$. Another fraction containing other bullvalene mixture was also collected. This fraction of bullvalene isomers was heated in a water bath at $55\text{ }^\circ\text{C}$ for 30 min, concentrated down under reduced pressure and resubjected to preparative HPLC separation. After eight successive HPLC separations, the combined fraction e was concentrated under reduced pressure and dried under vacuum at $0\text{ }^\circ\text{C}$. Approximately 1 mg of fraction e was obtained. Fraction e was dissolved in 150 μL of CD_2Cl_2 and transferred to a 3 mm outer diameter Shigemi NMR microtube that has magnetic susceptibility matched to CDCl_3 for NMR analysis (500 MHz, ^1H , ^{13}C , COSY, HSQC and HMBC) at $-20\text{ }^\circ\text{C}$. ^1H NMR (500 MHz, CD_2Cl_2 , $-20\text{ }^\circ\text{C}$) δ 7.43 (d, 2H, $J = 7.8\text{ Hz}$), 7.29 (t, 2H, $J = 7.5\text{ Hz}$), 7.25–7.23 (m, 1H), 7.21 (t, 1H, 7.5 Hz), 6.20–6.18 (m, 1H), 5.51–5.47 (m, 1H), 4.93 (d, 1H, $J = 17.1\text{ Hz}$), 4.78 (d, 1H, $J = 10.0\text{ Hz}$), 4.22–4.12 (m, 2H), 4.08 (s, 1H), 3.91 (dd, 2H, $J = 1.8\text{ Hz}$, $J = 6.7\text{ Hz}$), 2.82–2.81 (m, 2H), 2.68–2.65 (m, 2H), 2.51 (q, 1H, $J = 8.5\text{ Hz}$), 2.00–1.91 (m, 1H), 1.28 (t, 3H, $J = 7.2\text{ Hz}$), 0.92 (d, 6H, $J = 6.7\text{ Hz}$). ^{13}C NMR (500 MHz, CD_2Cl_2 , $-20\text{ }^\circ\text{C}$) δ 165.6, 153.8, 142.5, 139.5, 138.9, 138.4, 134.4, 128.7, 128.5, 127.1, 126.2, 124.5, 123.9, 116.5, 74.8, 61.3, 36.4, 36.3, 28.0, 26.4, 22.0, 20.4, 18.9, 14.4.

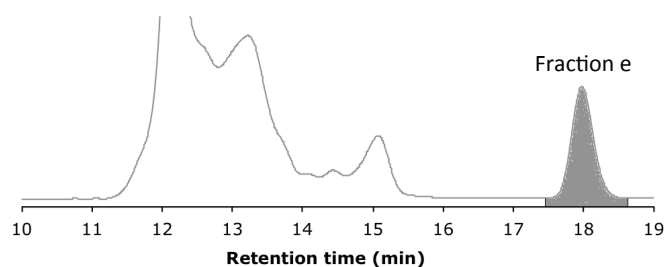
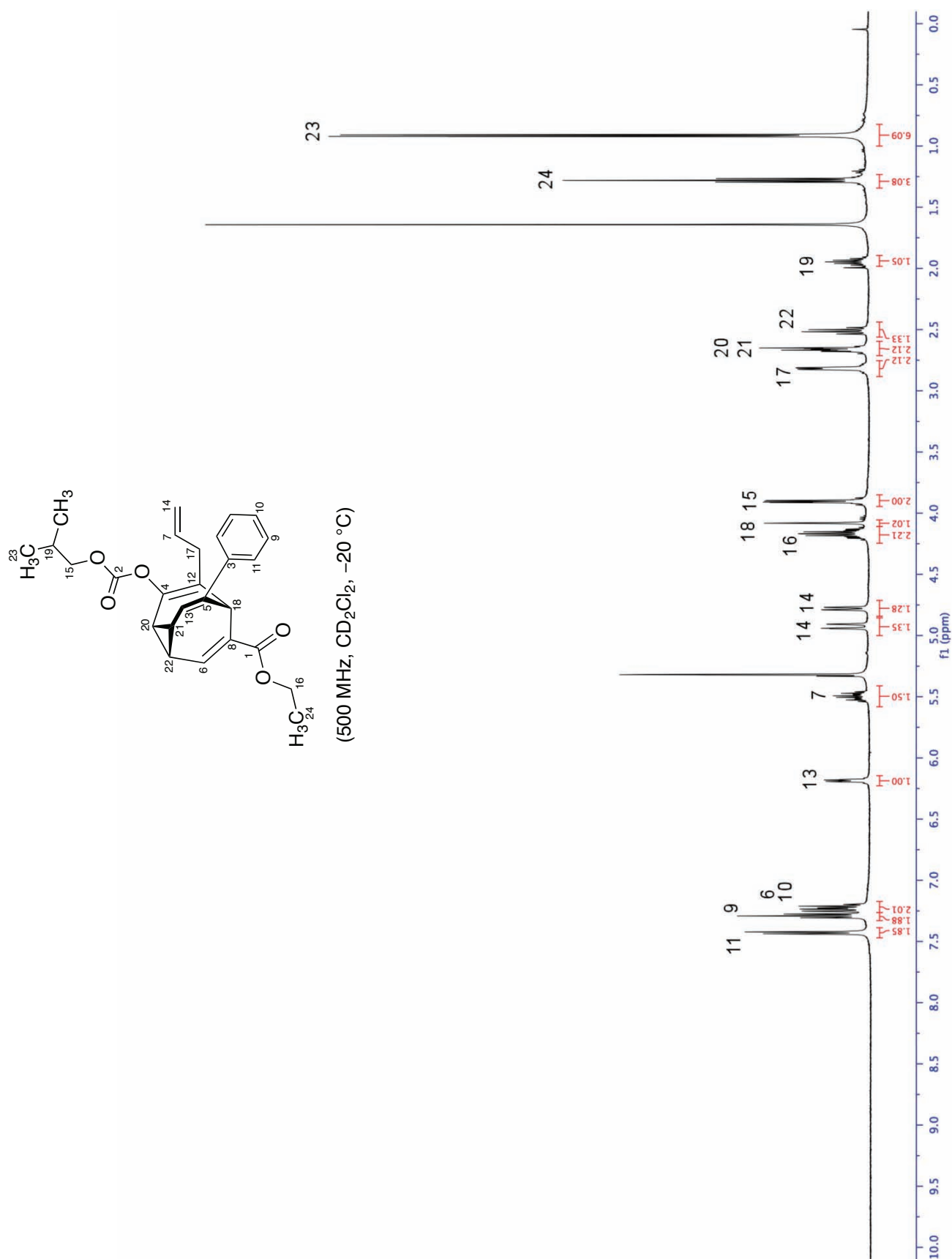
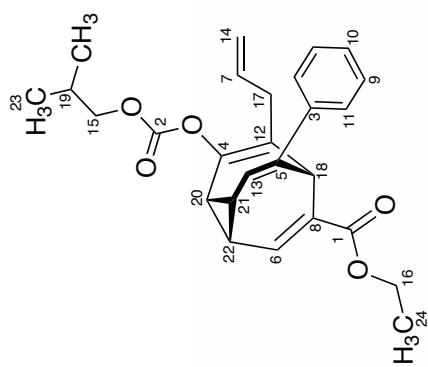
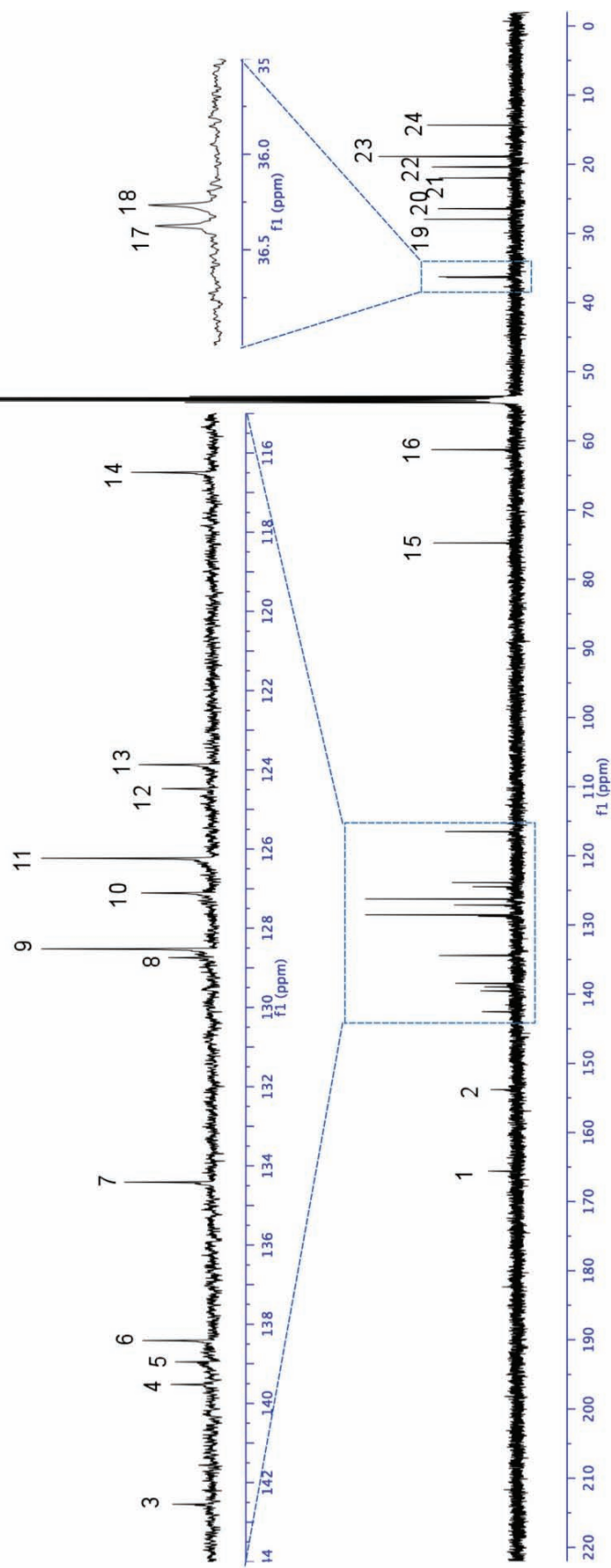


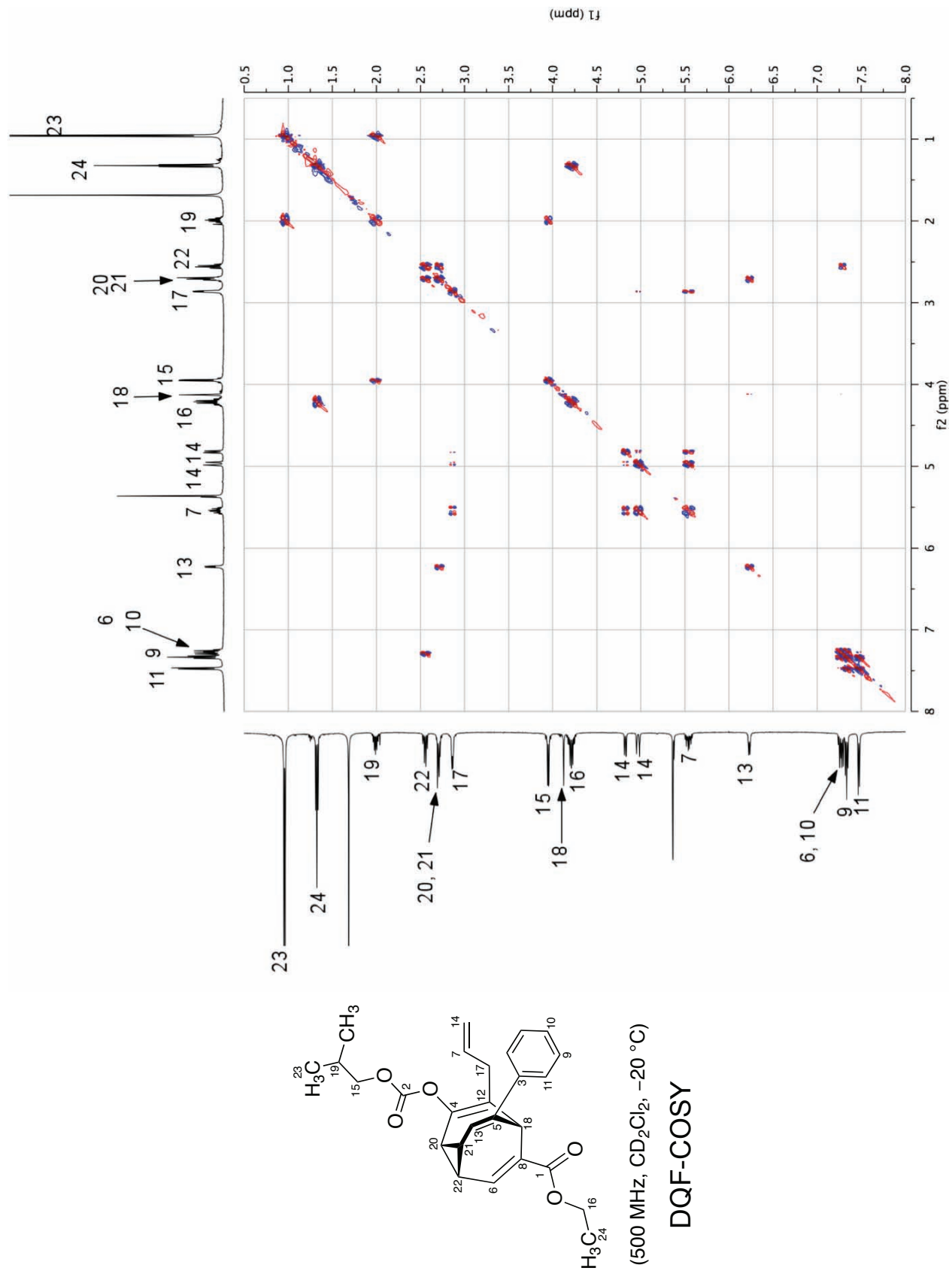
Figure S1. Preparative HPLC trace of bullvalene **6**.





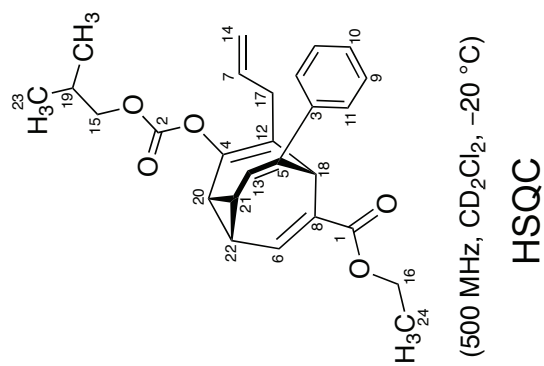
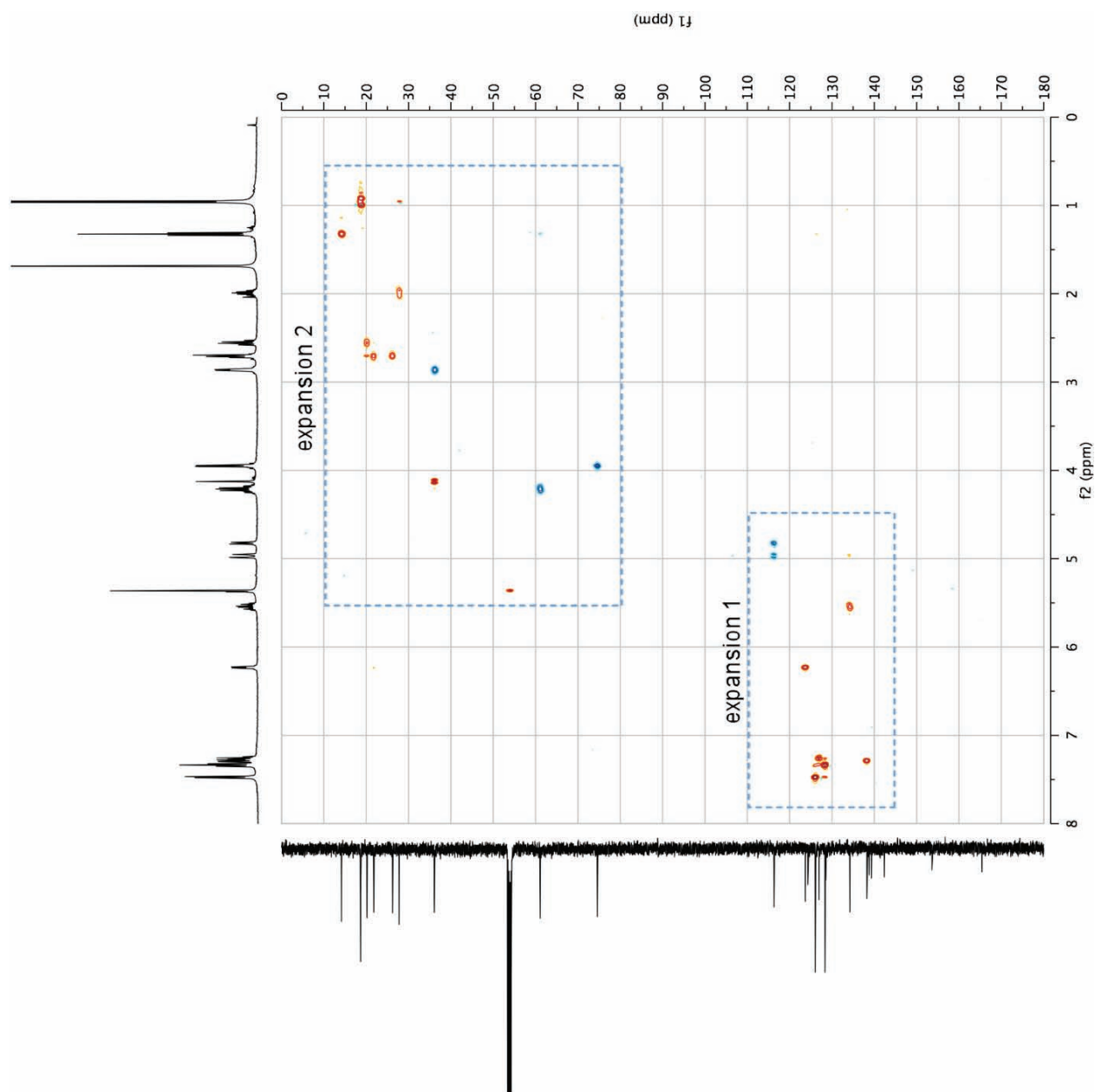
(500 MHz, CD₂Cl₂, -20 °C)

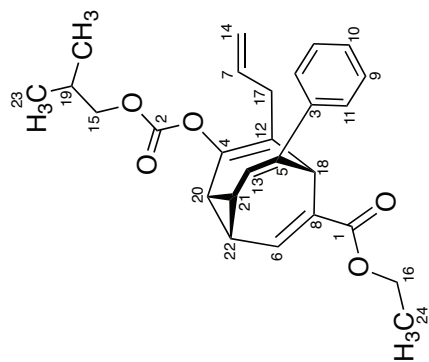
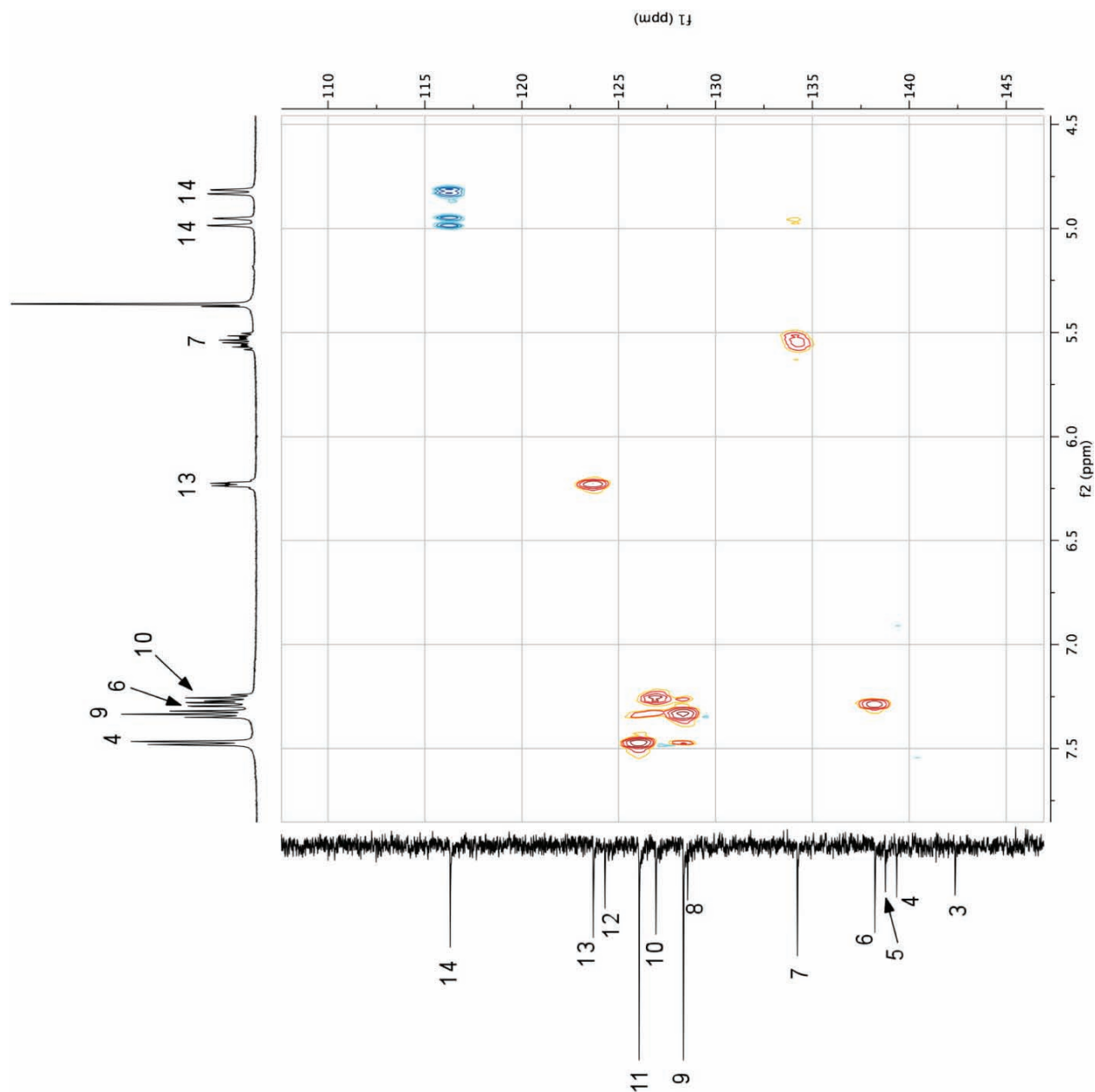




(500 MHz, CD₂Cl₂, -20 °C)

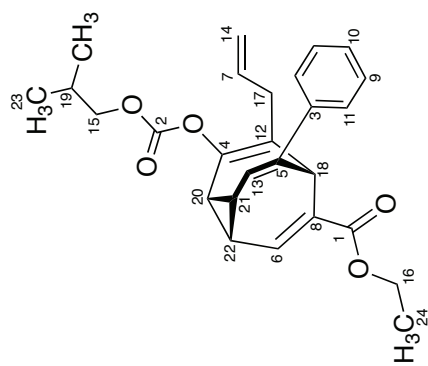
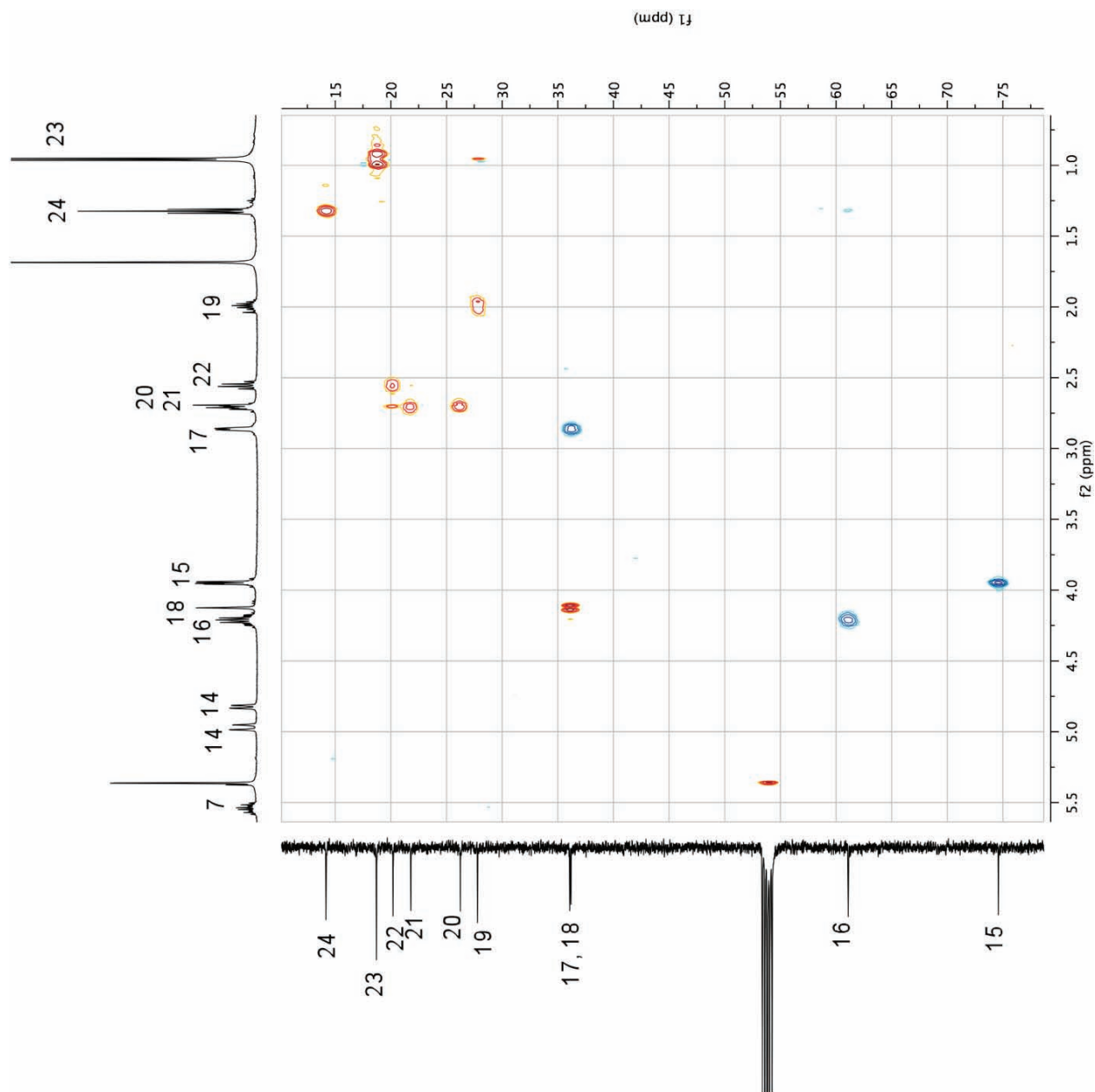
DQF-COSY





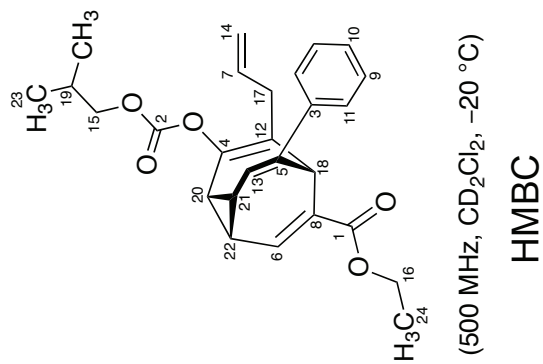
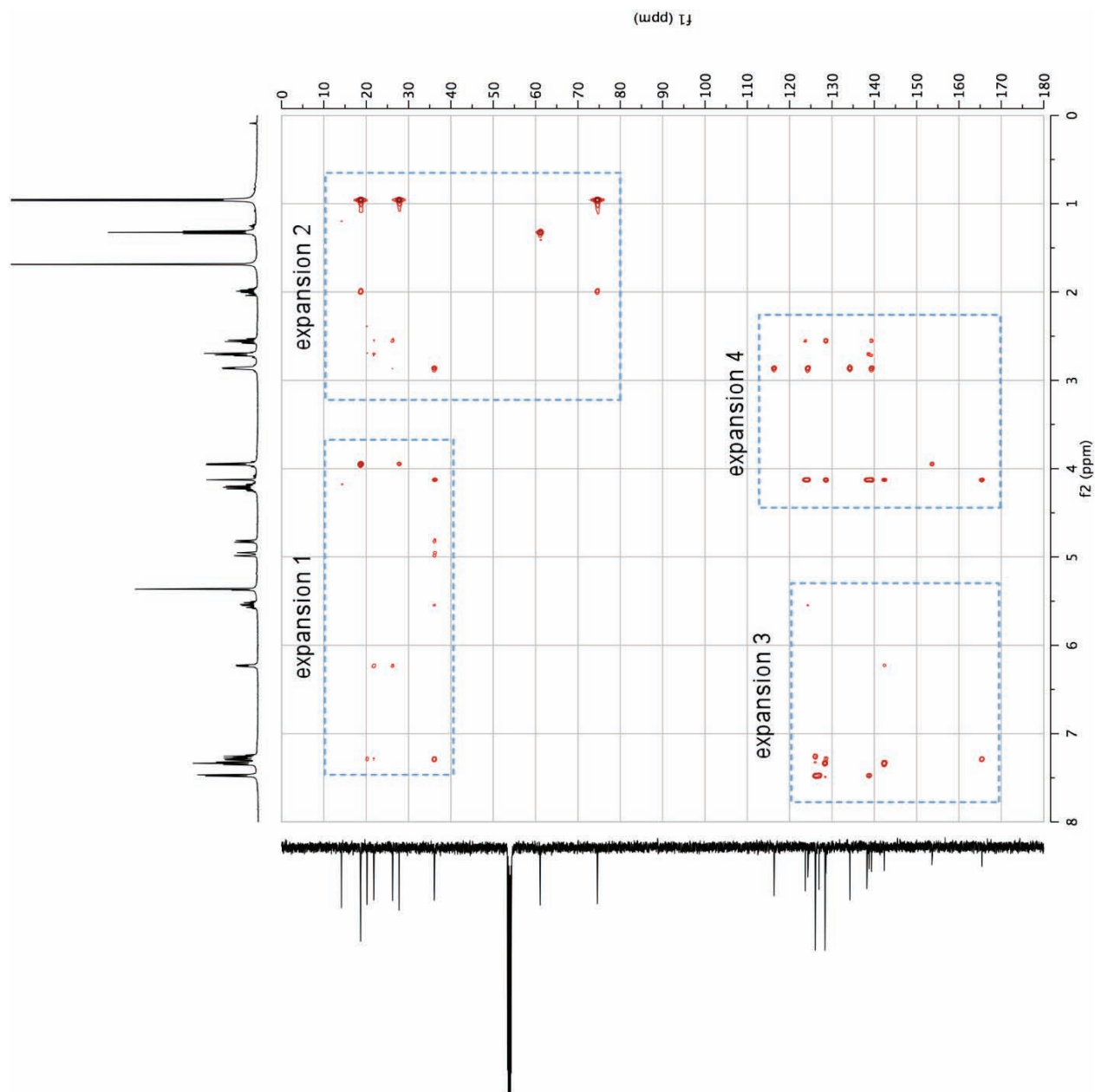
(500 MHz, CD₂Cl₂, -20 °C)

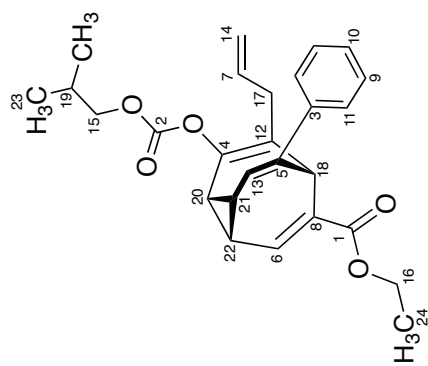
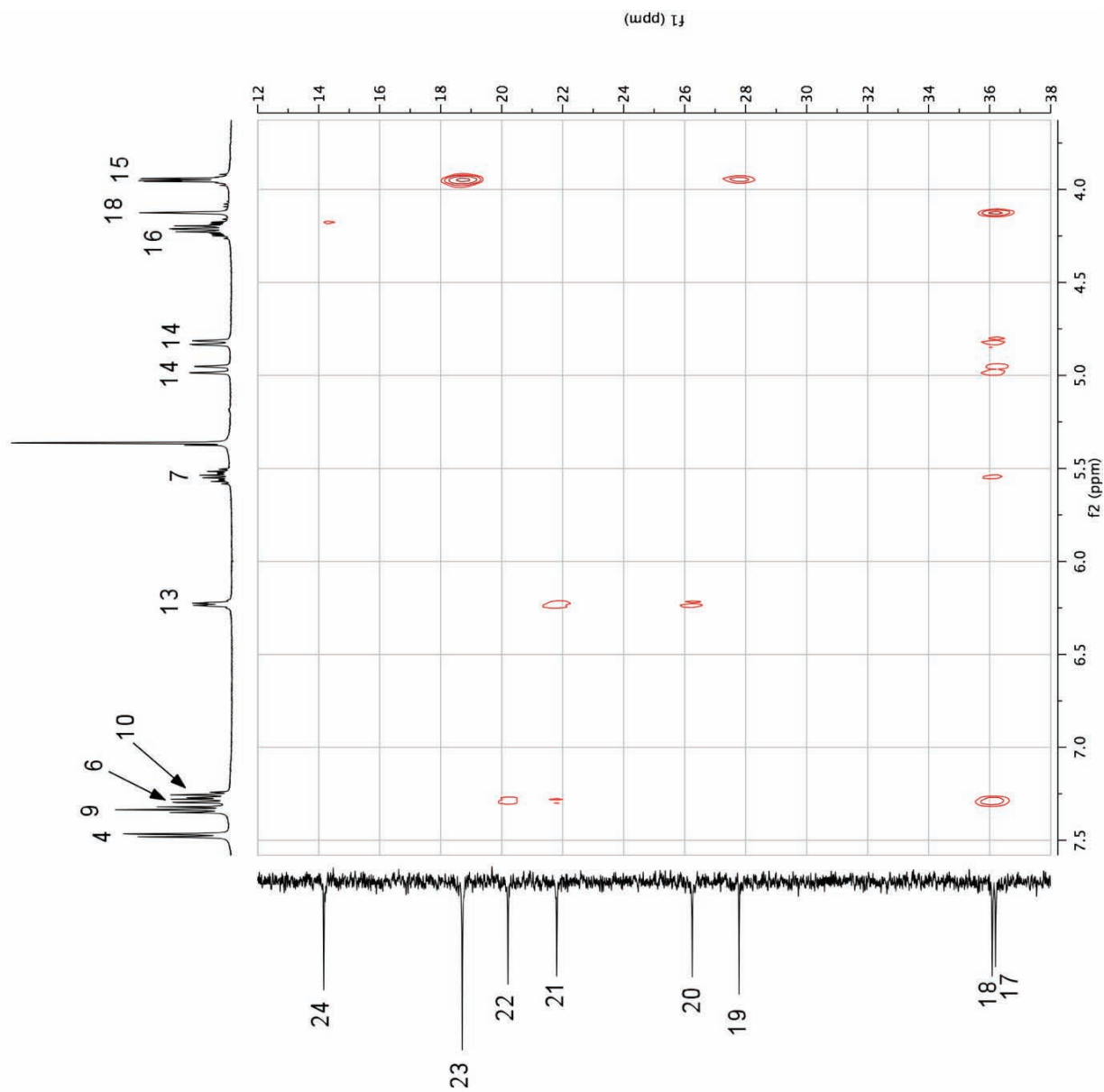
HSQC
Expansion 1



(500 MHz, CD_2Cl_2 , -20°C)

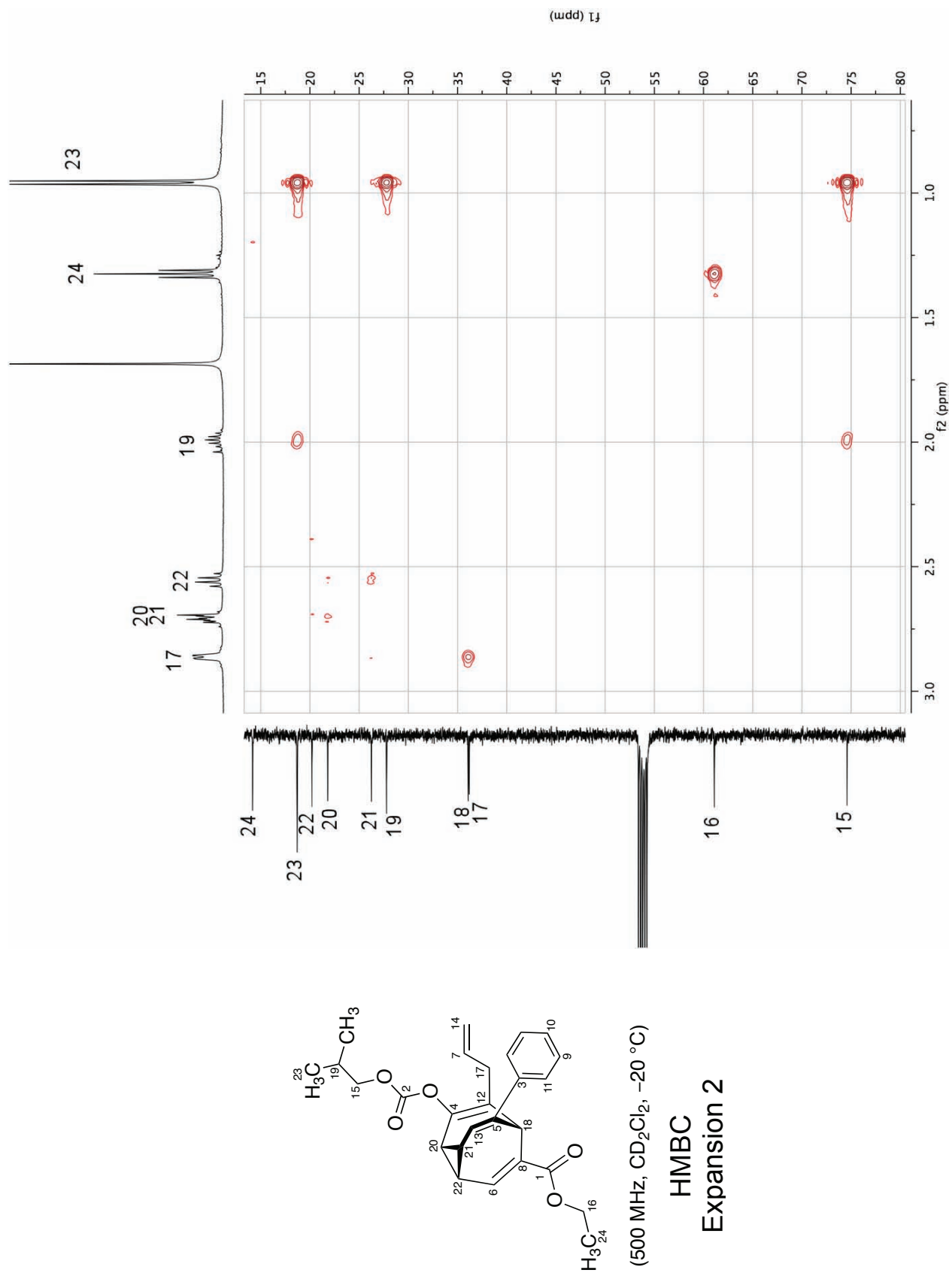
HSQC
Expansion 2

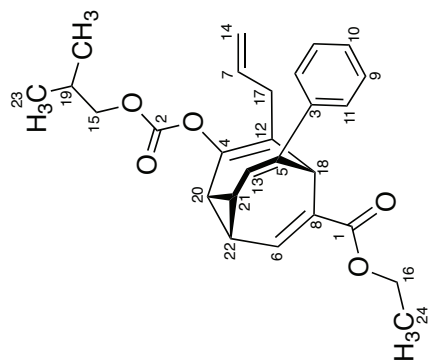
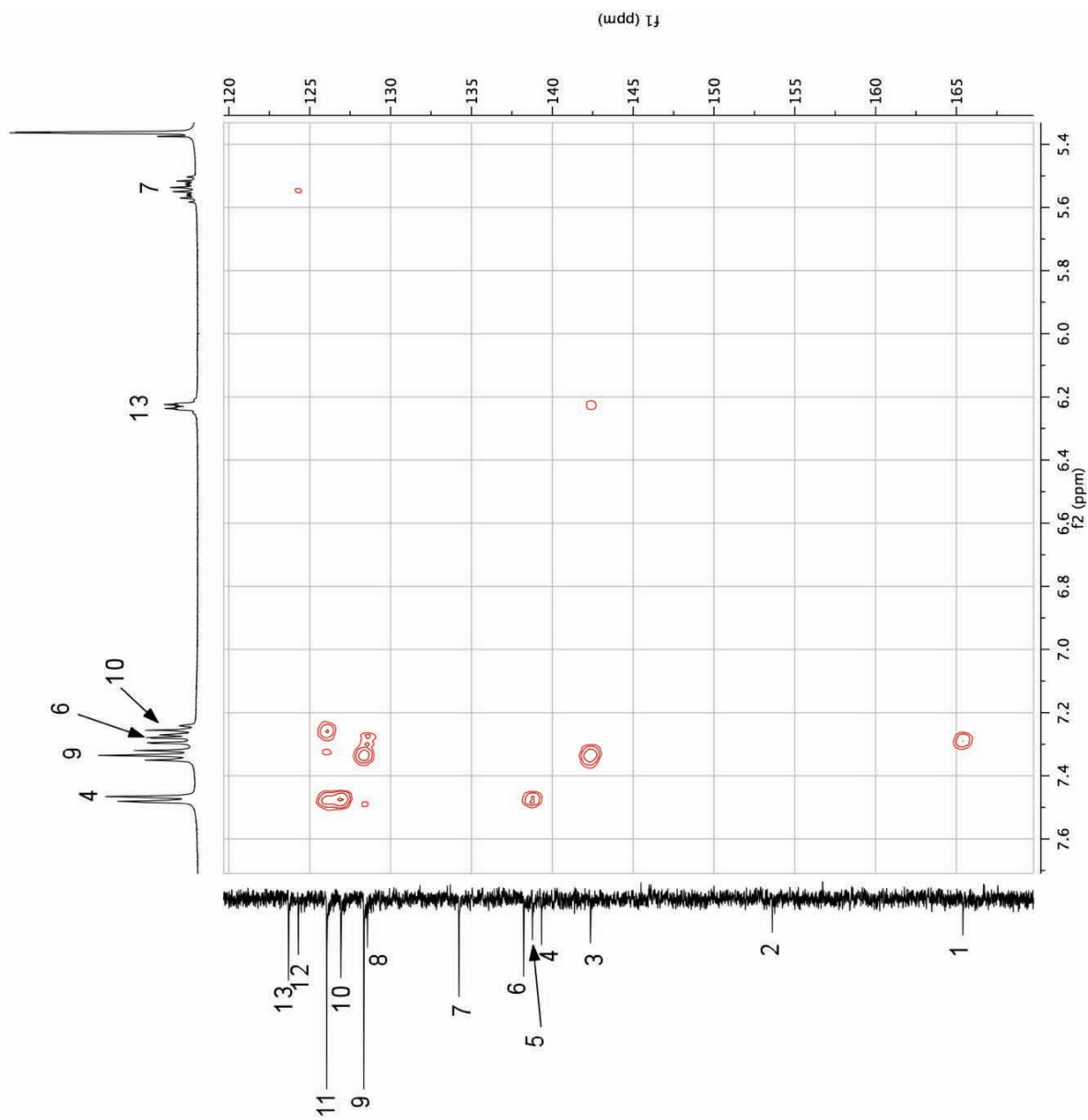




(500 MHz, CD₂Cl₂, -20 °C)

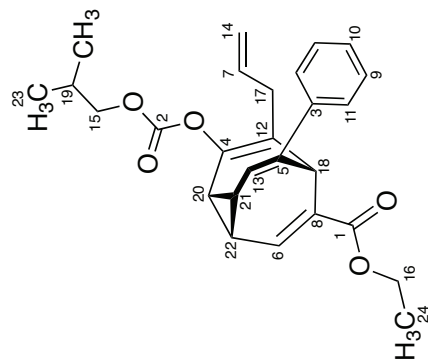
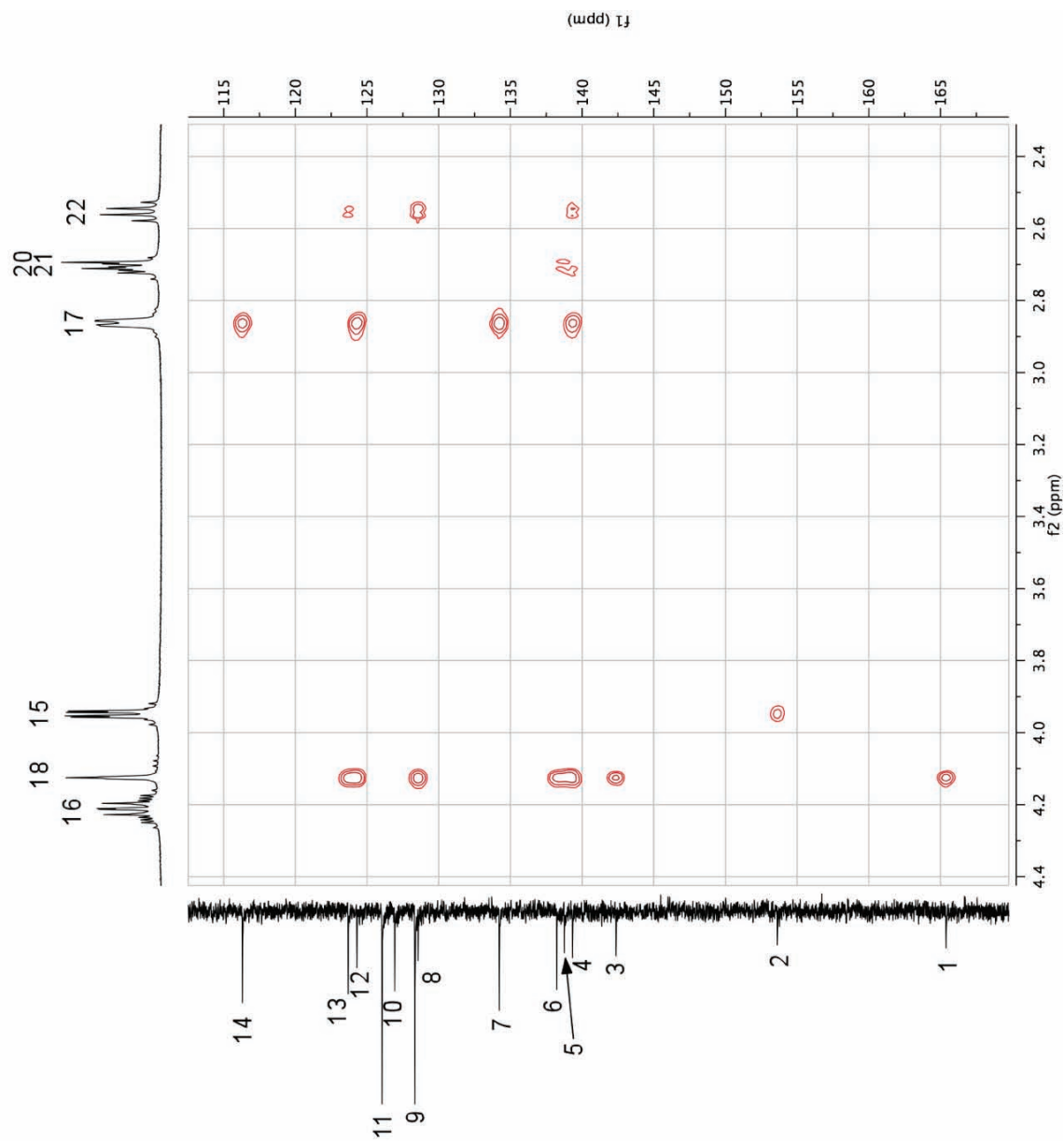
HMBC
Expansion 1





(500 MHz, CD_2Cl_2 , -20°C)

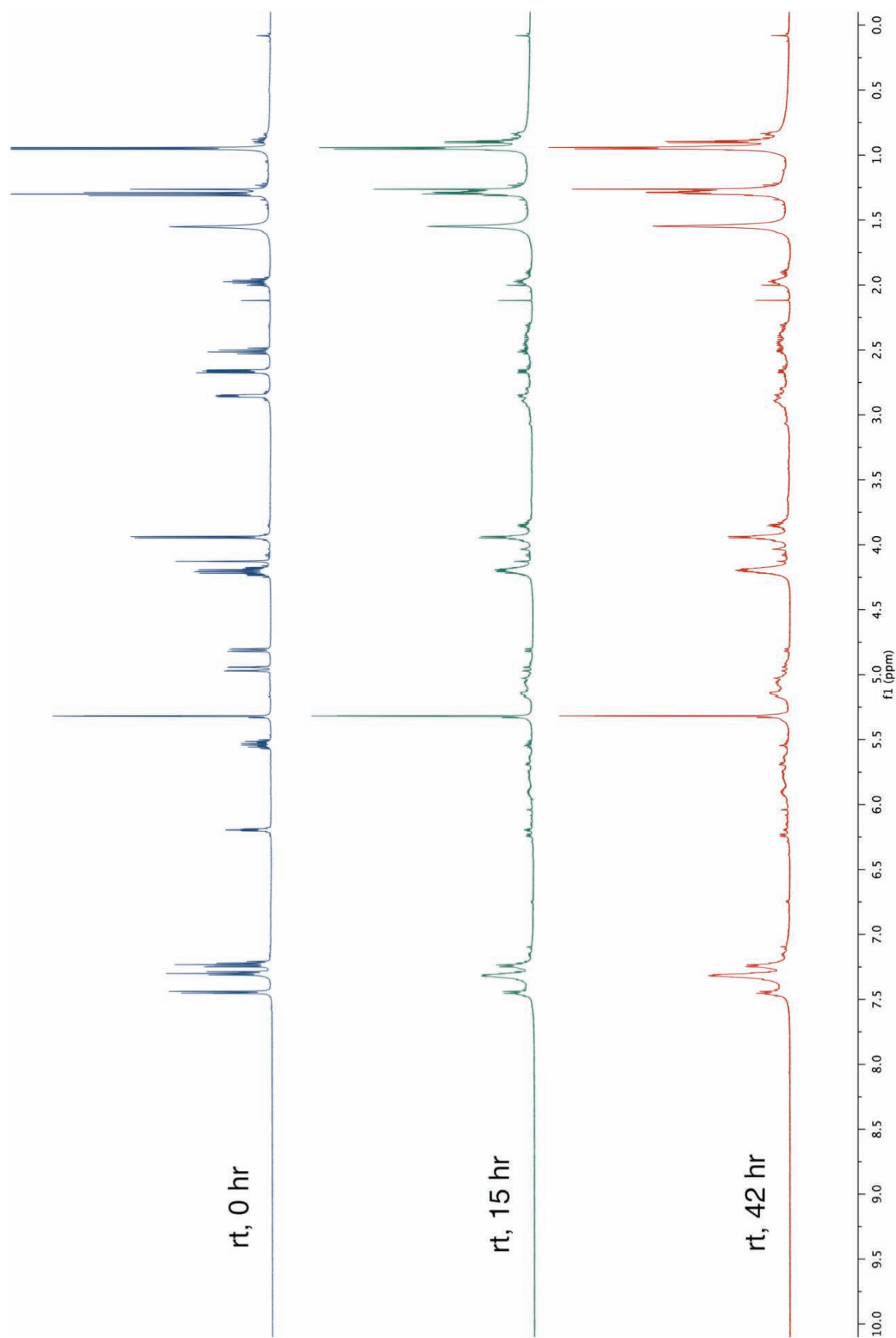
HMBC
Expansion 3



(500 MHz, CD_2Cl_2 , -20°C)

HMBC
Expansion 4

^1H NMR (600 MHz, CD_2Cl_2) of fraction e taken at different times upon standing at rt after it is removed from $-20\text{ }^\circ\text{C}$.



III. Evidence that fraction e was not induced by HPLC column

To ensure that the isomerization of fraction e is not induced by the HPLC column, the fraction shaded in gray below (Figure S2) was isolated (Alltima Silica column, 250×4.6 mm ID, EtOAc:Hex 1:9, 1 ml/min flow rate, 254 nm detection) concentrated at 0 °C under reduced pressure, and reinjected onto the HPLC. No fraction e was observed upon reinjection. This supported the conjecture that fraction e was not formed because of HPLC column.

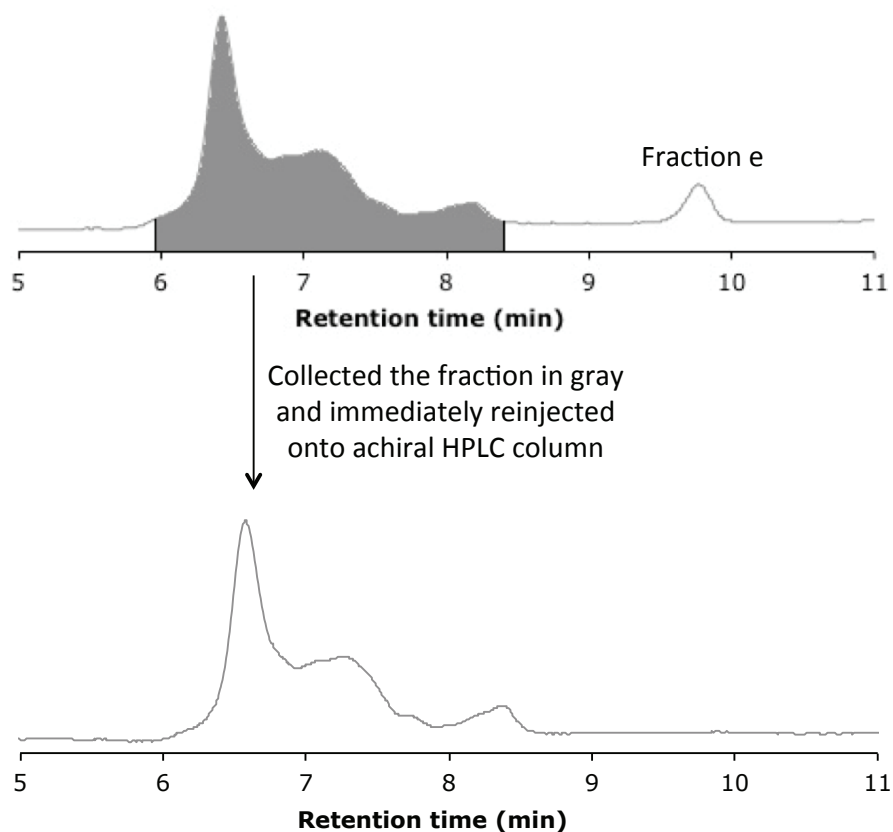


Figure S2. Isolation of bullvalene fraction and its reinjection HPLC trace.

IV. Code generation

Each isomer of bullvalene **6** can be represented by a 10-digit number. This 10-digit number codes the substitutions as well as their positions on the bullvalene core. Numbers 1, 2, 3, and 4 represents the substituents isobutyl carbonate, phenyl, ethyl ester and allyl respectively. Zero means no substitution, or just hydrogen, on the carbon. The position of the carbons of the bullvalene core is represented in the code in the order from left to right, coding arm 1, arm 2, arm 3 and methine carbon (Figure S3).

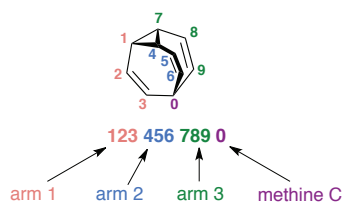


Figure S3. Position of bullvalene core carbons in the code.

To generate the complete interconversion network of bullvalene **6**. The codes for all 1680 isomers were created using the computer program Matlab 7.11.0.584 (R2010b).

Matlab command:

```
a=perms([1 2 3 4 0 0 0 0 0 0])
b=unique(a, 'rows')
arm1=b(:, 1:3)
arm2=b(:, 4:6)
arm3=b(:, 7:9)
methineC=b(:, 10)
c=cat(2, arm2, arm3, arm1, methineC)
d=cat(2, arm3, arm1, arm2, methineC)
dlmwrite('startcode1', b, ")
dlmwrite('startcode2', c, ")
dlmwrite('startcode3', d, ")
```

Import the text file “startcode1”, “startcode2”, “startcode3” back to Matlab. This was done by clicking [File], [Import Data...], select the file “startcode1”, [Open], select “Other” for column separator and leave it blank, [Next], [Finish].

```
e=cat(2, startcode1, startcode2, startcode3)
f=sort(e, 2)
g=f(:, 1)
smalleststartcode=unique(g)
h=sprintf('%010d\n', smalleststartcode)
dlmwrite('j', h, ' ')
```


The “perms” command generates all of the possible permutations of the 10 numbers. This gives 3,628,800 permutations. Most of these permutations repeats and therefore the “unique(a, ‘rows’)” command was used to remove the arrays that repeats. The “unique” command gives 5040 non-repetitive permutations. Since each bullvalene isomer can be represented by three codes (see main text Figure 3) we selected the 10-digit number with the smallest value to represent each isomer. The text file ‘j’ contains the numeric codes for all 1680 isomers of bullvalene **6**.

V. Cope rearrangements

Continued from Section IV – Code generation, the following commands and steps were carried out in Matlab.

Import the text file “j” by clicking [File], [Import Data...], select the file “j”, [Open], select “Space” for column separator, [Next], [Finish].

```
c1=j(:,1)
c2=j(:,2)
c3=j(:,3)
c4=j(:,4)
c5=j(:,5)
c6=j(:,6)
c7=j(:,7)
c8=j(:,8)
c9=j(:,9)
c10=j(:,10)
ra1code1=cat(2, c10, c9, c8, c6, c5, c4, c3, c2, c1, c7)
ra1code2=cat(2, c6, c5, c4, c3, c2, c1, c10, c9, c8, c7)
ra1code3=cat(2, c3, c2, c1, c10, c9, c8, c6, c5, c4, c7)
ra2code1=cat(2, c9, c8, c7, c6, c5, c4, c10, c3, c2, c1)
ra2code2=cat(2, c6, c5, c4, c10, c3, c2, c9, c8, c7, c1)
ra2code3=cat(2, c10, c3, c2, c9, c8, c7, c6, c5, c4, c1)
ra3code1=cat(2, c9, c8, c7, c10, c6, c5, c3, c2, c1, c4)
ra3code2=cat(2, c10, c6, c5, c3, c2, c1, c9, c8, c7, c4)
ra3code3=cat(2, c3, c2, c1, c9, c8, c7, c10, c6, c5, c4)
```

```
dlmwrite('ra1code1t', ra1code1, ")  
dlmwrite('ra1code2t', ra1code2, ")  
dlmwrite('ra1code3t', ra1code3, ")  
dlmwrite('ra2code1t', ra2code1, ")  
dlmwrite('ra2code2t', ra2code2, ")  
dlmwrite('ra2code3t', ra2code3, ")  
dlmwrite('ra3code1t', ra3code1, ")  
dlmwrite('ra3code2t', ra3code2, ")  
dlmwrite('ra3code3t', ra3code3, ")
```

Import the text file “ra1code1t”, “ra1code2t”, “ra1code3t”, “ra2code1t”, “ra2code2t”, “ra2code3t”, “ra3code1t”, “ra3code2t” and “ra3code3t” into Matlab separately by clicking [File], [Import Data...], select the file, [Open], select “Other” for column separator and leave it blank, [Next], [Finish].

```
k1=cat(2, ra1code1t, ra1code2t, ra1code3t)  
k2=cat(2, ra2code1t, ra2code2t, ra2code3t)  
k3=cat(2, ra3code1t, ra3code2t, ra3code3t)  
L1=sort(k1, 2)  
L2=sort(k2, 2)  
L3=sort(k3, 2)  
m1=L1(:, 1)  
m2=L2(:, 1)  
m3=L3(:, 1)  
n=cat(1, m1, m2, m3)  
p=cat(1, smalleststartcode, smalleststartcode, smalleststartcode)  
n10d=sprintf('%010d\n', n)  
p10d=sprintf('%010d\n', p)  
dlmwrite('NodeA', n10d, ")  
dlmwrite('NodeB', p10d, ")
```

Open Microsoft Excel for Mac 2011 (version 14.1.4). Click on cell A1, go to [File], [Import...], select “Text file”, then [Import]. Go to the folder where “NodeA” is saved, enable “Text Files”, select the file “NodeA” and click [Get Data]. When the Text Import Wizard come up, leave “Delimited” under Original data type selected, click [Next], [Next] again, select “Text” under Column data format and

click [Finish]. In the “Import Data” window, select “Existing sheet = \$A\$1” and click [OK]. Click on cell B1 and import the file “NodeB” using the same steps. Select cells A1:B5040, go to [File], [Save As...], save as “Network data” in the format of Tab Delimited Text (.txt). The “Network data” text file contains all the possible rearrangements of bullvalene **6**. Each line in this file represents one rearrangement between two isomers.

VI. Interconversion network

To visualize the interconversion network of bullvalene, the program NAViGaTOR2.2.1 (<<http://ophid.utoronto.ca/navigator/download.html>>) was used.

Open NAViGaTOR.

Click [Browse...].

Select “(.txt) Tab-delimited Data” for the File Format.

Select the text file “Network data” and click [Open].

Set Header Size (rows) = 0 and Title Row = 0, then click [Next].

Select “Node A ID” under NodeA and select “Node B ID” under NodeB.

Click [Next], then click [Done].

Further organization and formatting with NAViGaTOR generated the network map shown in Figure S4 with fraction e in the center and each ring of dots represents a successive generations of rearrangements.

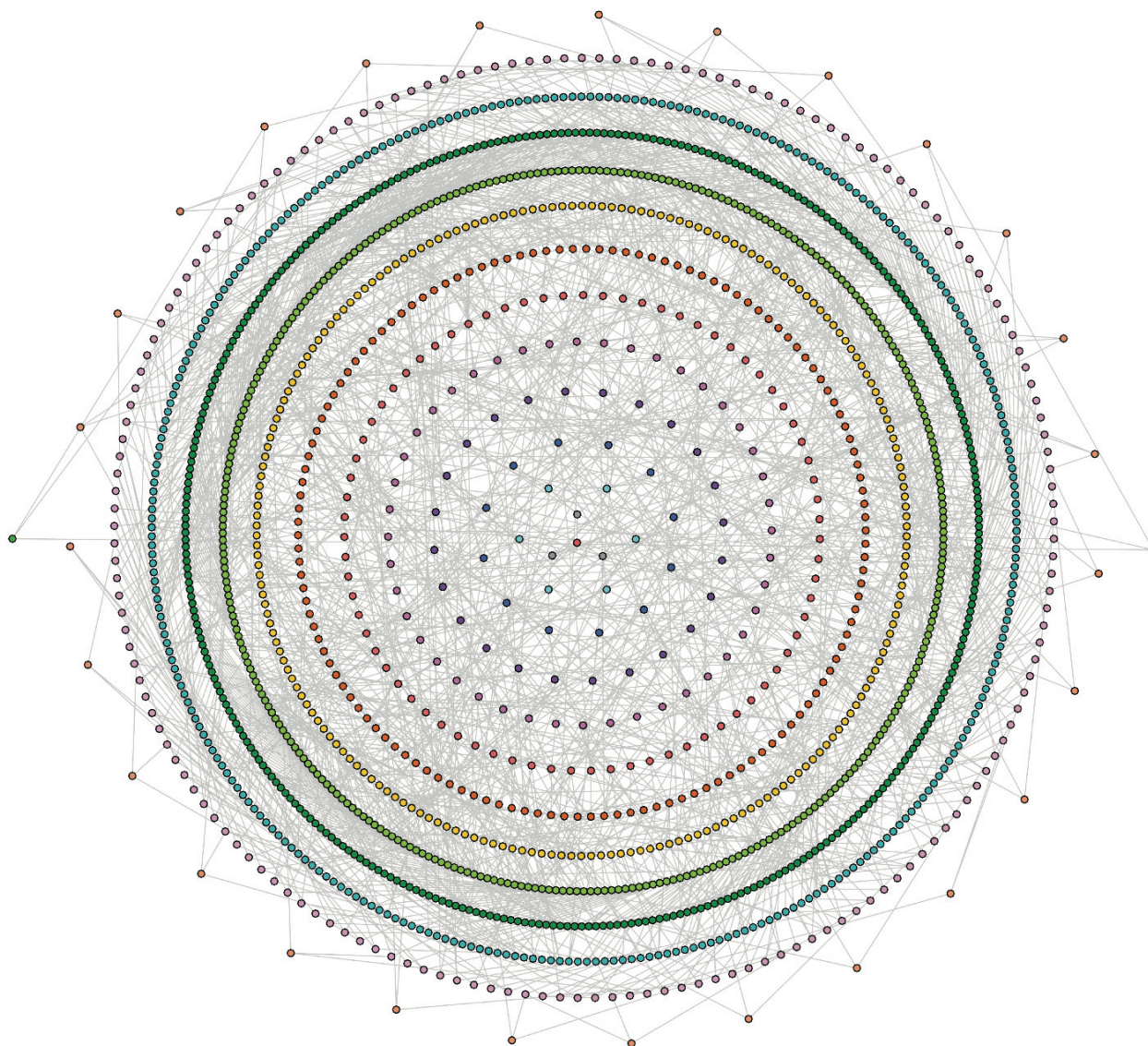


Figure S4. Interconversion network of bullvalene **6**.

VII. Experimental half-life of fraction **e**

Fraction **e** was isolated by preparative HPLC (Alltima Silica column, 250 × 22 mm ID, EtOAc:Hex 1:9, 10 mL/min flow rate, 286 nm detection) at rt (23 °C). The solvent was removed under reduced pressure at rt and a solution of naphthalene in EtOAc:Hex 1:9 was added. This sample was injected onto an analytical HPLC (Alltima Silica column, 250 × 4.6 mm ID, EtOAc:Hex 1:9, 1 mL/min flow rate, 286 nm detection) every hour to monitor the disappearance of fraction **e** peak relative to naphthalene internal standard. This experiment was repeated twice and the half-life was determined to be 262 min and 268 min (Table S1).

Table S1. Experimental half-life of fraction e

Half-life trial 1	
Time (s)	Fraction e/naphthalene
1260	0.28
4980	0.24
8280	0.20
11880	0.17
15480	0.15
19080	0.13
22680	0.11

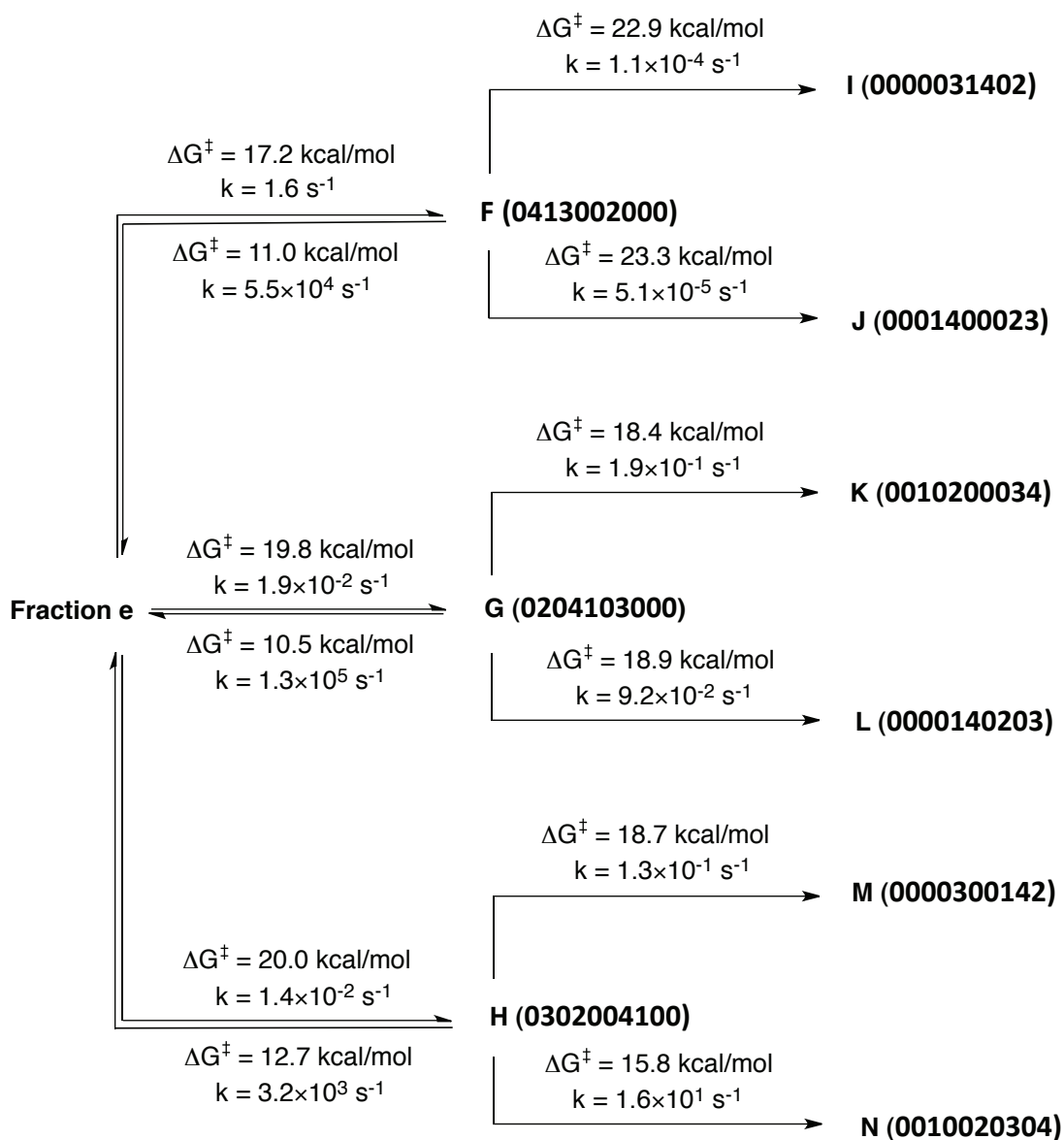
Half-life trial 2

Time (s)	Fraction e/naphthalene
0	0.35
3900	0.30
7320	0.26
11700	0.22
14580	0.19
18060	0.16
25260	0.11

VIII. Simulated half-life of fraction e

The first-order rate constants of the rearrangements of fraction e were obtained from the calculated free energy of activation at 25 °C at the M06-2X/6-31+G(d,p) level of theory (Scheme S1). The rearrangements and their rate constants were then inputted into the program KinTek_Explorer (<http://www.kintek-corp.com/KGExplorer/index.php>) to simulate the reaction and determine the half-life of fraction e (Figure S5).

$$k = \frac{k_B T}{h} e^{-\frac{\Delta G^\ddagger}{RT}}$$



Scheme S1. Calculated rate constants of rearrangements of fraction e.

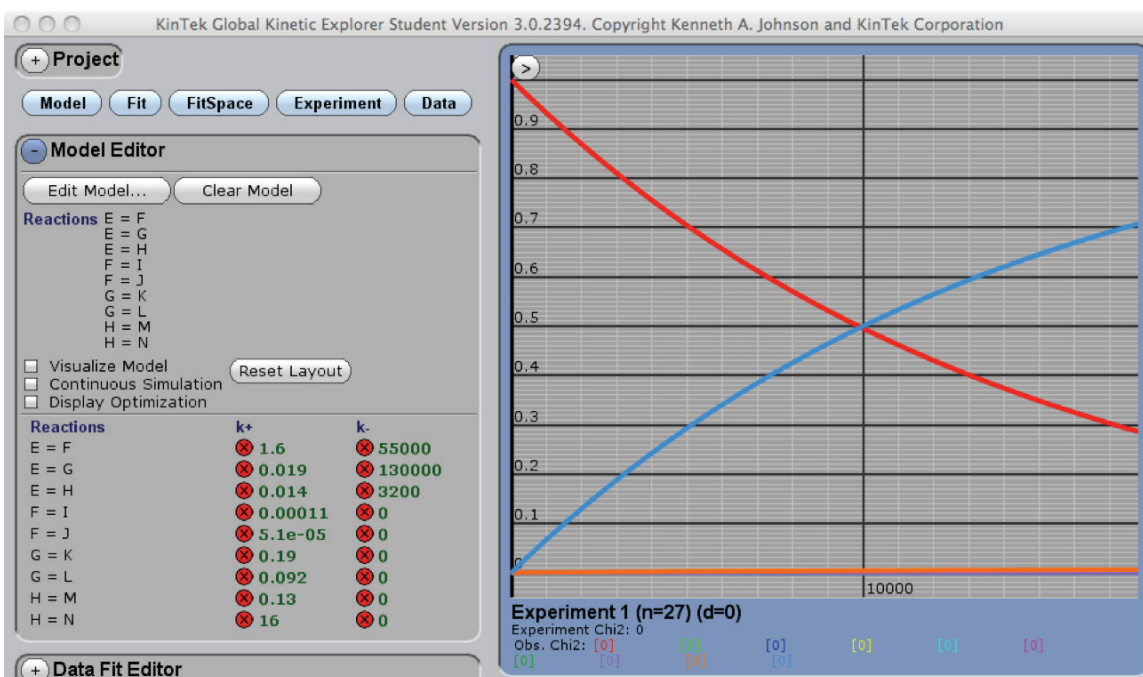
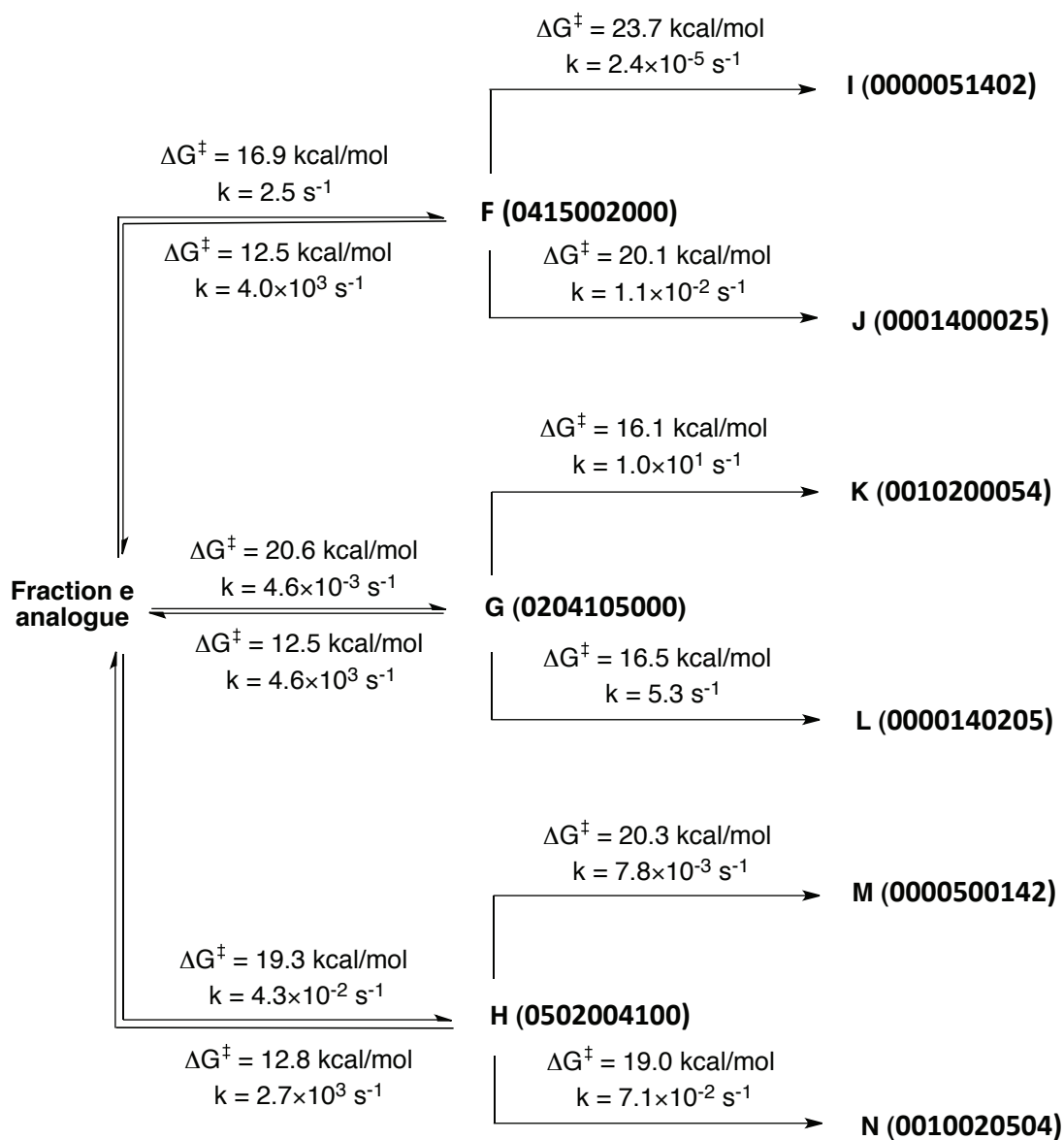


Figure S5. Half-life of fraction e.

IX. Simulated half-life of fraction e analogue without the ester

The half-life of fraction e analogue without the ester was simulated according to the procedure applied to fraction e (Scheme S2 and Figure S6).



Scheme S2. Calculated rate constants of rearrangements of fraction e analogue.



Figure S6. Half-life of fraction e analogue.

X. Computation details

Monte Carlo Multiple Minimum (MCMM) conformational search using the OPLS_2005 force field was carried out for all isomers using the MacroModel application within the Maestro program from Schrödinger. The lowest energy conformation of the MCMM conformational search was optimized with DFT method at the B3LYP/6-31G(d) level of theory. For isomers involved within two generations of rearrangements from fraction e and its analogues without the ester group, their B3LYP/6-31G(d) geometries were further optimized with M06-2X functional and the 6-31+G(d,p) basis set. All transition state calculations were optimized with B3LYP/6-31G(d) and M06-2X/6-31+G(d,p). The geometries for M06-2X/6-31+G(d,p) calculation were taken from B3LYP/6-31G(d) optimized geometries. Frequency calculations were performed to verify minima and transition states (no imaginary frequency for minimum and one imaginary frequency for transition state). Transition states were also verified by animating the negative frequency. For computational simplicity, the isobutyl and ethyl groups were replaced by methyl groups. All DFT calculations were performed in the gas phase at 1 atm and 298.15 K using the GAUSSIAN 09 program.

XI. Free energy comparison between B3LYP/6-31G(d) and M06-2X/6-31+G(d,p)

Fraction e

		Relative free energy		Forward barrier		Backward barrier	
		B3LYP/ 6-31G(d)	M06-2X/ 6-31+G(d,p)	B3LYP/ 6-31G(d)	M06-2X/ 6-31+G(d,p)	B3LYP/ 6-31G(d)	M06-2X/ 6-31+G(d,p)
Fraction e	0020030140	0.0	0.0				
TS	0020030140-0413002000	14.4	17.2	14.4	17.2	3.8	11.0
TS	0020030140-0204103000	16.8	19.8	16.8	19.8	4.3	10.5
TS	0020030140-0302004100	17.6	20.0	17.6	20.0	6.1	12.7
Isomer	0413002000	10.6	6.2				
Isomer	0204103000	12.6	9.3				
Isomer	0302004100	11.5	7.3				
TS	0413002000-0000031402	29.2	29.1	18.6	22.9	7.2	11.9
TS	0413002000-0001400023	30.8	29.5	20.2	23.3	14.0	17.9
TS	0204103000-0010200034	27.9	27.7	15.3	18.4	13.9	16.1
TS	0204103000-0000140203	29.7	28.2	17.2	18.9	15.4	18.8
TS	0302004100-0000300142	29.2	26.0	17.7	18.7	12.1	14.8
TS	0302004100-0010020304	24.3	23.1	12.8	15.8	13.0	14.7
Isomer	0000031402	22.0	17.2				
Isomer	0001400023	16.8	11.6				
Isomer	0010200034	13.9	11.6				
Isomer	0000140203	14.3	9.4				
Isomer	0000300142	17.0	11.2				
Isomer	0010020304	11.3	8.4				

Fraction e with the ester group replaced with a methyl group

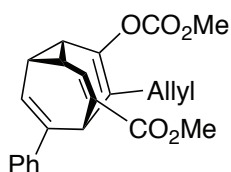
		Relative free energy		Forward barrier		Backward barrier	
		B3LYP/ 6-31G(d)	M06-2X/ 6-31+G(d,p)	B3LYP/ 6-31G(d)	M06-2X/ 6-31+G(d,p)	B3LYP/ 6-31G(d)	M06-2X/ 6-31+G(d,p)
Fraction e	0020050140	0.0	0.0				
TS	0020050140-0415002000	13.8	16.9	13.8	16.9	6.9	12.5
TS	0020050140-0204105000	17.4	20.6	17.4	20.6	6.9	12.5
TS	0020050140-0502004100	16.2	19.3	16.2	19.3	6.4	12.8
Isomer	0415002000	6.9	4.4				
Isomer	0204105000	10.5	8.2				
Isomer	0502004100	9.8	6.5				
TS	0415002000-0000051402	28.3	28.1	21.4	23.7	11.9	15.9
TS	0415002000-0001400025	24.2	24.5	17.3	20.1	13.6	17.8
TS	0204105000-0010200054	23.6	24.2	13.1	16.1	14.2	17.7
TS	0204105000-0000140205	24.3	24.7	13.9	16.5	16.6	20.5
TS	0502004100-0000500142	28.2	26.9	18.4	20.3	13.3	16.9
TS	0502004100-0010020504	24.5	25.6	14.7	19.0	15.4	18.8
Isomer	0000051402	16.4	12.2				
Isomer	0001400025	10.6	6.7				
Isomer	0010200054	9.4	6.6				
Isomer	0000140205	7.8	4.1				
Isomer	0000500142	15.0	10.0				
Isomer	0010020504	9.1	6.8				

XII. Full reference for Gaussian 09

Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

XIII. Cartesian coordinates of calculated structures

Isomer 0020030140 (fraction e)



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

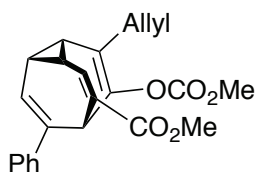
Sum of electronic and thermal Free Energies= -1265.391309 Hartree

Charge = 0 Multiplicity = 1

C	-0.17949	0.060976	0.051602
C	-0.182687	0.098569	1.568543
C	1.162779	0.021049	0.823633
H	-0.455458	-0.904869	-0.362038
H	-0.468178	-0.832847	2.046693
H	1.625205	-0.96109	0.854546
C	2.111809	1.133766	0.790451
C	1.793272	2.446449	0.752388
H	3.163129	0.861646	0.789967
C	-0.590175	1.289909	2.336516
C	-0.376304	2.576042	2.026971
C	-0.582359	1.202858	-0.78698
C	-0.388199	2.512133	-0.519974
H	-1.071224	0.932429	-1.720001
C	0.359168	2.956135	0.740149
H	0.41284	4.043787	0.730013
C	-0.87895	3.551936	-1.461578
C	-2.105748	3.390125	-2.13099
C	-0.131212	4.714643	-1.723797
C	-2.558932	4.341042	-3.043278
H	-2.721161	2.523168	-1.908339
C	-0.585651	5.664007	-2.638568
H	0.819409	4.873445	-1.222722
C	-1.798923	5.482597	-3.304531
H	-3.514926	4.196061	-3.540226
H	0.014578	6.549572	-2.831344
H	-2.15331	6.227546	-4.012117
C	2.856146	3.483406	0.702402
O	2.642837	4.681309	0.604831
O	4.110609	2.977617	0.773534
C	5.166716	3.946456	0.712407
H	6.09196	3.373655	0.785397

H	5.13031	4.498476	-0.230762
H	5.088031	4.655987	1.540478
O	-1.186759	0.97719	3.580204
C	-2.464361	0.536421	3.543686
O	-3.147968	0.395272	2.556779
O	-2.834107	0.28504	4.80724
C	-4.183676	-0.186653	4.950449
H	-4.322495	-0.338454	6.021006
H	-4.892437	0.554739	4.572455
H	-4.323164	-1.125287	4.407786
C	-0.840477	3.719988	2.907647
H	-0.006129	4.418583	3.055597
H	-1.120708	3.332767	3.893224
C	-2.007494	4.460813	2.296118
C	-1.993611	5.746393	1.943043
H	-2.903903	3.862971	2.128749
H	-2.861706	6.226111	1.499228
H	-1.11209	6.368834	2.083563

Isomer 0020030410



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

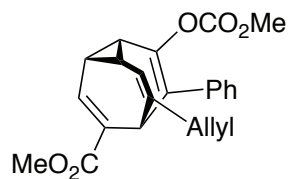
Sum of electronic and thermal Free Energies= -1265.388296 Hartree

Charge = 0 Multiplicity = 1

C	0.002109	-0.049917	-0.085336
C	0.019399	-0.112986	1.442435
C	1.348127	-0.099348	0.673544
H	-0.250082	-0.993698	-0.561017
H	-0.226531	-1.095886	1.836342
H	1.837988	-1.067867	0.630004
C	2.274832	1.036955	0.688094
C	1.927883	2.33942	0.723974
H	3.331505	0.789125	0.650361
C	-0.44852	0.993595	2.311983
C	-0.222743	2.280761	2.007089
C	-0.453525	1.130636	-0.838543
C	-0.289318	2.427315	-0.496601
H	-0.967867	0.905788	-1.770328
C	0.48217	2.807309	0.771329

H	0.500634	3.892351	0.852715
C	-0.849283	3.513251	-1.341656
C	-2.094188	3.357102	-1.978647
C	-0.151721	4.719872	-1.53741
C	-2.614492	4.357942	-2.796761
H	-2.670467	2.452868	-1.804323
C	-0.674044	5.718729	-2.358686
H	0.812918	4.872033	-1.061523
C	-1.904977	5.544171	-2.993288
H	-3.583216	4.216374	-3.269412
H	-0.112386	6.638152	-2.502929
H	-2.312164	6.328005	-3.626519
C	2.957565	3.408464	0.670492
O	2.714736	4.584758	0.460197
O	4.216721	2.950521	0.859877
C	5.246077	3.94661	0.788194
H	5.257987	4.421241	-0.197042
H	5.089348	4.714794	1.54992
H	6.180582	3.413528	0.96771
C	-1.191616	0.606048	3.584719
H	-1.660575	-0.375836	3.426902
C	-0.285937	0.53902	4.792991
C	-0.46486	1.242431	5.911629
H	0.569826	-0.132445	4.713286
H	0.216654	1.158644	6.754028
H	-1.300245	1.930656	6.024624
H	-1.998411	1.318829	3.778325
O	-0.773186	3.253941	2.859764
C	0.1032	4.021838	3.547251
O	1.308648	3.966169	3.484314
O	-0.613737	4.860842	4.306314
C	0.174382	5.768528	5.093216
H	0.796111	6.394871	4.448347
H	-0.547586	6.376799	5.63854
H	0.815481	5.218039	5.786662

Isomer 0030040120



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

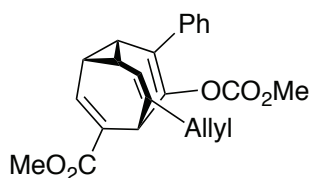
Sum of electronic and thermal Free Energies= -1265.388388 Hartree

Charge = 0 Multiplicity =1

C	-0.191425	0.057135	0.103681
C	-0.160814	0.101889	1.636864
C	1.151366	0.01118	0.869202
H	-0.508398	-0.900084	-0.29908
H	-0.474902	-0.826413	2.102077
H	1.59657	-0.979966	0.882897
C	2.131566	1.110568	0.820667
C	1.849985	2.424443	0.814096
H	3.175305	0.800858	0.78316
C	-0.558481	1.288886	2.41856
C	-0.317728	2.585209	2.141779
C	-0.592752	1.21196	-0.700032
C	-0.345369	2.506015	-0.402567
H	-1.142813	0.990662	-1.609478
C	0.415987	2.947731	0.839373
H	0.469502	4.034894	0.801993
C	-0.824798	3.591392	-1.296882
O	-0.694746	4.782446	-1.063264
O	-1.435017	3.139446	-2.418681
C	-1.934249	4.157659	-3.29681
H	-2.386061	3.624381	-4.134069
H	-2.679608	4.774817	-2.787757
H	-1.121003	4.800418	-3.644522
C	2.952887	3.46517	0.754984
H	3.914187	2.953871	0.604461
H	2.794852	4.117721	-0.115433
C	3.022469	4.31841	1.999321
C	2.830647	5.637554	2.031328
H	3.229002	3.782228	2.926231
H	2.881441	6.200321	2.959434
H	2.610841	6.205081	1.129205
O	-1.20075	0.954258	3.630152
C	-2.466579	0.486096	3.537364
O	-3.094656	0.309531	2.520245
O	-2.890761	0.242446	4.784896
C	-4.235618	-0.255327	4.868754
H	-4.939382	0.467125	4.447465
H	-4.329887	-1.203154	4.332189
H	-4.423369	-0.397083	5.93325
C	-0.748	3.703231	3.026077

C	-1.328636	4.857105	2.46855
C	-0.563791	3.660682	4.419714
C	-1.729435	5.918738	3.278568
H	-1.469169	4.927379	1.394022
C	-0.95731	4.7276	5.225755
H	-0.103074	2.789368	4.870942
C	-1.546262	5.860066	4.66078
H	-2.183244	6.79568	2.824183
H	-0.797791	4.673785	6.299759
H	-1.853701	6.690642	5.290908

Isomer 0030040210



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

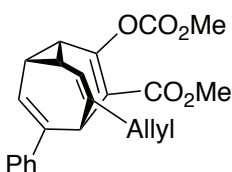
Sum of electronic and thermal Free Energies= -1265.387265 Hartree

Charge = 0 Multiplicity =1

C	0.006895	0.01509	-0.089202
C	-0.02058	0.013857	1.43198
C	1.337372	0.006003	0.680646
H	-0.215257	-0.950798	-0.53196
H	-0.267399	-0.952053	1.864641
H	1.835246	-0.959186	0.679224
C	2.251471	1.148671	0.721648
C	1.891285	2.450275	0.732397
H	3.309975	0.909992	0.769991
C	-0.465352	1.160532	2.247404
C	-0.285973	2.46144	1.961735
H	-0.971105	0.898109	3.175831
C	-0.449298	1.149628	-0.939491
C	-0.263279	2.427689	-0.563247
C	0.439125	2.902355	0.693182
H	0.440438	3.992489	0.65595
C	2.904034	3.5294	0.857165
O	2.632748	4.706119	1.020615
O	4.181248	3.080246	0.782961
C	5.191381	4.088102	0.92672
H	6.142888	3.562758	0.835258
H	5.094367	4.845896	0.1446
H	5.114962	4.576212	1.902345

C	-0.74808	3.558305	2.900731
H	0.119048	4.162757	3.203827
H	-1.153547	3.094449	3.811183
C	-1.787503	4.468996	2.290633
C	-1.631514	5.782448	2.115494
H	-2.706291	3.985642	1.961554
H	-2.412408	6.395594	1.672667
H	-0.718388	6.295753	2.410602
C	-1.135497	0.775968	-2.210282
C	-0.732568	1.309398	-3.445466
C	-2.184855	-0.157908	-2.196425
C	-1.362509	0.921662	-4.627748
H	0.080961	2.026868	-3.474952
C	-2.816295	-0.542671	-3.378589
H	-2.521716	-0.568484	-1.248228
C	-2.405698	-0.005777	-4.599966
H	-1.031843	1.341949	-5.574036
H	-3.632808	-1.259273	-3.343972
H	-2.89458	-0.30763	-5.522456
O	-0.686312	3.477648	-1.394163
C	-1.99821	3.815343	-1.37053
O	-2.862169	3.31375	-0.692406
O	-2.157792	4.81605	-2.246614
C	-3.503144	5.306417	-2.348666
H	-3.839984	5.707323	-1.388923
H	-3.465095	6.095475	-3.100119
H	-4.180746	4.508285	-2.662722

Isomer 0020040130



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

Sum of electronic and thermal Free Energies= -1265.383868 Hartree

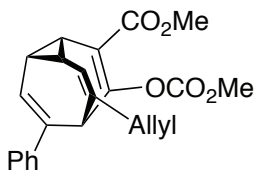
Charge = 0 Multiplicity = 1

C	0.092921	-0.032633	-0.124437
C	0.079122	-0.085849	1.413262
C	1.410711	-0.024968	0.65875
H	-0.148797	-0.98986	-0.578088
H	-0.163005	-1.057592	1.830518
H	1.934663	-0.97691	0.651008

C	2.297491	1.151692	0.696978
C	1.904144	2.435433	0.741217
H	3.364318	0.932304	0.675734
C	-0.438461	1.012399	2.242263
C	-0.299116	2.335518	2.00655
C	-0.385398	1.128648	-0.890961
C	-0.248847	2.429048	-0.553617
H	-0.905392	0.885844	-1.814819
C	0.431061	2.837209	0.755691
H	0.394985	3.923326	0.822896
C	-0.736446	3.497484	-1.465089
C	-1.354211	4.659572	-0.966579
C	-0.596994	3.367132	-2.85918
C	-1.831967	5.639828	-1.836012
H	-1.479911	4.7872	0.10449
C	-1.073679	4.349484	-3.725314
H	-0.084109	2.498208	-3.261952
C	-1.696292	5.491173	-3.2174
H	-2.31619	6.523679	-1.428528
H	-0.945687	4.228681	-4.79816
H	-2.064133	6.260611	-3.891167
C	2.915504	3.566394	0.779167
H	3.914929	3.15649	0.5772
H	2.694148	4.287317	-0.020111
C	2.925668	4.287249	2.107068
C	2.590385	5.565245	2.287732
H	3.215801	3.680534	2.965859
H	2.606919	6.0278	3.27101
H	2.286032	6.199783	1.457946
O	-1.080614	0.493082	3.36789
C	-2.410453	0.702166	3.539712
O	-3.158091	1.270916	2.784
O	-2.741224	0.124415	4.701265
C	-4.135994	0.217282	5.032705
H	-4.44325	1.263212	5.112488
H	-4.746131	-0.278052	4.272901
H	-4.236739	-0.287118	5.993907
C	-0.867782	3.413882	2.861456
O	-1.084525	4.544354	2.460939
O	-1.085139	3.055582	4.146584
C	-1.650152	4.082463	4.976775
H	-2.626175	4.391621	4.593377
H	-1.747838	3.631785	5.965081

H -0.990395 4.95299 5.013983

Isomer 0020040310



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

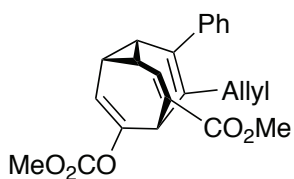
Sum of electronic and thermal Free Energies= -1265.383087 Hartree

Charge = 0 Multiplicity = 1

C	-0.055424	0.012757	-0.032601
C	-0.073226	0.038492	1.497315
C	1.265123	-0.000394	0.764138
H	-0.327907	-0.952055	-0.451331
H	-0.355329	-0.903397	1.952016
H	1.746444	-0.974032	0.795786
C	2.208692	1.129959	0.739099
C	1.888627	2.433812	0.704553
H	3.263486	0.85744	0.741993
C	-0.554809	1.191321	2.300812
C	-0.307415	2.471329	1.943051
C	-0.471609	1.155146	-0.861238
C	-0.278393	2.463186	-0.590574
H	-1.008167	0.895079	-1.771549
C	0.435043	2.901803	0.690503
H	0.44374	3.99189	0.721144
C	-0.747332	3.515872	-1.527306
C	-0.624349	3.349731	-2.918477
C	-1.33745	4.702229	-1.054004
C	-1.086572	4.323185	-3.802725
H	-0.136869	2.45862	-3.303638
C	-1.800531	5.674954	-1.938846
H	-1.461922	4.853202	0.015024
C	-1.677596	5.491126	-3.317394
H	-0.971875	4.174348	-4.873422
H	-2.263453	6.5776	-1.548471
H	-2.032778	6.253072	-4.005956
C	2.952208	3.514967	0.669413
H	3.93731	3.031768	0.603504
H	2.833917	4.123437	-0.239255
C	2.91634	4.422672	1.876127
C	2.748356	5.745564	1.826068

H	3.01549	3.928513	2.84186
H	2.734442	6.353983	2.726812
H	2.630599	6.273818	0.881562
C	-1.314855	0.763596	3.517882
O	-1.42889	-0.401614	3.852983
O	-1.896224	1.767471	4.208935
C	-2.63679	1.357549	5.369363
H	-3.049136	2.277225	5.785595
H	-3.437326	0.667892	5.0903
H	-1.979111	0.866011	6.091058
O	-0.787775	3.564944	2.658972
C	-0.197141	3.887899	3.836873
O	0.767571	3.355957	4.328386
O	-0.872456	4.929457	4.335651
C	-0.350278	5.435786	5.574098
H	-0.358773	4.657735	6.341652
H	0.67297	5.796845	5.440877
H	-1.012294	6.256546	5.85089

Isomer 0010030240



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

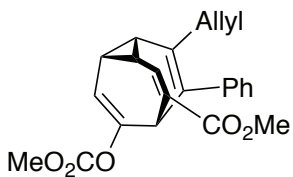
Sum of electronic and thermal Free Energies= -1265.384350 Hartree

Charge = 0 Multiplicity =1

C	0.025979	0.011761	0.001742
C	0.029139	-0.052439	1.544267
C	1.351102	0.017528	0.751969
H	-0.217202	-0.949013	-0.441084
H	-0.19584	-1.038039	1.941
H	1.872791	-0.935279	0.726093
C	2.267547	1.174397	0.788887
C	1.841241	2.444331	0.818683
H	3.326828	0.960073	0.784511
C	-0.45808	1.050322	2.370427
C	-0.323681	2.362892	2.085543
H	-0.982098	0.773297	3.280449
C	-0.506806	1.158722	-0.790367
C	-0.335305	2.458803	-0.450481
C	0.38561	2.86694	0.838069

H	0.381862	3.95565	0.899232
O	2.650915	3.586179	0.824342
C	3.999127	3.568419	0.873486
O	4.733383	2.608592	0.931684
O	4.393167	4.850065	0.846819
C	5.815984	5.038807	0.896444
H	6.298554	4.557875	0.041497
H	5.962308	6.118462	0.862077
H	6.227405	4.624639	1.820747
C	-0.899215	3.403803	2.973789
O	-0.903476	4.597456	2.720755
O	-1.438618	2.903451	4.11132
C	-2.0292	3.874251	4.986808
H	-2.843843	4.403035	4.484367
H	-1.282873	4.603513	5.313128
C	-1.239994	0.737752	-2.025959
C	-2.582587	1.091889	-2.234042
C	-0.609112	-0.071744	-2.98601
C	-3.267538	0.660939	-3.371181
H	-3.087604	1.707809	-1.49616
C	-1.292026	-0.500025	-4.124033
H	0.431494	-0.35376	-2.844736
C	-2.625738	-0.136007	-4.320383
H	-4.30778	0.943983	-3.510912
H	-0.780849	-1.116356	-4.859215
H	-3.160122	-0.472397	-5.204897
C	-0.773963	3.627224	-1.318475
H	0.096334	4.296872	-1.419942
H	-1.034693	3.293348	-2.325777
C	-1.918509	4.426411	-0.732373
C	-3.035534	4.735121	-1.39294
H	-1.791315	4.769153	0.294498
H	-3.823238	5.327063	-0.933799
H	-3.202862	4.415434	-2.419858
H	-2.408168	3.306847	5.837685

Isomer 0010030420



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

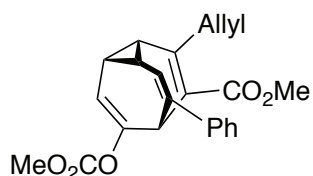
Sum of electronic and thermal Free Energies= -1265.382648 Hartree

Charge = 0 Multiplicity =1

C	-0.150329	0.046267	-0.05144
C	-0.125301	0.030855	1.469081
C	1.20458	-0.0152	0.682586
H	-0.428474	-0.906612	-0.493476
H	-0.369784	-0.94122	1.889713
H	1.671963	-0.995414	0.668655
C	2.147484	1.100218	0.69549
C	1.814165	2.407441	0.739757
H	3.201337	0.838231	0.683189
C	-0.55569	1.157426	2.340681
C	-0.382266	2.467428	2.032872
C	-0.592457	1.203363	-0.855257
C	-0.368742	2.473204	-0.491214
H	-1.125372	0.988478	-1.770463
C	0.37235	2.895485	0.761956
H	0.409034	3.983906	0.745194
O	-0.766413	3.614306	-1.195253
C	-1.471558	3.597205	-2.345127
O	-1.869905	2.637276	-2.964992
O	-1.658265	4.879186	-2.69111
C	-2.400754	5.068346	-3.90552
H	-3.399825	4.633245	-3.818058
H	-2.463428	6.148706	-4.036598
H	-1.881532	4.608253	-4.75049
C	2.8636	3.456286	0.804332
O	2.641385	4.642318	0.98251
O	4.120282	2.970684	0.656018
C	5.16724	3.947275	0.74339
H	6.095364	3.393181	0.597898
H	5.049396	4.709545	-0.031381
H	5.160722	4.434746	1.722268
C	-1.17756	0.678155	3.649158
H	-0.491319	-0.073096	4.075017
H	-1.237134	1.492246	4.374534
C	-2.537652	0.035236	3.491107
C	-3.605758	0.315401	4.238975
H	-2.626215	-0.719508	2.708411
H	-4.555202	-0.192643	4.091473
H	-3.570636	1.062196	5.029622
C	-0.89867	3.587442	2.872988
C	-2.246681	3.64165	3.267846

C	-0.055703	4.650554	3.246629
C	-2.729204	4.705636	4.030942
H	-2.921853	2.849291	2.960825
C	-0.538323	5.709832	4.013584
H	0.982276	4.653673	2.927167
C	-1.876195	5.74182	4.412276
H	-3.77762	4.72765	4.317995
H	0.134362	6.515685	4.29567
H	-2.252042	6.571869	5.004784

Isomer 0010020430



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

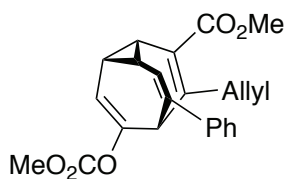
Sum of electronic and thermal Free Energies= -1265.382086 Hartree

Charge = 0 Multiplicity = 1

C	0.008357	0.003116	-0.084832
C	-0.043538	0.010337	1.445523
C	1.314427	-0.002332	0.71547
H	-0.247022	-0.964904	-0.507134
H	-0.310701	-0.95613	1.862391
H	1.807042	-0.969988	0.754687
C	2.242501	1.137673	0.740283
C	1.91019	2.445735	0.715648
H	3.29638	0.872829	0.791371
C	-0.528496	1.137923	2.270634
C	-0.352639	2.441617	1.927494
C	-0.423416	1.132033	-0.931331
C	-0.229205	2.412459	-0.590518
H	-0.905807	0.887418	-1.866985
C	0.441084	2.876866	0.687829
H	0.41223	3.964336	0.664913
O	-0.611113	3.532816	-1.338182
C	-1.167013	3.479701	-2.565769
O	-1.431468	2.501249	-3.226538
O	-1.383206	4.750808	-2.936111
C	-1.976236	4.901609	-4.235196
H	-2.085843	5.976998	-4.376212
H	-1.327795	4.477406	-5.00636
H	-2.950629	4.407423	-4.273908

C	2.963203	3.494211	0.69394
C	4.151002	3.298776	-0.034916
C	2.812808	4.699306	1.404806
C	5.159937	4.259915	-0.038114
H	4.267872	2.39596	-0.627688
C	3.824817	5.658975	1.400059
H	1.908882	4.878222	1.979466
C	5.00269	5.445545	0.682188
H	6.063914	4.088339	-0.617195
H	3.69011	6.578313	1.964302
H	5.786112	6.198852	0.675824
C	-1.212246	0.659271	3.548985
H	-1.236775	1.456865	4.292843
H	-0.614511	-0.161906	3.965505
C	-2.617492	0.169543	3.290878
C	-3.0435	-1.075616	3.506872
H	-3.302062	0.91811	2.894675
H	-4.069757	-1.371366	3.30557
H	-2.38569	-1.846579	3.904203
C	-0.862512	3.598039	2.718126
O	-0.337932	4.699397	2.731134
O	-2.016409	3.356681	3.388856
C	-2.531522	4.469381	4.140252
H	-3.446871	4.104092	4.606893
H	-1.813128	4.790549	4.899013
H	-2.745289	5.310983	3.476659

Isomer 0010020340



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

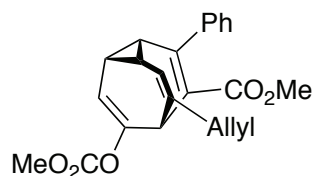
Sum of electronic and thermal Free Energies= -1265.380822 Hartree

Charge = 0 Multiplicity = 1

C	0.086924	0.009209	-0.097744
C	0.034147	0.00209	1.436042
C	1.386705	0.002134	0.694757
H	-0.171032	-0.945976	-0.539303
H	-0.232853	-0.963404	1.856601
H	1.884133	-0.963638	0.703254
C	2.327575	1.137205	0.737915

C	1.929399	2.414513	0.72397
H	3.381863	0.901318	0.780471
C	-0.445417	1.143813	2.22794
C	-0.281488	2.453057	1.940876
H	-0.963607	0.882609	3.148535
C	-0.384551	1.150437	-0.926328
C	-0.259718	2.45692	-0.578823
C	0.489245	2.88013	0.688787
H	0.535392	3.968826	0.668398
O	2.766893	3.535444	0.820339
C	4.102036	3.502033	0.631661
O	4.79116	2.552637	0.338587
O	4.542094	4.754382	0.830458
C	5.959449	4.920219	0.667983
H	6.14958	5.974052	0.872274
H	6.504898	4.287438	1.373022
C	-0.830464	3.509438	2.827706
C	-2.093301	3.36152	3.429695
C	-0.102363	4.682172	3.101981
C	-2.601835	4.338275	4.284136
H	-2.688893	2.48216	3.201434
C	-0.611511	5.658184	3.957525
H	0.883846	4.819298	2.666537
C	-1.863227	5.49205	4.553121
H	-3.584119	4.203331	4.729783
H	-0.02436	6.549676	4.162554
H	-2.261631	6.256609	5.214592
C	-1.076817	0.668959	-2.165874
O	-1.588744	-0.430341	-2.270871
O	-1.033381	1.539435	-3.204479
C	-1.673858	1.083749	-4.408105
H	-2.732563	0.87879	-4.229423
H	-1.19417	0.172354	-4.774093
C	-0.860434	3.63724	-1.328596
H	-1.670068	3.310908	-1.983303
H	-1.290011	4.323395	-0.586708
C	0.17929	4.372266	-2.142077
C	0.56983	5.62895	-1.925419
H	0.627206	3.793279	-2.948501
H	1.326857	6.106242	-2.542148
H	0.142475	6.233184	-1.127365
H	6.262631	4.665972	-0.351094
H	-1.55434	1.896355	-5.125375

Isomer 0010040230



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

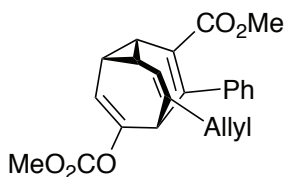
Sum of electronic and thermal Free Energies= -1265.379638 Hartree

Charge = 0 Multiplicity = 1

C	0.041557	0.01453	0.031306
C	0.044273	0.016097	1.570043
C	1.369686	0.026468	0.792267
H	-0.215757	-0.953791	-0.38863
H	-0.206253	-0.95177	1.992021
H	1.876621	-0.934853	0.804173
C	2.286614	1.182009	0.784985
C	1.930275	2.476757	0.784406
H	3.347725	0.93464	0.773788
C	-0.451882	1.145835	2.393752
C	-0.239557	2.450453	2.079515
C	-0.443126	1.144058	-0.783785
C	-0.259959	2.427118	-0.445181
H	-0.983713	0.896734	-1.687132
C	0.464018	2.900292	0.797402
H	0.413509	3.989591	0.782844
O	-0.655942	3.530208	-1.209255
C	-1.620391	3.483197	-2.152064
O	-2.292854	2.534536	-2.484258
O	-1.702911	4.718327	-2.668865
C	-2.698239	4.870911	-3.692354
H	-2.628644	5.912633	-4.006067
H	-2.493791	4.201686	-4.532357
H	-3.694027	4.655486	-3.296087
C	2.961307	3.588913	0.792253
H	3.957248	3.151103	0.636955
H	2.774292	4.274224	-0.046459
C	2.949442	4.373544	2.083421
C	2.628729	5.663543	2.193211
H	3.205737	3.805111	2.978287
H	2.626606	6.172556	3.153401
H	2.356855	6.262117	1.326151
C	-1.282768	0.719198	3.560407

C	-2.612057	1.150905	3.687224
C	-0.774086	-0.175192	4.514918
C	-3.404225	0.716242	4.749619
H	-3.025991	1.820948	2.938563
C	-1.563283	-0.603498	5.581629
H	0.253978	-0.518615	4.43208
C	-2.881872	-0.160037	5.702487
H	-4.433513	1.056724	4.827506
H	-1.147423	-1.28434	6.31989
H	-3.499121	-0.500083	6.529777
C	-0.700208	3.589987	2.929959
O	-1.144693	4.630087	2.480436
O	-0.513157	3.382445	4.25184
C	-0.981029	4.434443	5.107381
H	-2.063653	4.556646	5.009893
H	-0.723353	4.122051	6.11993
H	-0.493456	5.38024	4.856915

Isomer 0010040320



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

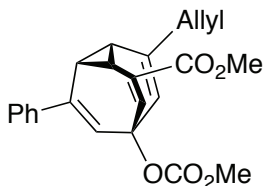
Sum of electronic and thermal Free Energies= -1265.378156 Hartree

Charge = 0 Multiplicity = 1

C	-0.065655	0.010495	0.029978
C	-0.058089	0.012283	1.560307
C	1.267923	0.03474	0.793136
H	-0.305332	-0.956935	-0.402353
H	-0.280282	-0.948762	2.010255
H	1.784031	-0.921373	0.801406
C	2.170499	1.198055	0.780397
C	1.804183	2.490421	0.782563
H	3.234023	0.963065	0.749818
C	-0.559901	1.143802	2.378423
C	-0.363482	2.460016	2.105466
C	-0.567455	1.141932	-0.774354
C	-0.400041	2.42439	-0.425247
H	-1.103853	0.898537	-1.680685
C	0.333954	2.903997	0.810658
H	0.300394	3.994039	0.788171

O	-0.880241	3.542015	-1.126686
C	-1.523566	3.485391	-2.310671
O	-1.787212	2.509306	-2.974308
O	-1.828052	4.752399	-2.633857
C	-2.524471	4.898119	-3.881743
H	-3.472722	4.354715	-3.859418
H	-2.698541	5.968931	-3.988805
H	-1.915592	4.523476	-4.708779
C	2.830704	3.606711	0.727827
H	2.664033	4.216552	-0.172409
H	3.828692	3.157109	0.627377
C	2.801965	4.508844	1.938134
C	2.561713	5.820201	1.905823
H	2.981009	4.019449	2.895959
H	2.545973	6.42173	2.810464
H	2.371999	6.343057	0.970174
C	-1.311397	0.664443	3.586749
O	-0.997949	-0.320296	4.230022
O	-2.419614	1.388256	3.846001
C	-3.153269	0.990857	5.013504
H	-2.539669	1.108695	5.911247
H	-4.017321	1.654697	5.05293
H	-3.469217	-0.052616	4.933861
C	-0.729381	3.557476	3.041786
C	-0.288214	3.542383	4.375216
C	-1.471073	4.664276	2.596573
C	-0.596442	4.59007	5.242126
H	0.313681	2.708056	4.725548
C	-1.786805	5.707103	3.465638
H	-1.815959	4.699422	1.566342
C	-1.350396	5.675189	4.791929
H	-0.238775	4.562138	6.268269
H	-2.373993	6.547682	3.105059
H	-1.589382	6.493239	5.466284

Isomer 0200300401



RB3LYP/6-31G(d) Geometry
Imaginary frequency: none

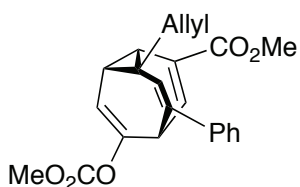
Sum of electronic and thermal Free Energies= -1265.386257 Hartree

Charge = 0 Multiplicity =1

C	0.015084	0.051447	0.035569
C	0.017705	0.071605	1.570298
C	1.341587	0.073836	0.803547
H	-0.240842	-0.903616	-0.409158
H	-0.206755	-0.892195	2.015614
H	1.843171	-0.889516	0.82745
C	2.281027	1.218498	0.764491
C	1.903585	2.505899	0.758138
H	2.653441	3.28972	0.714794
C	-0.477007	1.221386	2.369532
C	-0.292906	2.510021	2.022146
H	-0.73196	3.294223	2.628661
C	-0.453804	1.197988	-0.768366
C	-0.266784	2.495278	-0.456044
H	-0.649428	3.274288	-1.105636
C	0.458695	2.965757	0.787752
C	-1.188599	0.821965	-2.01401
O	-1.400046	-0.325799	-2.359909
O	-1.603205	1.889714	-2.732481
C	-2.314869	1.577472	-3.938659
H	-2.568272	2.539985	-4.384211
H	-1.68648	0.993331	-4.616388
H	-3.220369	1.006901	-3.715207
C	3.756919	0.851035	0.720048
H	3.954009	0.213478	-0.153605
H	4.342367	1.770421	0.584725
C	4.222081	0.137482	1.966841
C	4.761462	-1.082035	1.993708
H	4.085383	0.686341	2.899136
H	5.081599	-1.545672	2.922997
H	4.912851	-1.661264	1.08448
C	-1.23246	0.902402	3.613684
C	-1.018785	1.644961	4.787533
C	-2.179926	-0.135053	3.645937
C	-1.738659	1.368777	5.949188
H	-0.263692	2.425989	4.787823
C	-2.900374	-0.40994	4.807699
H	-2.374648	-0.714049	2.747118
C	-2.683076	0.340704	5.96458
H	-1.55144	1.950464	6.84815
H	-3.636891	-1.209322	4.80675

H	-3.240791	0.122526	6.871383
O	0.396805	4.419071	0.673208
C	0.939808	5.165211	1.64911
O	1.490382	4.77122	2.653633
O	0.761242	6.452219	1.309438
C	1.283287	7.397288	2.25639
H	1.060847	8.377935	1.835154
H	0.797304	7.277968	3.228342
H	2.361928	7.266955	2.3773

Isomer 0014020300



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

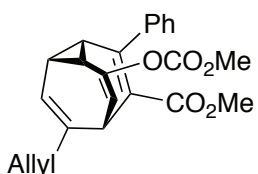
Sum of electronic and thermal Free Energies= -1265.386926 Hartree

Charge = 0 Multiplicity = 1

C	-0.030799	0.039686	-0.080574
C	-0.013527	0.031839	1.459619
C	1.304856	0.032249	0.66145
H	-0.304221	-0.910598	-0.527295
H	1.79161	-0.939654	0.649216
C	2.273864	1.147314	0.652649
C	1.922566	2.439932	0.648705
H	3.321061	0.878868	0.654815
C	-0.424758	1.220201	2.236899
C	-0.234347	2.524813	1.943426
H	-0.925521	0.986267	3.174151
C	-0.506941	1.193487	-0.86937
C	-0.280531	2.484272	-0.556983
H	-0.690811	3.254787	-1.201044
C	0.493815	2.944596	0.662966
H	0.542844	4.033185	0.628502
C	-1.312493	0.829529	-2.073575
O	-1.598281	-0.31287	-2.383294
O	-1.703682	1.901315	-2.800679
C	-2.487385	1.598721	-3.963708
H	-2.707453	2.562002	-4.425231
H	-1.925242	0.961978	-4.6521
H	-3.412141	1.086866	-3.683654

O	2.793258	3.538369	0.671454
C	4.138459	3.450318	0.603677
O	4.81808	2.455557	0.500975
O	4.600685	4.70823	0.669741
C	6.031579	4.821773	0.606727
H	6.236798	5.890174	0.675085
H	6.497178	4.286656	1.438438
H	6.408412	4.417614	-0.336451
C	-0.397705	-1.301518	2.114703
H	0.020885	-2.117973	1.509353
H	0.071794	-1.371366	3.105253
C	-1.886652	-1.48975	2.239307
C	-2.536912	-1.708478	3.383285
H	-2.448411	-1.432595	1.306017
H	-3.615081	-1.841965	3.412703
H	-2.013666	-1.771959	4.335749
C	-0.720598	3.589537	2.857695
C	-1.957897	3.465788	3.515372
C	0.044171	4.745035	3.101376
C	-2.406139	4.450716	4.393679
H	-2.580755	2.599216	3.312987
C	-0.404774	5.729395	3.980864
H	1.011658	4.863105	2.620605
C	-1.631696	5.587803	4.631546
H	-3.369898	4.335394	4.883106
H	0.209598	6.607853	4.160774
H	-1.983641	6.358645	5.311833

Isomer 0040100230



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

Sum of electronic and thermal Free Energies= -1265.378885 Hartree

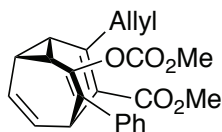
Charge = 0 Multiplicity = 1

C	0.026352	0.025736	0.010486
C	-0.005933	0.033776	1.538772
C	1.342404	0.01625	0.80323
H	-0.221	-0.92382	-0.452993
H	-0.27018	-0.92874	1.96882
H	1.822253	-0.956982	0.793765

C	2.316812	1.137062	0.813555
C	1.947194	2.443656	0.841712
C	-0.476945	1.188566	2.327214
C	-0.280812	2.482236	2.024658
C	-0.400586	1.181061	-0.799519
C	-0.204551	2.470301	-0.503268
C	0.489913	2.904304	0.777085
H	0.5212	3.994332	0.755562
C	-0.799521	3.592791	2.91782
H	-1.417491	4.284319	2.327777
H	-1.450328	3.156162	3.688252
C	0.315038	4.368874	3.580119
C	0.571807	5.662468	3.380643
H	0.951724	3.792194	4.252154
H	1.394924	6.166274	3.880396
H	-0.034024	6.269908	2.711239
H	-1.035338	0.939834	3.228927
O	-0.996262	0.699836	-1.978072
H	-0.551021	3.241076	-1.177201
C	-1.858897	1.423152	-2.722119
O	-2.255688	2.54724	-2.52361
O	-2.212426	0.640499	-3.7542
C	-3.136251	1.246986	-4.671407
H	-3.308274	0.496147	-5.442891
H	-4.072068	1.499301	-4.165752
H	-2.708136	2.153935	-5.106435
C	3.741467	0.697804	0.712009
C	4.556226	1.148531	-0.3382
C	4.276027	-0.224467	1.625287
C	5.872775	0.705085	-0.460394
H	4.146206	1.841118	-1.068299
C	5.594508	-0.662506	1.507677
H	3.660593	-0.583103	2.446522
C	6.397982	-0.200146	0.463431
H	6.485756	1.061233	-1.284327
H	5.994898	-1.365618	2.233508
H	7.423247	-0.547395	0.367455
C	2.924398	3.57386	0.899083
O	2.792215	4.611426	0.276604
O	3.938216	3.36192	1.766513
C	4.915298	4.410393	1.832057
H	4.445469	5.356823	2.112469
H	5.631232	4.093824	2.591314

H 5.413198 4.534136 0.866042

Isomer 0000120430



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

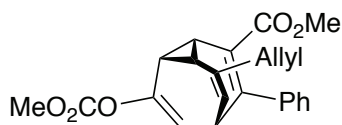
Sum of electronic and thermal Free Energies= -1265.377557 Hartree

Charge = 0 Multiplicity = 1

C	0.132162	0.044903	0.106021
C	0.172713	0.076476	1.646075
C	1.471991	0.114144	0.84932
H	-0.094408	-0.937543	-0.298999
H	-0.009493	-0.895467	2.094485
H	2.018433	-0.82333	0.868164
C	2.368507	1.282966	0.788117
C	2.023586	2.583588	0.769932
C	-0.338269	1.188382	2.483601
C	-0.130994	2.497656	2.173143
C	-0.387783	1.172013	-0.683796
C	-0.222494	2.46173	-0.361803
H	-0.939249	0.911047	-1.585023
H	-0.64397	3.227921	-1.008478
C	0.532557	2.9423	0.863498
H	0.467813	4.02757	0.859999
O	3.725683	0.917612	0.650188
C	4.365905	0.529538	1.775213
O	3.889813	0.448587	2.88381
O	5.628351	0.240435	1.434951
C	6.459141	-0.181489	2.528679
H	6.524993	0.604311	3.285511
H	6.059946	-1.089971	2.987289
H	7.437868	-0.372356	2.088167
C	3.002631	3.697349	0.645398
C	2.84616	4.865623	1.414256
C	4.080513	3.640245	-0.25748
C	3.746235	5.924364	1.300985
H	2.014676	4.951479	2.107048
C	4.973809	4.703608	-0.374384
H	4.211353	2.760656	-0.876949
C	4.815001	5.849407	0.407047
H	3.606514	6.812066	1.912407

H	5.793484	4.637229	-1.085316
H	5.512575	6.677745	0.314822
C	-1.132946	0.672756	3.671378
H	-1.809514	1.437011	4.056068
H	-1.776132	-0.141217	3.299487
C	-0.311621	0.12552	4.819708
C	1.015792	0.149759	4.941136
H	-0.909885	-0.327257	5.61207
H	1.499233	-0.274438	5.817594
H	1.672946	0.579003	4.190149
C	-0.532873	3.658494	3.024822
O	-0.54332	4.813757	2.627478
O	-0.831257	3.357285	4.309341
C	-1.165527	4.47967	5.140307
H	-1.361725	4.058982	6.127067
H	-0.332483	5.18604	5.181924
H	-2.049109	4.997107	4.757265

Isomer 0100400320



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

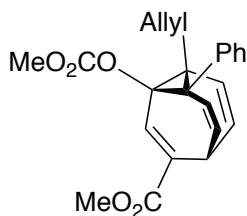
Sum of electronic and thermal Free Energies= -1265.378889 Hartree

Charge = 0 Multiplicity =1

C	0.00746	0.039411	-0.077758
C	-0.008741	0.066235	1.454917
C	1.323463	0.019322	0.698629
H	-0.272828	-0.921706	-0.493349
H	-0.290264	-0.888695	1.890314
H	1.824689	-0.942999	0.719059
C	2.271094	1.149421	0.667658
C	1.951421	2.447896	0.61871
H	2.729423	3.19658	0.588325
C	-0.465724	1.233055	2.242354
C	-0.247206	2.504762	1.869501
H	-0.62103	3.30944	2.499909
C	-0.429394	1.167079	-0.939562
C	-0.262228	2.483126	-0.645032
C	0.504002	2.914743	0.614856
H	0.531854	4.005832	0.603271
O	3.571707	0.618785	0.698263

C	4.697285	1.35015	0.58129
O	4.8036	2.546633	0.437536
O	5.71842	0.481873	0.654297
C	7.019531	1.080422	0.547671
H	7.131891	1.589679	-0.413104
H	7.180823	1.798932	1.355656
H	7.722941	0.251297	0.626257
C	-1.219705	0.911135	3.523641
H	-1.43426	1.853334	4.046274
H	-0.580656	0.315049	4.191025
C	-2.508882	0.163117	3.281978
C	-2.802602	-1.036786	3.784668
H	-3.229574	0.665284	2.63555
H	-3.749082	-1.528713	3.577129
H	-2.108345	-1.571021	4.430897
C	-1.11133	0.680653	-2.184292
O	-1.768324	-0.343373	-2.237172
O	-0.868988	1.449864	-3.265293
C	-1.53208	1.042299	-4.470609
H	-1.212526	1.754495	-5.23187
H	-1.241534	0.024827	-4.745306
H	-2.61784	1.079168	-4.344176
C	-0.867415	3.594716	-1.429121
C	-2.255913	3.662506	-1.626164
C	-0.070383	4.641286	-1.921031
C	-2.828367	4.733955	-2.311066
H	-2.886896	2.873687	-1.225558
C	-0.641395	5.707006	-2.614752
H	1.006811	4.606031	-1.778508
C	-2.023151	5.758526	-2.8115
H	-3.906177	4.771157	-2.447242
H	-0.005671	6.499143	-3.001743
H	-2.468701	6.59412	-3.344638

Isomer 1032004000



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

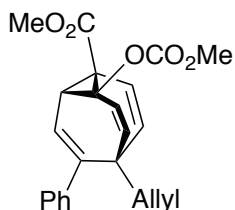
Sum of electronic and thermal Free Energies= -1265.366911 Hartree

Charge = 0 Multiplicity =1

C	-0.020703	0.007667	-0.043349
C	-0.024154	-0.024079	1.50399
C	1.325588	-0.001545	0.759774
C	2.188229	1.209258	0.809034
C	1.806127	2.491181	0.876274
H	3.254223	0.993802	0.795734
H	2.574684	3.260727	0.905813
C	-0.538066	1.087591	2.324414
C	-0.386069	2.405664	2.095388
H	-1.103908	0.783363	3.197477
C	-0.476638	1.238577	-0.758524
C	-0.328396	2.516374	-0.383873
H	-0.988185	1.03687	-1.696472
H	-0.726634	3.294896	-1.031278
C	0.363156	2.95283	0.892117
H	0.335673	4.040698	0.96144
C	-0.405772	-1.232514	-0.822484
C	-1.569676	-1.961833	-0.544265
C	0.347449	-1.582432	-1.953899
C	-1.951218	-3.029755	-1.358052
H	-2.175285	-1.699389	0.315676
C	-0.033307	-2.64905	-2.768148
H	1.234463	-1.00563	-2.20315
C	-1.183803	-3.380578	-2.469348
H	-2.854887	-3.585843	-1.122449
H	0.567275	-2.904604	-3.637285
H	-1.482904	-4.212804	-3.101018
C	2.142971	-1.306647	0.732327
H	1.466332	-2.163614	0.808413
H	2.627077	-1.391415	-0.248354
C	3.197086	-1.391159	1.809501
C	4.482092	-1.665656	1.57806
H	2.856614	-1.224298	2.829841
H	5.203744	-1.74239	2.387172
H	4.862888	-1.831859	0.571589
O	-0.441531	-1.292138	2.018162
C	0.001968	-1.651715	3.24137
O	0.724473	-1.008997	3.969111
O	-0.514449	-2.85801	3.507908
C	-0.143422	-3.399175	4.787277
H	-0.475667	-2.740863	5.594009
H	-0.647229	-4.363922	4.846403

H	0.940222	-3.527162	4.849913
C	-0.979635	3.410883	3.018488
O	-0.871077	4.615321	2.874006
O	-1.662952	2.858864	4.049602
C	-2.242098	3.794649	4.969239
H	-2.742327	3.188636	5.725537
H	-1.467166	4.416024	5.426251
H	-2.960139	4.44285	4.459397

Isomer 0021003004



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

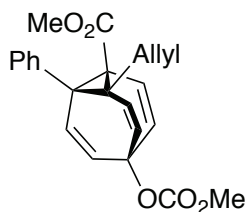
Sum of electronic and thermal Free Energies= -1265.364395 Hartree

Charge = 0 Multiplicity = 1

C	0.037313	0.003511	-0.062207
C	0.166264	-0.033063	1.482612
C	1.416951	-0.023075	0.542687
H	-0.246686	-0.970673	-0.448915
C	2.329687	1.132894	0.473186
C	1.981828	2.425696	0.467834
H	3.377788	0.866007	0.365061
H	2.778884	3.158284	0.353546
C	-0.173012	1.162898	2.284396
C	-0.039229	2.444795	1.919067
H	-0.60002	0.951654	3.258184
H	-0.360355	3.203917	2.628199
C	-0.508142	1.158178	-0.799201
C	-0.302404	2.470563	-0.570252
H	-1.142215	0.890513	-1.642125
C	0.564843	2.965862	0.619688
C	-0.963429	3.448999	-1.490348
C	-2.34369	3.685185	-1.400458
C	-0.233765	4.12336	-2.483134
C	-2.975949	4.574284	-2.272037
H	-2.91957	3.165043	-0.639847
C	-0.864603	5.010592	-3.354943
H	0.831838	3.933003	-2.582755
C	-2.238079	5.24145	-3.250267

H	-4.046367	4.74279	-2.186275
H	-0.283789	5.516256	-4.122013
H	-2.729314	5.932781	-3.929738
O	2.090532	-1.248529	0.299343
C	2.766303	-1.80448	1.327512
O	2.811742	-1.395838	2.465478
O	3.382799	-2.893001	0.852074
C	4.124823	-3.634822	1.831872
H	4.580832	-4.458999	1.28305
H	4.891995	-3.007103	2.292552
H	3.457716	-4.016487	2.609461
C	-0.164768	-1.374381	2.083347
O	-0.216865	-2.41946	1.465035
O	-0.396332	-1.295274	3.408796
C	-0.653407	-2.547899	4.06106
H	-1.515468	-3.047932	3.612332
H	0.220982	-3.199059	3.981872
H	-0.850537	-2.297194	5.103711
C	0.612684	4.521201	0.681505
H	1.087621	4.886293	-0.239031
H	-0.409822	4.913812	0.675964
C	1.351635	5.076008	1.870771
C	0.853302	5.977112	2.719212
H	2.370062	4.719224	2.027066
H	1.436953	6.364221	3.550208
H	-0.156613	6.368487	2.611048

Isomer 2004003001



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

Sum of electronic and thermal Free Energies= -1265.354441 Hartree

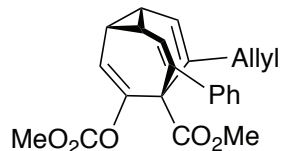
Charge = 0 Multiplicity = 1

C	0.047234	0.019403	0.015179
C	0.030675	0.021487	1.57303
C	1.391066	0.044279	0.834864
C	2.247948	1.268139	0.820543
C	1.883677	2.555366	0.788738
H	3.313608	1.055975	0.841092

H	2.649106	3.324504	0.783783
C	-0.446279	1.237657	2.291747
C	-0.281539	2.528667	1.985032
H	-1.012761	1.017358	3.192992
H	-0.691039	3.302164	2.628904
C	-0.413407	1.204129	-0.765172
C	-0.264238	2.502209	-0.481069
H	-0.944542	0.960169	-1.678757
H	-0.678886	3.243926	-1.155729
C	0.444658	3.015681	0.751821
C	-0.252881	-1.272488	-0.720407
O	-0.669235	-2.313279	-0.258051
O	0.006713	-1.133199	-2.045015
C	-0.251508	-2.299483	-2.845059
H	-0.011534	-2.007366	-3.867766
H	0.380173	-3.130755	-2.521196
H	-1.299903	-2.597633	-2.76414
C	2.271343	-1.190859	0.84395
C	2.753395	-1.705754	2.056093
C	2.755639	-1.738696	-0.352024
C	3.662797	-2.763532	2.073771
H	2.417861	-1.270491	2.992765
C	3.666094	-2.796822	-0.336531
H	2.423985	-1.327267	-1.300356
C	4.118831	-3.31694	0.876236
H	4.017918	-3.151754	3.02477
H	4.027279	-3.208741	-1.275352
H	4.826982	-4.141078	0.88884
C	-0.377309	-1.243393	2.361522
H	0.044869	-1.145652	3.370627
H	0.057055	-2.133483	1.90945
C	-1.868493	-1.424773	2.466622
C	-2.553763	-1.440747	3.611416
H	-2.39034	-1.571142	1.523047
H	-3.628971	-1.598551	3.632721
H	-2.064717	-1.31022	4.575549
O	0.355198	4.466056	0.843648
C	0.912244	5.207435	-0.127354
O	1.504181	4.806758	-1.105304
O	0.694912	6.496387	0.181436
C	1.23177	7.434511	-0.764072
H	0.974299	8.417972	-0.370216
H	2.316548	7.324673	-0.843515

H 0.784392 7.286883 -1.750571

Isomer 0010020043



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

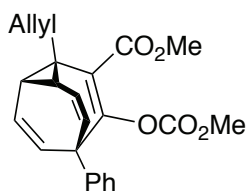
Sum of electronic and thermal Free Energies= -1265.349906 Hartree

Charge = 0 Multiplicity = 1

C	-0.122514	-0.136977	-0.099993
C	-0.318484	-0.104522	1.404411
C	1.102449	-0.250768	0.796435
H	-0.418342	-1.07301	-0.565756
H	-0.712031	-1.023037	1.830277
H	1.520554	-1.250102	0.873909
C	2.090439	0.824176	0.927806
C	1.885587	2.149425	0.876081
H	3.106445	0.513136	1.156117
C	-0.677596	1.104741	2.150377
C	-0.336176	2.389664	1.910793
H	-1.200712	0.914457	3.085292
C	-0.350684	1.044057	-0.942506
C	-0.111971	2.341542	-0.682135
H	-0.758962	0.81049	-1.924212
C	0.510575	2.821349	0.671071
C	-0.455993	3.327413	-1.797825
H	-0.85585	2.72242	-2.623042
H	-1.269209	3.992158	-1.487099
C	0.686116	4.156284	-2.34686
C	0.544722	5.395932	-2.819483
H	1.662123	3.67635	-2.375488
H	1.381456	5.938667	-3.250942
H	-0.41351	5.913646	-2.80313
O	2.980763	2.936004	1.257469
C	3.692693	3.533773	0.272697
O	3.572596	3.341113	-0.913992
O	4.593548	4.325454	0.861302
C	5.425037	5.057058	-0.051088
H	6.100811	5.637627	0.577557
H	5.988479	4.375019	-0.693495
H	4.815768	5.718538	-0.67225

C	-0.656803	3.377592	2.988047
C	-1.97868	3.535417	3.433076
C	0.35582	4.116069	3.62546
C	-2.283055	4.401645	4.483199
H	-2.771041	2.981885	2.936955
C	0.04832	4.985749	4.672565
H	1.389361	4.001398	3.311708
C	-1.270556	5.132446	5.106982
H	-3.314579	4.510058	4.809011
H	0.847306	5.540431	5.157847
H	-1.506312	5.809068	5.924103
C	0.573773	4.370816	0.648929
O	1.558781	5.072717	0.665307
O	-0.674994	4.876099	0.61841
C	-0.757103	6.310779	0.66548
H	-0.229262	6.74743	-0.185428
H	-1.822203	6.539765	0.624609
H	-0.320368	6.680563	1.596527

Isomer 0000004312



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

Sum of electronic and thermal Free Energies= -1265.349750 Hartree

Charge = 0 Multiplicity = 1

C	0.055937	0.064751	-0.027523
C	0.031823	0.03311	1.505403
C	1.378228	0.052504	0.744352
H	-0.233206	-0.941023	1.907649
H	1.883312	-0.909757	0.716348
C	2.290271	1.200329	0.847437
C	1.953074	2.494896	0.932064
H	3.348043	0.949268	0.904374
H	2.74606	3.222616	1.073483
C	-0.377959	1.154443	2.364702
C	-0.176482	2.463684	2.154572
H	-0.871018	0.864233	3.290419
H	-0.496749	3.154524	2.925606
C	-0.382906	1.297023	-0.75113

C	-0.220089	2.564522	-0.333089
C	0.522343	3.047823	0.929299
C	-0.292349	-1.279915	-0.685975
H	-1.373504	-1.349951	-0.841174
H	-0.025458	-2.066415	0.034363
C	0.438752	-1.553995	-1.975983
C	-0.130241	-2.022562	-3.08789
H	1.51494	-1.375559	-1.960999
H	0.452938	-2.241709	-3.978648
H	-1.200854	-2.206658	-3.145608
C	-1.17095	1.098917	-2.024799
O	-2.283301	0.616112	-2.075561
O	-0.481942	1.512763	-3.103166
C	-1.16563	1.375087	-4.358341
H	-0.492198	1.799221	-5.103645
H	-1.359002	0.319954	-4.570526
H	-2.113253	1.919552	-4.341335
O	-0.745829	3.563789	-1.169397
C	-1.947646	4.087521	-0.819749
O	-2.600949	3.796359	0.15263
O	-2.272471	4.982432	-1.759858
C	-3.520083	5.656478	-1.529723
H	-3.644221	6.327957	-2.379609
H	-4.342323	4.937999	-1.482253
H	-3.48085	6.223034	-0.595729
C	0.578897	4.591462	0.944491
C	-0.294337	5.378996	1.705489
C	1.515506	5.253515	0.133793
C	-0.207557	6.773961	1.688705
H	-1.074323	4.918232	2.299491
C	1.60221	6.643851	0.110565
H	2.178675	4.674087	-0.501847
C	0.745414	7.413694	0.89906
H	-0.89389	7.357008	2.297441
H	2.338868	7.124635	-0.527704
H	0.814421	8.498204	0.889252

Isomer 0020030140 (Fraction e)

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

Sum of electronic and thermal Free Energies= -1264.944185 Hartree

Charge = 0 Multiplicity = 1

C	-0.106209	0.05657	0.178098
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C	-0.076949	0.11059	1.693453
C	1.234472	0.021328	0.926215
H	-0.397228	-0.909567	-0.219487
H	-0.362391	-0.8116	2.188427
H	1.691736	-0.961234	0.959469
C	2.191794	1.128679	0.853468
C	1.8722	2.433394	0.808778
H	3.242115	0.854795	0.814912
C	-0.503229	1.314154	2.430118
C	-0.301799	2.591519	2.099003
C	-0.541509	1.197593	-0.648343
C	-0.335955	2.503237	-0.394038
H	-1.089145	0.929602	-1.548865
C	0.452837	2.952707	0.828322
H	0.5147	4.041504	0.805831
C	-0.899975	3.553141	-1.279355
C	-2.186871	3.415906	-1.815331
C	-0.170762	4.713905	-1.573042
C	-2.725689	4.402742	-2.637172
H	-2.78071	2.544898	-1.552777
C	-0.709267	5.698424	-2.397031
H	0.824326	4.849325	-1.155043
C	-1.988284	5.54797	-2.932751
H	-3.729185	4.283358	-3.034639
H	-0.127615	6.587765	-2.620135
H	-2.409245	6.320509	-3.568833
C	2.938095	3.463678	0.675587
O	2.720498	4.6483	0.520514
O	4.184263	2.964785	0.734869
C	5.232048	3.924172	0.585847
H	6.159786	3.360214	0.665489
H	5.160283	4.415152	-0.387045
H	5.168551	4.679357	1.371977
O	-1.197435	1.023368	3.618532
C	-2.454102	0.578962	3.458931
O	-3.021998	0.422551	2.407217
O	-2.963421	0.339415	4.665422
C	-4.310972	-0.139897	4.656435
H	-4.567314	-0.299901	5.701825
H	-4.973139	0.601412	4.20499
H	-4.376764	-1.073671	4.09474
C	-0.909798	3.75026	2.854575
H	-0.129889	4.491232	3.069913

H	-1.324342	3.405901	3.805684
C	-1.977041	4.381676	1.994578
C	-1.864828	5.575567	1.415226
H	-2.850343	3.760683	1.791842
H	-2.632118	5.958743	0.749402
H	-0.987354	6.199545	1.574248

Transition state 0020030140–0413002000

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -319.05 cm⁻¹

Sum of electronic and thermal Free Energies= -1264.916806 Hartree

Charge = 0 Multiplicity = 1

C	-0.863988	0.256264	0.344611
C	-0.427633	0.215397	1.770944
C	0.985832	0.112319	1.276911
H	-1.167686	-0.69662	-0.077983
H	-0.738424	-0.718869	2.235737
H	1.389452	-0.892767	1.208335
C	1.778455	1.158917	0.850304
C	1.392347	2.498805	0.719305
H	2.757674	0.905191	0.458341
C	-0.801683	1.356814	2.663167
C	-0.585948	2.644881	2.416584
C	-0.893978	1.362924	-0.483509
C	-0.422406	2.654889	-0.203213
H	-1.218513	1.188166	-1.505716
C	0.078051	3.091813	1.144133
H	0.185851	4.176061	1.163204
C	-0.41112	3.651164	-1.308181
C	0.061544	3.293321	-2.577681
C	-0.870657	4.957036	-1.104988
C	0.062694	4.213597	-3.621932
H	0.458699	2.293384	-2.733589
C	-0.877112	5.875325	-2.150969
H	-1.233333	5.250878	-0.123808
C	-0.410418	5.508198	-3.411967
H	0.442847	3.922877	-4.596604
H	-1.243169	6.882831	-1.978859
H	-0.407164	6.228654	-4.224104
C	2.327119	3.480219	0.110085
O	2.147976	4.680294	0.098452
O	3.408141	2.908933	-0.454053
C	4.317916	3.820713	-1.069563

H	5.123079	3.206467	-1.469667
H	3.815267	4.370819	-1.868191
H	4.702266	4.531049	-0.334473
O	-1.358771	0.988348	3.896506
C	-2.545238	0.362957	3.842363
O	-3.159457	0.099686	2.838935
O	-2.921744	0.080862	5.08667
C	-4.180297	-0.592651	5.186215
H	-4.346691	-0.73714	6.251728
H	-4.971628	0.019246	4.749125
H	-4.136798	-1.552575	4.667883
C	-1.002662	3.746625	3.36294
H	-0.1406	4.396581	3.558689
H	-1.319491	3.31428	4.31592
C	-2.119401	4.566285	2.768655
C	-2.031019	5.864306	2.480981
H	-3.040304	4.024692	2.550237
H	-2.864245	6.407163	2.045382
H	-1.118803	6.424119	2.676757

Transition state 0020030140–0204103000

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -346.17 cm⁻¹

Sum of electronic and thermal Free Energies= -1264.912645 Hartree

Charge = 0 Multiplicity = 1

C	-0.071543	0.006195	-0.136433
C	0.07298	-0.007883	1.351019
C	1.429132	-0.02341	-0.230052
H	-0.480057	-0.947127	-0.469476
H	0.026524	-0.974723	1.84312
H	1.881056	-1.001312	-0.364945
C	2.268649	1.059661	-0.094242
C	1.900769	2.374341	0.248097
H	3.334374	0.862397	-0.131414
C	0.305377	1.081906	2.156035
C	0.592506	2.402187	1.780762
C	-0.815125	1.128428	-0.790637
C	-0.582196	2.425385	-0.567206
H	-1.579902	0.845858	-1.510311
C	0.494685	2.896114	0.370491
H	0.524961	3.983919	0.386316
C	-1.377244	3.4743	-1.2584
C	-2.756895	3.318053	-1.44446

C	-0.761854	4.63343	-1.75136
C	-3.497981	4.281961	-2.12291
H	-3.252347	2.445588	-1.028409
C	-1.502786	5.595862	-2.431778
H	0.307905	4.776943	-1.619315
C	-2.873056	5.423458	-2.621768
H	-4.567917	4.147014	-2.24942
H	-1.007244	6.48223	-2.815798
H	-3.4502	6.178032	-3.14689
C	2.959156	3.404299	0.406866
O	2.744757	4.590439	0.570818
O	4.206131	2.907962	0.337926
C	5.252302	3.873673	0.451046
H	6.18024	3.313074	0.352276
H	5.164909	4.62216	-0.339207
H	5.203692	4.372718	1.421233
O	0.496744	0.81043	3.52288
C	-0.615967	0.612151	4.253763
O	-1.738163	0.499811	3.835937
O	-0.246662	0.538291	5.53256
C	-1.33162	0.367137	6.44689
H	-0.872565	0.282241	7.43009
H	-1.996583	1.23306	6.403223
H	-1.896392	-0.534636	6.203261
C	0.881959	3.418808	2.86748
H	1.360745	4.292528	2.414824
H	1.560246	3.002947	3.617762
C	-0.40904	3.833247	3.528747
C	-0.643906	3.738677	4.836794
H	-1.183568	4.220872	2.866344
H	-1.590694	4.055454	5.263284
H	0.107133	3.342513	5.517117

Transition 0020030140-0302004100

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -355.86 cm⁻¹

Sum of electronic and thermal Free Energies= -1264.912368 Hartree

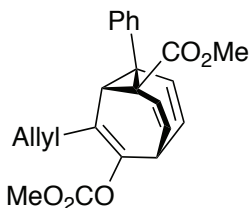
Charge = 0 Multiplicity = 1

C	0.061178	-0.019292	0.040004
C	0.07813	-0.019118	2.098435
C	1.158467	-0.008533	1.065193
H	-0.196743	-0.994163	-0.361778
H	-0.199602	-0.984239	2.508771

H	1.681317	-0.96367	1.068919
C	2.144928	1.111633	1.037586
C	1.799765	2.401745	1.035134
H	3.198053	0.849306	0.999605
C	-0.621163	1.077867	2.554171
C	-0.605179	2.38924	2.074465
C	-0.654185	1.074847	-0.413968
C	-0.611777	2.394788	0.064342
H	-1.426725	0.866884	-1.149957
C	0.389041	2.894686	1.069783
H	0.407298	3.982168	1.097029
C	-1.564626	3.385572	-0.503761
C	-2.91771	3.061628	-0.669905
C	-1.127422	4.659636	-0.890828
C	-3.807388	3.980076	-1.220809
H	-3.274301	2.090127	-0.337585
C	-2.017039	5.57761	-1.443614
H	-0.080486	4.928785	-0.772051
C	-3.359728	5.24167	-1.610477
H	-4.854404	3.715336	-1.33298
H	-1.658847	6.556515	-1.746971
H	-4.053906	5.960076	-2.035016
C	2.837456	3.470661	0.948628
O	2.58125	4.651946	0.847501
O	4.094054	3.003071	0.985608
C	5.11677	3.996595	0.891905
H	6.058483	3.454617	0.956943
H	5.04113	4.528159	-0.059071
H	5.024228	4.713112	1.710498
O	-1.662408	0.798594	3.46042
C	-1.308556	0.676239	4.752042
O	-0.18893	0.649358	5.190659
O	-2.429965	0.566332	5.466142
C	-2.220145	0.473601	6.876043
H	-1.720303	1.374623	7.239859
H	-3.212935	0.380554	7.312455
H	-1.609412	-0.399314	7.114696
C	-1.571474	3.400516	2.659279
H	-2.579202	2.978549	2.728679
H	-1.622536	4.264978	1.98744
C	-1.11532	3.851014	4.023829
C	-1.863899	3.77949	5.12369
H	-0.100333	4.244555	4.08521

H	-1.489672	4.120148	6.084164
H	-2.873616	3.375591	5.091411

Isomer 0413002000



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

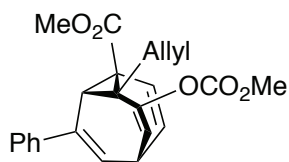
Sum of electronic and thermal Free Energies= -1264.934304 Hartree

Charge = 0 Multiplicity = 1

C	0.112093	-0.007465	-0.143233
C	0.071441	0.015055	1.426363
C	1.387311	-0.035767	0.669901
H	1.822672	-1.030938	0.724382
C	2.411804	1.038424	0.697739
C	2.096913	2.336319	0.689299
C	-0.389007	1.203565	2.174564
C	-0.105494	2.476213	1.87758
H	-1.006957	0.993409	3.042064
H	-0.499439	3.260703	2.517662
C	-0.293935	1.203513	-0.902188
C	-0.031928	2.477872	-0.592603
H	-0.839808	0.996074	-1.819042
H	-0.358904	3.262319	-1.268479
C	0.69514	2.901888	0.664537
H	0.780493	3.989528	0.666198
C	3.843685	0.54545	0.702585
H	3.968075	-0.187608	1.50892
H	4.520444	1.380404	0.900904
C	4.18605	-0.100909	-0.615051
C	4.489823	-1.389497	-0.766473
H	4.147308	0.551787	-1.487701
H	4.717888	-1.808898	-1.741521
H	4.522531	-2.064903	0.085856
O	3.135971	3.273222	0.786577
C	3.252016	4.139938	-0.230287
O	2.556994	4.173186	-1.215432
O	4.266676	4.957632	0.037807
C	4.521583	5.939058	-0.971414
H	5.389275	6.494548	-0.621334

H	4.730801	5.453661	-1.92651
C	-0.330401	-1.311474	2.010491
O	0.341106	-2.315924	1.994757
O	-1.569497	-1.269646	2.526714
C	-2.059254	-2.518943	3.021307
H	-1.403248	-2.899606	3.806695
H	-2.105368	-3.247065	2.207777
C	-0.333301	-1.286707	-0.800239
C	0.572741	-2.147914	-1.417683
C	-1.696691	-1.598778	-0.820637
C	0.123067	-3.309955	-2.043491
H	1.632873	-1.907602	-1.403465
C	-2.146705	-2.760236	-1.442804
H	-2.401369	-0.925971	-0.335835
C	-1.235152	-3.620093	-2.055725
H	0.836896	-3.976096	-2.518407
H	-3.2069	-2.995139	-1.448913
H	-1.582666	-4.527957	-2.539121
H	-3.05325	-2.310674	3.413387
H	3.659211	6.599494	-1.082221

Isomer 0204103000



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

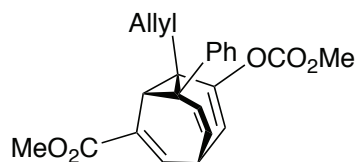
Sum of electronic and thermal Free Energies= -1264.929336 Hartree

Charge = 0 Multiplicity = 1

C	0.146245	0.101109	0.028588
C	0.015444	0.012036	1.542723
C	1.417032	0.12643	0.855019
H	0.003585	-0.872423	-0.432482
C	2.179075	1.391913	1.028204
C	1.7174	2.641223	1.03327
H	2.434638	3.443761	1.176874
C	-0.558087	1.11179	2.354875
C	-0.495528	2.418712	2.078051
H	-1.087501	0.794683	3.247538
H	-0.980259	3.115936	2.756209
C	-0.373522	1.223158	-0.793893
C	-0.328961	2.510292	-0.417319

H	-0.760966	3.259925	-1.075898
C	0.253278	2.989863	0.89325
H	0.166985	4.077562	0.922445
C	-0.976301	0.840691	-2.100442
C	-1.843357	-0.256404	-2.192617
C	-0.694964	1.573525	-3.259893
C	-2.431183	-0.595854	-3.408026
H	-2.074131	-0.836927	-1.302618
C	-1.281086	1.231803	-4.476329
H	0.008464	2.39955	-3.206517
C	-2.153126	0.147569	-4.554492
H	-3.108559	-1.442798	-3.458743
H	-1.043804	1.805478	-5.367105
H	-2.60666	-0.121994	-5.503225
C	2.282126	-1.128555	0.748462
H	1.626916	-2.004703	0.753274
H	2.953799	-1.204416	1.609236
C	3.073778	-1.150381	-0.53251
C	4.366467	-1.460094	-0.616043
H	2.518335	-0.905165	-1.439087
H	4.877268	-1.489371	-1.573648
H	4.951221	-1.691466	0.271486
O	3.542351	1.183567	1.272802
C	4.413932	1.518962	0.30175
O	4.15767	2.063699	-0.738666
O	5.626064	1.151748	0.715304
C	6.66727	1.391331	-0.233479
H	7.582858	1.053689	0.248583
H	6.477604	0.822641	-1.14693
C	-0.337243	-1.361811	2.046665
O	-0.612379	-2.314398	1.351796
O	-0.300023	-1.42855	3.384574
C	-0.629473	-2.703663	3.943227
H	0.071617	-3.461797	3.588696
H	-1.642926	-2.991076	3.655944
H	-0.552158	-2.579085	5.021633
H	6.72586	2.454428	-0.474912

Isomer 0302004100



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

Sum of electronic and thermal Free Energies= -1264.932570 Hartree

Charge = 0 Multiplicity = 1

C	0.035895	0.138115	0.08816
C	0.16269	0.149436	1.604582
C	1.427386	0.070337	0.705705
H	-0.320974	-0.816683	-0.286729
C	2.361684	1.22048	0.586239
C	2.054883	2.522371	0.539656
H	3.409431	0.939471	0.50997
H	2.859487	3.244837	0.432526
C	-0.107862	1.391749	2.374129
C	0.070223	2.65776	1.998606
H	-0.177163	3.440176	2.709271
C	-0.455477	1.269415	-0.725796
C	-0.209127	2.567482	-0.491637
H	-0.6337	3.306559	-1.163631
C	0.642802	3.053934	0.656116
H	0.676102	4.143968	0.615327
C	-1.28788	0.861161	-1.897922
O	-1.517246	-0.291793	-2.195632
O	-1.763965	1.898129	-2.604404
C	-2.564278	1.549447	-3.735064
H	-3.432393	0.967381	-3.419263
H	-1.979485	0.961744	-4.445938
C	2.150529	-1.249258	0.661855
C	2.078065	-2.096369	-0.444641
C	2.957077	-1.614057	1.745531
C	2.794945	-3.293489	-0.464858
H	1.459389	-1.817946	-1.294203
C	3.670816	-2.808384	1.7284
H	3.011609	-0.954757	2.609341
C	3.590225	-3.653236	0.620596
H	2.731868	-3.943468	-1.332184
H	4.286089	-3.082973	2.579745
H	4.145265	-4.58592	0.60509
C	-0.307281	-1.139399	2.276068
H	0.052083	-1.982678	1.676427
H	0.136147	-1.241495	3.272109
C	-1.807582	-1.219729	2.360775
C	-2.486364	-1.559204	3.455572
H	-2.348717	-0.994222	1.4404

H	-3.56989	-1.62871	3.447942
H	-1.976748	-1.772479	4.392659
O	-0.53217	1.140177	3.684842
C	-1.806634	1.434034	4.005421
O	-2.61924	1.97535	3.304211
O	-2.001174	1.029541	5.260046
C	-3.333757	1.221671	5.738218
H	-4.036045	0.651305	5.125779
H	-3.329959	0.855532	6.763196
H	-2.873666	2.494759	-4.177566
H	-3.6017	2.279513	5.705997

Transition state 0413002000–0000031402

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -376 cm^{-1}

Sum of electronic and thermal Free Energies= -1264.897877 Hartree

Charge = 0 Multiplicity = 1

C	-0.209149	0.2843	-0.726291
C	-0.412804	0.274654	0.748637
C	0.778613	0.377955	1.651306
H	-0.713706	-0.492782	-1.292977
H	-1.07128	-0.536171	1.053279
H	0.694519	-0.154858	2.593117
C	1.952868	1.087812	1.421041
C	2.190847	2.0415	0.432358
H	2.689274	1.049011	2.217844
C	-0.806837	1.533087	1.436609
C	-0.454323	2.853863	1.13239
C	0.547799	1.167528	-1.368075
C	1.278708	2.340626	-0.748472
H	0.644309	1.08529	-2.446879
C	0.523358	3.206508	0.20943
H	0.855707	4.242133	0.217742
C	1.95479	3.090003	-1.887127
C	3.123276	2.563993	-2.44389
C	1.375804	4.216377	-2.46471
C	3.717513	3.169666	-3.546053
H	3.571747	1.6751	-2.002734
C	1.968873	4.825757	-3.571047
H	0.456299	4.622592	-2.05207
C	3.141811	4.307365	-4.112547
H	4.630789	2.755905	-3.962741
H	1.511171	5.707779	-4.008484

H	3.605059	4.784218	-4.970541
C	3.366747	2.942966	0.621804
O	3.418939	4.108011	0.296853
O	4.40035	2.310018	1.210126
C	5.547821	3.127265	1.448102
H	6.279078	2.474242	1.921548
H	5.932303	3.521044	0.504923
H	5.290845	3.962659	2.103104
O	-1.642251	1.360344	2.544866
C	-2.912984	1.008593	2.258562
O	-3.354035	0.795812	1.159223
O	-3.578039	0.923436	3.405709
C	-4.96793	0.619006	3.25913
H	-5.366008	0.590267	4.271481
H	-5.459643	1.396939	2.670929
H	-5.095512	-0.346105	2.765272
C	-1.036827	3.946482	2.016512
H	-0.502346	4.878079	1.798702
H	-0.874733	3.713415	3.074793
C	-2.509147	4.155537	1.770213
C	-3.448197	4.097763	2.713791
H	-2.79328	4.358481	0.737484
H	-4.494872	4.269671	2.481271
H	-3.195061	3.874884	3.748065

Transition state 0413002000-0001400023

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -413.51 cm⁻¹

Sum of electronic and thermal Free Energies= -1264.897171 Hartree

Charge = 0 Multiplicity = 1

C	-0.422981	0.370472	0.094233
C	-0.104548	0.099277	1.562534
C	1.3152	0.123653	1.080664
H	1.713459	-0.853856	0.833405
C	2.185199	1.199743	0.9348
C	1.77839	2.534736	1.013027
C	-0.569853	1.090586	2.590204
C	-0.290341	2.38945	2.573021
H	-1.181506	0.680968	3.387677
H	-0.672409	3.019664	3.371304
C	-0.397136	1.641694	-0.478644
C	0.080362	2.830424	0.066629
H	-0.611233	1.667875	-1.544218

H	0.18993	3.673352	-0.608209
C	0.473016	3.075242	1.490805
H	0.582949	4.139348	1.691857
C	3.589985	0.891167	0.426035
H	4.259031	1.706743	0.728412
H	3.589703	0.868405	-0.671437
C	4.150448	-0.394879	0.963011
C	4.560648	-1.409651	0.203703
H	4.215216	-0.473819	2.048384
H	4.975243	-2.313888	0.637614
H	4.494323	-1.362724	-0.880963
O	2.698701	3.554734	0.750959
C	3.162143	3.719938	-0.50303
O	2.802007	3.128655	-1.487048
O	4.09027	4.673429	-0.460361
C	4.673124	4.990755	-1.727694
H	5.406388	5.768013	-1.522174
H	5.153649	4.107953	-2.153727
C	-0.584642	-1.290098	1.981075
O	-1.600852	-1.476363	2.609145
O	0.199502	-2.281917	1.554063
C	-0.315808	-3.600271	1.756442
H	-1.252007	-3.714046	1.2034
H	-0.493903	-3.778437	2.818406
C	-0.821385	-0.771749	-0.784921
C	0.005786	-1.192317	-1.830794
C	-2.050774	-1.414099	-0.591797
C	-0.380141	-2.242998	-2.660705
H	0.961196	-0.694204	-1.97672
C	-2.437313	-2.464083	-1.422337
H	-2.705222	-1.085681	0.211239
C	-1.600775	-2.88478	-2.455417
H	0.274838	-2.563554	-3.465163
H	-3.395902	-2.949325	-1.264529
H	-1.900664	-3.705191	-3.100074
H	0.445033	-4.274464	1.368072
H	3.907265	5.353616	-2.415905

Transition state 0204103000-0010200034

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -399.17 cm⁻¹

Sum of electronic and thermal Free Energies= -1264.899964 Hartree

Charge = 0 Multiplicity =1

C	-0.896731	0.17763	0.092189
C	-1.033297	0.103401	1.572939
C	0.498805	0.296953	-0.439518
H	-1.426472	-0.64815	-0.379106
H	-1.520973	-0.769818	1.995944
H	0.725303	-0.266567	-1.338812
C	1.531905	1.030389	0.132214
C	1.476743	1.984372	1.160266
H	2.476906	0.988541	-0.398377
C	-0.483911	0.969008	2.411095
C	0.27178	2.232331	2.06446
C	-1.116403	1.437053	-0.670405
C	-0.863597	2.742407	-0.25159
H	-1.533299	1.304152	-1.664304
C	-0.194424	3.077342	0.924877
H	0.093825	4.119944	1.040887
C	-1.108118	3.848018	-1.222862
C	-1.699812	5.043021	-0.795827
C	-0.74205	3.724944	-2.56894
C	-1.918528	6.088334	-1.689917
H	-2.003358	5.141142	0.243572
C	-0.964426	4.768295	-3.464352
H	-0.254723	2.814638	-2.908677
C	-1.554237	5.953755	-3.028456
H	-2.382449	7.006195	-1.341552
H	-0.665272	4.659183	-4.502516
H	-1.726288	6.766631	-3.726967
C	2.70174	2.823549	1.337638
O	2.730558	3.978735	1.707109
O	3.823076	2.154508	1.016881
C	5.03005	2.910956	1.12018
H	5.825132	2.23509	0.810029
H	4.987431	3.787045	0.469428
H	5.182696	3.239912	2.150278
O	-0.619519	0.676	3.777401
C	0.481318	0.19492	4.380177
O	1.552393	0.019994	3.857892
O	0.18125	-0.03853	5.654689
C	1.268576	-0.541768	6.437032
H	0.862379	-0.684041	7.436355
H	1.625361	-1.487338	6.024594
H	2.088161	0.179474	6.451275
C	0.47308	3.116008	3.317164

H	1.079096	3.978089	3.046029
H	1.035527	2.563461	4.077235
C	-0.847621	3.598552	3.856886
C	-1.200726	4.883848	3.866504
H	-1.536965	2.849847	4.242926
H	-2.161707	5.205938	4.255502
H	-0.532041	5.655916	3.491398

Transition state 0204103000–0000140203

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -434.73 cm⁻¹

Sum of electronic and thermal Free Energies= -1264.899277 Hartree

Charge = 0 Multiplicity = 1

C	0.614956	-0.187476	-0.302679
C	0.29463	-0.010206	1.144894
C	2.027869	-0.010184	-0.743092
H	0.217611	-1.135231	-0.661478
H	-0.438824	-0.685508	1.572116
H	2.465352	-0.812039	-1.3319
C	2.782164	1.035502	-0.422314
C	2.302208	2.226789	0.362157
H	3.818055	1.061195	-0.747275
C	0.849809	0.923965	2.005516
C	1.643772	2.037967	1.718441
C	-0.397805	0.899914	-0.484815
C	-0.178637	2.275407	-0.416031
H	-1.406457	0.566167	-0.707913
C	1.00313	2.876745	0.022687
H	1.006348	3.956377	0.14588
C	-1.348307	3.180171	-0.620487
C	-2.56761	2.940231	0.025908
C	-1.234733	4.294683	-1.459636
C	-3.650195	3.793605	-0.176882
H	-2.645689	2.107968	0.719668
C	-2.317194	5.149007	-1.657536
H	-0.293696	4.479139	-1.971382
C	-3.530761	4.89796	-1.019702
H	-4.587564	3.601419	0.336745
H	-2.214853	6.005122	-2.317655
H	-4.376233	5.561067	-1.175635
C	3.430991	3.245994	0.433974
O	3.37127	4.39239	0.063113
O	4.524552	2.705664	0.987517

C	5.638655	3.590907	1.134669
H	6.421042	3.001954	1.609091
H	5.964076	3.95623	0.158565
H	5.360803	4.442477	1.760041
O	0.427301	0.840283	3.34751
C	-0.851038	1.14165	3.623846
O	-1.710805	1.42956	2.830255
O	-1.013071	1.040524	4.941851
C	-2.321927	1.379488	5.402959
H	-2.288402	1.259908	6.484274
H	-2.55815	2.411574	5.134313
H	-3.065411	0.711395	4.963518
C	1.87966	3.057437	2.824468
H	2.617418	3.797241	2.496264
H	2.310815	2.543588	3.691223
C	0.640507	3.805795	3.250628
C	0.226998	3.913276	4.512016
H	0.075611	4.286072	2.451221
H	-0.656821	4.490241	4.766826
H	0.75473	3.4199	5.325132

Transition state 0302004100-0000300142

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -411.84 cm⁻¹

Sum of electronic and thermal Free Energies= -1264.902828 Hartree

Charge = 0 Multiplicity = 1

C	-0.340377	0.010342	-0.564949
C	-0.056815	-0.0805	1.981821
C	0.532399	-0.226745	0.614537
H	-0.332503	-0.750093	-1.341403
H	0.288287	-0.774226	2.740573
H	1.071701	-1.167656	0.528732
C	1.407573	0.841283	1.179579
C	1.162771	2.220156	1.165351
H	2.332767	0.507541	1.633491
C	-1.036657	0.824258	2.383515
C	-1.538632	1.953843	1.733786
C	-1.14782	1.05715	-0.701728
C	-1.277628	2.222569	0.249397
H	-1.770178	1.118079	-1.589922
C	-0.046718	2.830274	0.835902
H	-0.111662	3.8905	1.065236
C	-2.22823	3.220046	-0.392477

C	-3.593211	2.916737	-0.456584
C	-1.764946	4.382358	-1.004098
C	-4.480001	3.771003	-1.102174
H	-3.956639	2.005575	0.015418
C	-2.652904	5.240004	-1.657582
H	-0.705263	4.619779	-0.98051
C	-4.010391	4.940034	-1.70498
H	-5.537703	3.528086	-1.134192
H	-2.277335	6.143219	-2.128454
H	-4.701046	5.609473	-2.208046
C	2.1	3.110453	1.909704
O	1.881134	4.27546	2.170346
O	3.240241	2.497047	2.268624
C	4.125615	3.285881	3.062106
H	4.979941	2.645493	3.275759
H	4.436915	4.176896	2.512745
H	3.628331	3.589357	3.985997
O	-1.397053	0.710525	3.741694
C	-0.489016	1.15444	4.630766
O	0.593875	1.615724	4.372082
O	-0.991848	0.973998	5.849154
C	-0.167851	1.470535	6.905519
H	-0.029614	2.54858	6.795008
H	-0.704962	1.242542	7.824284
H	0.805907	0.976634	6.893128
C	-2.368642	2.944031	2.542592
H	-3.219402	2.415975	2.989672
H	-2.784434	3.691332	1.861266
C	-1.614264	3.679252	3.623656
C	-2.062316	3.836598	4.868283
H	-0.657243	4.115443	3.333081
H	-1.503848	4.417652	5.596128
H	-2.997975	3.389854	5.197481

Transition state 0302004100–0010020304

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -394.84 cm^{-1}

Sum of electronic and thermal Free Energies= -1264.907405 Hartree

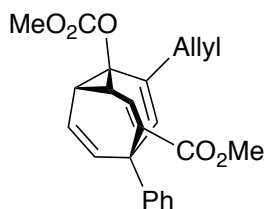
Charge = 0 Multiplicity = 1

C	0.962946	0.322954	0.663987
C	0.801011	0.339642	3.213279
C	1.657296	0.313802	1.994419
H	1.395318	-0.302828	-0.109538

H	0.933969	-0.454481	3.941926
H	2.379782	-0.497614	2.054693
C	2.282311	1.534169	1.420768
C	1.760433	2.828985	1.462703
H	3.244172	1.394147	0.942558
C	-0.182073	1.204199	3.417851
C	-0.584761	2.355551	2.534911
C	-0.218568	0.998132	0.359799
C	-0.890628	1.986536	1.090306
H	-0.586994	0.859146	-0.653809
C	0.468561	3.170444	1.858937
H	0.185965	4.20582	1.686906
C	-2.056504	2.64138	0.420412
C	-3.350659	2.195199	0.714771
C	-1.880069	3.667751	-0.511124
C	-4.450396	2.773405	0.084984
H	-3.478071	1.391924	1.436499
C	-2.983261	4.246999	-1.138019
H	-0.873874	4.016071	-0.732412
C	-4.269563	3.802014	-0.840206
H	-5.450846	2.41933	0.315132
H	-2.83564	5.045961	-1.858121
H	-5.128181	4.253751	-1.32745
C	2.498019	3.919161	0.76358
O	2.045782	5.017034	0.517208
O	3.757081	3.573092	0.431439
C	4.507812	4.583838	-0.241148
H	5.497263	4.158071	-0.399882
H	4.037596	4.835005	-1.194608
H	4.566695	5.4842	0.373677
O	-0.940548	1.023304	4.586989
C	-2.154859	0.479049	4.415971
O	-2.6421	0.154755	3.361343
O	-2.731488	0.373119	5.608622
C	-4.048041	-0.187822	5.584344
H	-4.020614	-1.195673	5.165912
H	-4.371667	-0.208229	6.622847
H	-4.712428	0.436852	4.984212
C	-1.602835	3.295423	3.212357
H	-2.50944	2.740077	3.477433
H	-1.912798	4.048296	2.482695
C	-1.015941	3.986005	4.413736
C	-0.833116	5.303794	4.483409

H	-0.723305	3.356441	5.252176
H	-0.397992	5.769741	5.361744
H	-1.11243	5.958866	3.661101

Isomer 0000031402



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

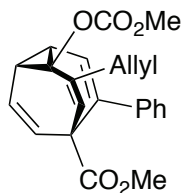
Sum of electronic and thermal Free Energies= -1264.916838 Hartree

Charge = 0 Multiplicity = 1

C	0.228834	-0.013342	0.045862
C	0.008561	-0.019259	1.538926
C	1.423074	0.004436	1.03739
H	0.059203	-0.986853	-0.401433
H	1.915823	-0.95662	1.13481
C	2.325391	1.158185	1.101954
C	1.991891	2.453611	0.970508
H	3.384071	0.91602	1.138842
C	-0.625991	1.123569	2.239515
C	-0.363609	2.397815	1.928033
H	-0.912672	3.15822	2.478128
C	-0.057815	1.139831	-0.826224
C	0.080532	2.440068	-0.52504
H	-0.35203	0.882963	-1.840224
H	-0.075841	3.164937	-1.316856
C	0.548412	2.950564	0.827091
C	3.100555	3.40039	0.644062
O	3.037473	4.240206	-0.223134
O	4.204135	3.189157	1.383849
C	5.320435	4.015771	1.045846
H	6.117935	3.725068	1.727437
H	5.616464	3.848476	0.007774
H	5.061634	5.068811	1.176756
O	-0.40332	-1.3012	1.984495
C	0.158179	-1.730287	3.124809
O	0.978199	-1.141059	3.782452
O	-0.357213	-2.926077	3.4087
C	0.153401	-3.523089	4.604518
H	1.234344	-3.655894	4.529408

H	-0.074613	-2.895122	5.468025
H	-0.348675	-4.485217	4.684322
C	-1.712455	0.804996	3.247574
H	-1.38908	0.039607	3.960437
H	-1.905472	1.715102	3.825646
C	-2.9823	0.369197	2.559537
C	-3.531196	-0.837836	2.67426
H	-3.445612	1.119058	1.918008
H	-4.44595	-1.096593	2.15072
H	-3.070019	-1.611661	3.284048
C	0.47217	4.473876	0.9893
C	-0.270256	5.304122	0.153997
C	1.095364	5.042783	2.108027
C	-0.358143	6.675479	0.407072
H	-0.797789	4.901935	-0.703451
C	1.012983	6.406213	2.361939
H	1.654795	4.403254	2.789569
C	0.28677	7.233814	1.504351
H	-0.937719	7.304422	-0.26183
H	1.51257	6.823911	3.230878
H	0.220462	8.30001	1.696489

Isomer 0001400023



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

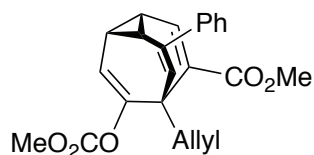
Sum of electronic and thermal Free Energies= -1264.925741 Hartree

Charge = 0 Multiplicity = 1

C	-0.060997	-0.033999	0.065313
C	-0.077537	0.00924	1.580017
C	1.249331	-0.027851	0.814377
H	-0.355762	-0.945432	2.013558
H	1.72124	-1.004447	0.821502
C	2.199406	1.095007	0.780407
C	1.920845	2.407384	0.757579
H	3.248714	0.809009	0.7949
C	-0.496714	1.198174	2.342864
C	-0.258922	2.473188	2.015247
H	-1.028279	0.997177	3.269027

H	-0.596287	3.272097	2.668592
C	-0.52857	1.099842	-0.770964
C	-0.277711	2.383004	-0.477249
H	-0.665884	3.135972	-1.15763
C	0.458801	2.905333	0.750946
O	-0.430563	-1.317299	-0.413658
C	0.304932	-1.796453	-1.426968
O	1.253781	-1.258546	-1.94046
O	-0.205275	-2.97654	-1.779826
C	0.477839	-3.617609	-2.861055
H	-0.05494	-4.551878	-3.026587
H	0.446272	-2.99002	-3.753842
H	1.518296	-3.809113	-2.591476
C	-1.418368	0.768357	-1.953947
H	-1.480395	1.663955	-2.581606
H	-0.983818	-0.021153	-2.575602
C	-2.803777	0.372457	-1.50749
C	-3.348014	-0.826972	-1.698244
H	-3.363409	1.14601	-0.981442
H	-4.351122	-1.0557	-1.352697
H	-2.798424	-1.624759	-2.193162
C	3.050258	3.379579	0.724716
C	3.222339	4.338827	1.732019
C	3.972742	3.331557	-0.326663
C	4.293858	5.228568	1.683363
H	2.520144	4.381779	2.560155
C	5.044222	4.220539	-0.373343
H	3.83028	2.600072	-1.116911
C	5.206389	5.174217	0.630174
H	4.41896	5.961061	2.475058
H	5.74881	4.17151	-1.198029
H	6.040051	5.868612	0.594319
C	0.463953	4.436033	0.6834
O	0.167397	5.176739	1.590108
O	0.87681	4.867468	-0.512627
C	1.126157	6.272344	-0.606796
H	1.926577	6.546061	0.086502
H	1.43337	6.447075	-1.636185
H	0.223704	6.837076	-0.365462

Isomer 0010200034



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

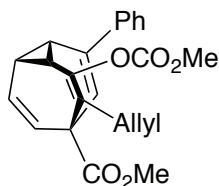
Sum of electronic and thermal Free Energies= -1264.925673 Hartree

Charge = 0 Multiplicity = 1

C	0.296192	-0.128805	-0.205914
C	0.17272	-0.029154	1.320166
C	1.540301	-0.051489	0.642403
H	0.092493	-1.121127	-0.592869
H	-0.102012	-0.958791	1.806127
H	2.057026	-1.000834	0.731961
C	2.427178	1.130584	0.673117
C	1.991994	2.396457	0.587024
H	2.736759	3.181444	0.688418
C	-0.375718	1.163124	1.978041
C	-0.256956	2.464148	1.63345
H	-0.988715	0.945277	2.845756
C	-0.193065	0.955903	-1.069247
C	-0.102817	2.258949	-0.8084
H	-0.744169	0.666227	-1.959306
C	0.564469	2.900923	0.4059
O	-0.717118	3.125041	-1.723097
C	-1.901937	3.629958	-1.331814
O	-2.501154	3.328354	-0.332042
O	-2.287527	4.521968	-2.239434
C	-3.528444	5.169251	-1.9389
H	-3.688631	5.877062	-2.74959
H	-4.33629	4.435833	-1.899131
H	-3.459029	5.685612	-0.979492
C	3.881707	0.869023	0.857468
C	4.832704	1.601079	0.134932
C	4.331022	-0.101218	1.762887
C	6.194451	1.379363	0.323553
H	4.49406	2.335102	-0.591189
C	5.692725	-0.32287	1.952017
H	3.609998	-0.669345	2.34496
C	6.630015	0.416711	1.232647
H	6.91656	1.952307	-0.250251
H	6.0228	-1.070519	2.666914
H	7.691433	0.240886	1.37671

C	-1.024042	3.457911	2.45078
O	-1.186551	4.626917	2.183416
O	-1.547883	2.91823	3.572123
C	-2.334451	3.811021	4.358983
H	-3.200154	4.155497	3.788857
H	-2.649593	3.234977	5.227638
H	-1.741153	4.675727	4.662957
C	0.69308	4.437153	0.203226
H	-0.290469	4.890457	0.070933
H	1.094577	4.866546	1.126277
C	1.586907	4.801537	-0.952223
C	2.659706	5.585269	-0.843857
H	1.306532	4.414824	-1.930922
H	3.257789	5.85045	-1.710078
H	2.967875	5.995128	0.115946

Isomer 0000140203



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

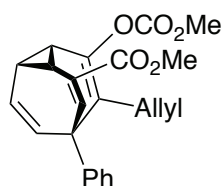
Sum of electronic and thermal Free Energies= -1264.929214 Hartree

Charge = 0 Multiplicity = 1

C	-0.021298	0.030614	-0.020572
C	-0.025799	0.024518	1.505977
C	1.288636	0.052886	0.752471
H	-0.249594	-0.936004	-0.456473
H	-0.266432	-0.941378	1.936483
H	1.835826	-0.883041	0.757782
C	2.173057	1.228526	0.770602
C	1.875145	2.533163	0.735499
C	-0.501626	1.174284	2.306043
C	-0.313878	2.464035	1.98134
H	-0.661847	3.220356	2.678209
C	-0.481168	1.179787	-0.818406
C	-0.303353	2.4717	-0.523593
H	-1.00437	0.933292	-1.738611
H	-0.668634	3.237187	-1.200796
C	0.392434	2.965225	0.728889
O	3.539164	0.89961	0.771072

C	4.011043	0.383253	1.91799
O	3.352168	0.063191	2.875962
O	5.331107	0.269402	1.803776
C	5.983125	-0.247087	2.966727
H	5.79671	0.40636	3.821498
H	5.619249	-1.251726	3.19126
H	7.042582	-0.266941	2.719178
C	3.001876	3.545245	0.721105
H	3.79423	3.176046	0.060499
H	2.665998	4.487693	0.270714
C	3.621669	3.836445	2.069385
C	3.241866	3.321864	3.237704
H	4.463627	4.528196	2.038947
H	3.759258	3.586077	4.154857
H	2.411046	2.624055	3.314506
C	-1.212445	0.841538	3.571828
C	-2.412162	1.479472	3.905892
C	-0.683112	-0.107089	4.457056
C	-3.064093	1.186145	5.101539
H	-2.842133	2.194476	3.21024
C	-1.334713	-0.399318	5.652522
H	0.260671	-0.592201	4.219283
C	-2.527747	0.245251	5.978401
H	-3.99772	1.685498	5.342167
H	-0.90609	-1.126699	6.335245
H	-3.036905	0.013429	6.908653
C	0.359379	4.497549	0.727724
O	0.126535	5.191843	-0.232753
O	0.679682	4.992452	1.927477
C	0.833971	6.41031	1.995987
H	1.099824	6.625888	3.029097
H	1.629385	6.732571	1.318548
H	-0.096834	6.908658	1.717772

Isomer 0000300142



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

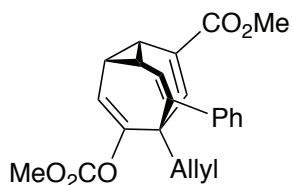
Sum of electronic and thermal Free Energies= -1264.926351 Hartree

Charge = 0 Multiplicity =1

C	0.053889	0.047133	-0.073417
C	0.001745	0.02597	1.461254
C	1.328191	0.065882	0.734725
H	-0.174003	-0.895485	-0.555618
H	-0.245216	-0.944226	1.87804
H	1.87145	-0.872176	0.731042
C	2.217607	1.238979	0.752847
C	1.927824	2.545543	0.781112
C	-0.525969	1.170858	2.214586
C	-0.34333	2.468407	1.938812
H	-1.165484	0.921516	3.057598
H	-0.87414	3.189071	2.551682
C	-0.410182	1.221756	-0.829722
C	-0.250363	2.513775	-0.489088
H	-0.718218	3.251675	-1.130683
C	0.451633	3.025491	0.761642
C	-1.184897	0.878446	-2.063261
O	-1.474458	-0.252604	-2.385822
O	-1.53592	1.949227	-2.795226
C	-2.285434	1.658063	-3.97552
H	-2.479293	2.621393	-4.444058
H	-1.707093	1.013119	-4.640317
H	-3.220986	1.157243	-3.717328
O	3.580653	0.892543	0.767061
C	4.06265	0.361576	-0.368925
O	3.417766	0.064079	-1.34267
O	5.376391	0.207468	-0.224114
C	6.037182	-0.333234	-1.371297
H	5.642567	-1.324176	-1.604506
H	5.895352	0.325475	-2.230499
H	7.089041	-0.390943	-1.098391
C	3.070648	3.537509	0.742825
H	2.784094	4.473747	1.23014
H	3.910454	3.138485	1.322061
C	3.576412	3.858417	-0.645276
C	3.177414	3.29623	-1.786181
H	4.350961	4.624974	-0.675822
H	3.61671	3.595062	-2.733097
H	2.416545	2.51929	-1.81259
C	0.426369	4.561744	0.791021
C	0.518453	5.309755	-0.3869
C	0.427627	5.255428	2.00711

C	0.576259	6.702386	-0.353749
H	0.580629	4.80942	-1.347851
C	0.485206	6.646775	2.045508
H	0.414741	4.709476	2.945206
C	0.552458	7.379119	0.862394
H	0.647526	7.255389	-1.285347
H	0.484127	7.156453	3.004191
H	0.594765	8.463393	0.889159

Isomer 0010020304



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

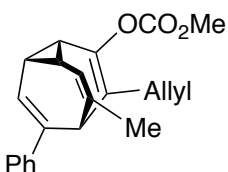
Sum of electronic and thermal Free Energies= -1264.930808 Hartree

Charge = 0 Multiplicity = 1

C	-0.045659	-0.042137	-0.150841
C	0.122649	-0.085502	1.365991
C	1.340419	-0.140285	0.456817
H	-0.414291	-0.95677	-0.599153
H	-0.142189	-1.039062	1.809491
H	1.786335	-1.124763	0.369579
C	2.315521	0.958902	0.408518
C	2.039357	2.257526	0.511814
H	3.361433	0.685328	0.300452
C	-0.193833	1.073977	2.218143
C	0.0086	2.380118	1.97363
H	-0.676428	0.825254	3.161202
C	-0.531178	1.175087	-0.822936
C	-0.239805	2.44212	-0.482532
H	-0.689681	3.239546	-1.067336
C	0.655938	2.883842	0.6643
O	3.129498	3.137955	0.411986
C	3.645039	3.597621	1.56032
O	3.291025	3.291323	2.671515
O	4.613432	4.457968	1.25973
C	5.26978	5.035594	2.392498
H	5.744895	4.256127	2.991216
H	6.014344	5.713208	1.97978
H	4.551153	5.580323	3.007897

C	-0.492826	3.369108	2.977461
C	-1.851991	3.702023	3.003175
C	0.368147	3.961088	3.90863
C	-2.343677	4.612222	3.938011
H	-2.52255	3.239391	2.283231
C	-0.125507	4.868759	4.844545
H	1.421237	3.697439	3.894421
C	-1.480029	5.199502	4.86049
H	-3.401118	4.85902	3.946438
H	0.551182	5.314153	5.567808
H	-1.861357	5.90702	5.590336
C	-1.452132	0.909899	-1.972041
O	-1.760071	-0.200575	-2.347192
O	-1.913448	2.02377	-2.562819
C	-2.779892	1.805552	-3.676344
H	-3.66144	1.24029	-3.366706
H	-3.06027	2.796933	-4.02789
H	-2.258004	1.250871	-4.459026
C	0.729823	4.43246	0.636294
H	-0.270118	4.814503	0.868829
H	1.378918	4.773401	1.452223
C	1.182249	5.01833	-0.674345
C	0.440344	5.85632	-1.398203
H	2.172284	4.740448	-1.029325
H	0.804765	6.270034	-2.333138
H	-0.553766	6.158953	-1.0757

Isomer 0020050140



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

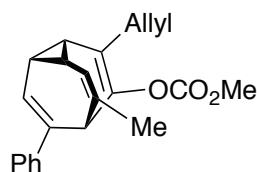
Sum of electronic and thermal Free Energies= -1076.835958 Hartree

Charge = 0 Multiplicity = 1

C	-0.113649	0.02582	-0.014732
C	-0.101507	0.042892	1.516478
C	1.222253	0.012647	0.744712
H	-0.388963	-0.936822	-0.436687
H	-0.374236	-0.896664	1.987008
H	1.707908	-0.959319	0.757215
C	2.159749	1.150199	0.727671

C	1.836294	2.454812	0.719207
H	3.215158	0.880308	0.727162
C	-0.532821	1.21732	2.293155
C	-0.340344	2.512713	2.006864
C	-0.561746	1.175882	-0.81569
C	-0.380762	2.483141	-0.53126
H	-1.080766	0.919172	-1.736672
C	0.382935	2.927016	0.721424
H	0.388522	4.019668	0.722892
C	-0.930403	3.523303	-1.439745
C	-2.203036	3.369662	-2.019156
C	-0.199643	4.680362	-1.762738
C	-2.714643	4.322022	-2.899031
H	-2.80425	2.506008	-1.750398
C	-0.709726	5.633404	-2.643064
H	0.790934	4.827797	-1.341115
C	-1.969919	5.458983	-3.217537
H	-3.704657	4.18152	-3.325611
H	-0.11783	6.512882	-2.883898
H	-2.370022	6.204668	-3.899317
C	2.897478	3.52459	0.715983
O	-1.146602	0.857685	3.518037
C	-2.485164	0.673326	3.500688
O	-3.226297	0.835421	2.559265
O	-2.846262	0.282328	4.73183
C	-4.255592	0.059302	4.896325
H	-4.378109	-0.249492	5.934703
H	-4.816147	0.977125	4.70014
H	-4.603484	-0.724679	4.218609
C	-0.845015	3.628504	2.901241
H	-0.040531	4.360052	3.059769
H	-1.102655	3.21959	3.884732
C	-2.045835	4.32763	2.306094
C	-2.099619	5.625164	2.003908
H	-2.903288	3.684705	2.108719
H	-2.988756	6.074683	1.570258
H	-1.256201	6.290424	2.180754
H	3.904299	3.094188	0.730524
H	2.820136	4.166805	-0.172824
H	2.799689	4.186335	1.588174

Isomer 0020050410



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

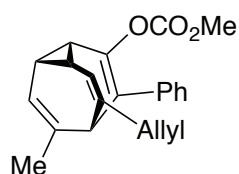
Sum of electronic and thermal Free Energies= -1076.835596 Hartree

Charge = 0 Multiplicity = 1

C	-0.016593	-0.009879	-0.008705
C	-0.001439	0.003483	1.525597
C	1.319687	0.011397	0.75204
H	-0.263282	-0.980152	-0.431078
H	-0.250701	-0.959506	1.963297
H	1.832966	-0.946456	0.757118
C	2.229129	1.172459	0.727844
C	1.873195	2.467665	0.708716
H	3.291305	0.930195	0.730132
C	-0.485467	1.143201	2.340398
C	-0.310435	2.417573	1.960409
C	-0.493377	1.122991	-0.819279
C	-0.343719	2.436014	-0.547151
H	-1.010807	0.846818	-1.735835
C	0.405037	2.894304	0.708734
H	0.373042	3.985277	0.744328
C	-0.920307	3.466767	-1.447021
C	-2.196937	3.294838	-2.011394
C	-0.21235	4.638143	-1.769834
C	-2.733262	4.243415	-2.880444
H	-2.781777	2.422667	-1.735527
C	-0.747657	5.587549	-2.639184
H	0.780038	4.799516	-1.357137
C	-2.010803	5.394244	-3.201075
H	-3.7262	4.09002	-3.295531
H	-0.173456	6.478361	-2.88122
H	-2.430999	6.136751	-3.874218
C	2.899306	3.570106	0.703321
C	-1.233009	0.769092	3.609987
H	-1.319214	1.651032	4.254047
C	-2.606682	0.21401	3.312055
C	-3.030833	-0.999473	3.667388
H	-3.263346	0.880024	2.752917
H	-4.031489	-1.348527	3.426223
H	-2.396714	-1.689255	4.221939

H	-0.651214	0.022134	4.166763
O	-0.745189	3.466564	2.800421
C	-1.993401	3.944104	2.591883
O	-2.811669	3.511408	1.81432
O	-2.161921	4.985659	3.4188
C	-3.45412	5.608112	3.33547
H	-3.426733	6.423827	4.058272
H	-3.631354	5.992332	2.327698
H	-4.241974	4.894721	3.591309
H	3.918732	3.170652	0.719909
H	2.803628	4.207194	-0.187447
H	2.777767	4.229214	1.574217

Isomer 0050040120



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

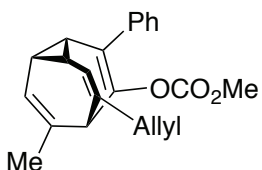
Sum of electronic and thermal Free Energies= -1076.834432 Hartree

Charge = 0 Multiplicity = 1

C	-0.216116	0.114002	0.096949
C	-0.203913	0.127249	1.622593
C	1.120913	0.030618	0.853896
H	-0.544861	-0.832985	-0.322045
H	-0.522968	-0.801756	2.083201
H	1.559044	-0.963749	0.869842
C	2.109182	1.122094	0.835429
C	1.845292	2.440592	0.83306
H	3.151399	0.804553	0.815379
C	-0.569218	1.311402	2.419123
C	-0.318698	2.605524	2.146426
C	-0.595529	1.288318	-0.709247
C	-0.338515	2.574399	-0.417229
H	-1.131623	1.064476	-1.630485
C	0.416407	2.982405	0.847258
H	0.49089	4.072537	0.851154
C	-0.763463	3.687303	-1.340245
C	2.968381	3.461578	0.801132
H	3.923556	2.929568	0.687048
H	2.858838	4.109646	-0.081149
C	3.019712	4.327407	2.037197

C	2.904602	5.65595	2.046583
H	3.148276	3.793468	2.979289
H	2.942518	6.227708	2.969746
H	2.769521	6.224464	1.128082
O	-1.181258	0.986695	3.649845
C	-2.452599	0.529807	3.598339
O	-3.121839	0.371345	2.605006
O	-2.832323	0.275581	4.85916
C	-4.177211	-0.211032	4.987252
H	-4.88998	0.521588	4.59976
H	-4.300265	-1.152254	4.444796
H	-4.327273	-0.362698	6.056447
C	-0.720274	3.711662	3.059403
C	-0.399974	3.695236	4.427703
C	-1.409365	4.828341	2.556018
C	-0.760913	4.754171	5.259753
H	0.13817	2.847182	4.836983
C	-1.776362	5.884398	3.388864
H	-1.677452	4.861884	1.503416
C	-1.451896	5.852956	4.745982
H	-0.497173	4.720669	6.313824
H	-2.318335	6.731436	2.976019
H	-1.733063	6.677234	5.396126
H	0.10074	4.275309	-1.680717
H	-1.279185	3.301559	-2.225774
H	-1.440615	4.392483	-0.838057

Isomer 0050040210



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

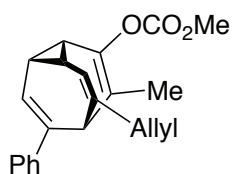
Sum of electronic and thermal Free Energies= -1076.834003 Hartree

Charge = 0 Multiplicity = 1

C	0.016622	0.02092	-0.062641
C	-0.032645	0.007733	1.468104
C	1.32291	0.03617	0.740411
H	-0.194874	-0.943529	-0.513714
H	-0.286954	-0.963092	1.885494
H	1.840094	-0.919542	0.73915
C	2.228706	1.199396	0.78675

C	1.869821	2.494483	0.793465
H	3.29089	0.958862	0.818275
C	-0.517186	1.144016	2.273204
C	-0.344288	2.448548	2.002531
H	-1.052608	0.872863	3.182598
C	-0.442592	1.157325	-0.906002
C	-0.275132	2.435686	-0.520592
C	0.400302	2.912263	0.751742
H	0.354616	4.004128	0.719012
C	2.886025	3.604343	0.842358
C	-0.86017	3.524652	2.939626
H	-0.017547	4.124237	3.316668
H	-1.314986	3.036065	3.813179
C	-1.868241	4.450263	2.301096
C	-1.732311	5.774774	2.212611
H	-2.747458	3.969447	1.874854
H	-2.491373	6.397554	1.746213
H	-0.861005	6.29058	2.612973
C	-1.105586	0.789536	-2.191262
C	-0.684455	1.330122	-3.417167
C	-2.151954	-0.147779	-2.199815
C	-1.293929	0.946919	-4.611748
H	0.128094	2.049233	-3.429817
C	-2.763209	-0.52795	-3.393984
H	-2.500975	-0.565515	-1.259252
C	-2.334919	0.016689	-4.605892
H	-0.948752	1.372724	-5.550444
H	-3.577653	-1.247598	-3.376313
H	-2.807941	-0.281726	-5.537772
O	-0.684619	3.488765	-1.360184
C	-1.997379	3.817996	-1.37338
O	-2.877842	3.317471	-0.715624
O	-2.139833	4.814671	-2.258796
C	-3.486334	5.290374	-2.40454
H	-3.858121	5.690724	-1.457465
H	-3.43344	6.077239	-3.157487
H	-4.145267	4.484049	-2.736768
H	3.909062	3.214707	0.872715
H	2.797533	4.262661	-0.033141
H	2.739363	4.240614	1.726735

Isomer 0020040150



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

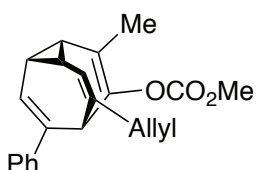
Sum of electronic and thermal Free Energies= -1076.836921 Hartree

Charge = 0 Multiplicity = 1

C	-0.007225	0.053623	0.16682
C	0.043136	0.139449	1.699229
C	1.343497	0.085148	0.904805
H	-0.278469	-0.93014	-0.206533
H	-0.211069	-0.784576	2.207265
H	1.840013	-0.880112	0.949339
C	2.267067	1.2296	0.815472
C	1.92506	2.52738	0.756292
H	3.325432	0.971584	0.804382
C	-0.398894	1.342444	2.429159
C	-0.256315	2.625358	2.065471
C	-0.481995	1.160784	-0.67698
C	-0.312135	2.482353	-0.454104
H	-1.016613	0.857366	-1.574867
C	0.469089	2.986318	0.764164
H	0.475078	4.077881	0.72428
C	-0.901059	3.478825	-1.386526
C	-2.179409	3.27954	-1.94014
C	-0.205002	4.644561	-1.754231
C	-2.729112	4.194708	-2.836317
H	-2.754892	2.408726	-1.639754
C	-0.753066	5.560406	-2.651088
H	0.789011	4.826918	-1.355248
C	-2.018235	5.340401	-3.198174
H	-3.722335	4.018662	-3.241609
H	-0.186942	6.446707	-2.926219
H	-2.448319	6.057488	-3.892152
C	2.990081	3.608575	0.703717
H	3.969021	3.130672	0.558731
H	2.826833	4.265043	-0.163521
C	3.029752	4.450324	1.957286
C	2.822168	5.767617	2.006635
H	3.237604	3.904228	2.878133
H	2.867135	6.320037	2.941553
H	2.610371	6.347697	1.110192

O	-1.164354	1.061448	3.586718
C	-0.516557	0.50403	4.631176
O	0.654732	0.208684	4.683603
O	-1.418496	0.332015	5.61042
C	-0.890788	-0.259417	6.807597
H	-0.486657	-1.254037	6.600863
H	-0.100865	0.366357	7.231294
H	-1.736402	-0.324861	7.492713
C	-0.797714	3.778763	2.867223
H	0.015297	4.459534	3.151812
H	-1.501521	4.36534	2.260884
H	-1.316841	3.450957	3.769297

Isomer 0020040510



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

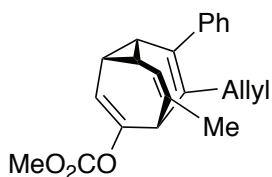
Sum of electronic and thermal Free Energies= -1076.836896 Hartree

Charge = 0 Multiplicity = 1

C	0.015084	-0.01259	-0.024618
C	0.007178	-0.018232	1.511991
C	1.339074	-0.019348	0.761284
H	-0.243528	-0.972471	-0.463426
H	-0.249381	-0.987061	1.933299
H	1.838013	-0.98484	0.765282
C	2.265375	1.127912	0.744062
C	1.924634	2.426832	0.730617
H	3.323822	0.87033	0.723113
C	-0.490058	1.112633	2.335192
C	-0.262022	2.388508	1.992047
C	-0.429901	1.140823	-0.824245
C	-0.252997	2.447097	-0.531686
H	-0.976627	0.888949	-1.73094
C	0.464227	2.873571	0.752974
H	0.456656	3.963432	0.804987
C	-0.757172	3.505578	-1.443029
C	-0.64965	3.370064	-2.838817
C	-1.36709	4.668831	-0.938317
C	-1.145223	4.350315	-3.697242
H	-0.148173	2.497501	-3.247904

C	-1.864208	5.647966	-1.7972
H	-1.479729	4.79466	0.13523
C	-1.755896	5.494553	-3.180762
H	-1.041703	4.225535	-4.772221
H	-2.341993	6.531994	-1.3827
H	-2.137464	6.261794	-3.849124
C	2.974327	3.520909	0.677643
H	3.96442	3.0511	0.590429
H	2.8294	4.129116	-0.227535
C	2.953137	4.42759	1.885235
C	2.769296	5.748542	1.839534
H	3.07837	3.934239	2.848169
H	2.767787	6.356737	2.740624
H	2.624382	6.27536	0.897989
C	-1.246807	0.730745	3.584037
O	-0.803491	3.438506	2.766553
C	-0.128886	3.816304	3.875112
O	0.870917	3.308402	4.325721
O	-0.788079	4.860793	4.399081
C	-0.204508	5.390875	5.598786
H	-0.162447	4.625874	6.378545
H	0.806048	5.759904	5.404269
H	-0.85894	6.209387	5.899691
H	-0.557808	0.393819	4.369922
H	-1.829127	1.565275	3.980261
H	-1.937177	-0.095926	3.377417

Isomer 0010050240



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

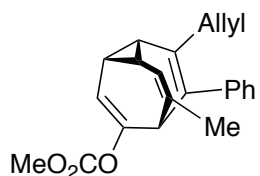
Sum of electronic and thermal Free Energies= -1076.830554 Hartree

Charge = 0 Multiplicity = 1

C	-0.00127	0.035775	-0.063039
C	0.001953	0.06542	1.472065
C	1.328055	0.023298	0.69893
H	-0.259946	-0.934866	-0.474666
H	-0.269552	-0.883285	1.927659
H	1.807743	-0.95151	0.710399
C	2.295475	1.137233	0.671809

C	1.928055	2.424148	0.632822
H	3.344333	0.876134	0.677271
C	-0.435135	1.242335	2.243268
C	-0.240975	2.528363	1.90815
H	-0.963048	1.024439	3.171109
C	-0.463365	1.163306	-0.921667
C	-0.262877	2.470681	-0.631094
C	0.494811	2.915599	0.624508
H	0.556305	4.006642	0.601243
O	2.79092	3.531816	0.58689
C	4.13654	3.456003	0.604657
O	4.831592	2.468713	0.675989
O	4.585507	4.719739	0.528404
C	6.016079	4.844892	0.537194
H	6.210182	5.915486	0.468886
H	6.433087	4.437225	1.461889
H	6.454352	4.31982	-0.315623
C	-0.727726	3.661261	2.772735
C	-1.191513	0.716249	-2.151694
C	-0.724736	1.033133	-3.43713
C	-2.341298	-0.084033	-2.040452
C	-1.394366	0.576726	-4.573868
H	0.170744	1.638452	-3.540527
C	-3.012737	-0.537557	-3.175451
H	-2.717452	-0.34002	-1.052935
C	-2.540867	-0.208994	-4.448066
H	-1.013418	0.830828	-5.559863
H	-3.90647	-1.146649	-3.065658
H	-3.060936	-0.565254	-5.333377
C	-0.800588	3.616447	-1.473685
H	-1.549444	3.265562	-2.187957
H	-1.316574	4.314303	-0.79248
C	0.27967	4.382107	-2.206893
C	0.244846	4.689166	-3.504354
H	1.136718	4.698786	-1.611123
H	1.04424	5.252366	-3.978962
H	-0.586265	4.392606	-4.141129
H	0.105267	4.301326	3.095899
H	-1.425831	4.310616	2.225415
H	-1.240559	3.294094	3.667929

Isomer 0010050420



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

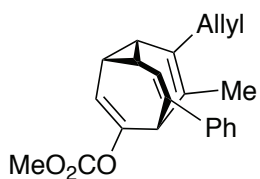
Sum of electronic and thermal Free Energies= -1076.830234 Hartree

Charge = 0 Multiplicity =1

C	-0.110404	0.036358	-0.025065
C	-0.097811	0.020474	1.506093
C	1.227149	0.01503	0.730393
H	-0.377529	-0.919757	-0.467124
H	-0.341065	-0.953767	1.923008
H	1.718722	-0.954115	0.721414
C	2.160489	1.155023	0.730447
C	1.825254	2.455332	0.753331
H	3.217486	0.893166	0.695095
C	-0.560485	1.144374	2.360006
C	-0.377714	2.451354	2.059966
C	-0.574185	1.187834	-0.823859
C	-0.368848	2.462104	-0.464224
H	-1.105605	0.96697	-1.738765
C	0.364564	2.901574	0.788768
H	0.347302	3.993069	0.777948
O	-0.768941	3.597573	-1.184606
C	-1.511601	3.568702	-2.308488
O	-1.960779	2.605784	-2.887297
O	-1.672465	4.847274	-2.68665
C	-2.452835	5.022188	-3.878998
H	-3.461917	4.624686	-3.741348
H	-2.485097	6.099283	-4.044458
H	-1.981475	4.51729	-4.726443
C	2.863946	3.545486	0.712374
C	-1.244062	0.683506	3.643283
H	-0.598141	-0.081804	4.104482
H	-1.320155	1.503776	4.360576
C	-2.611768	0.079216	3.41726
C	-3.717562	0.428779	4.075663
H	-2.673199	-0.70227	2.658714
H	-4.673853	-0.049578	3.880383
H	-3.707957	1.205948	4.837226
C	-0.892763	3.5626	2.916237
C	-2.270422	3.755982	3.107804

C	-0.006349	4.478618	3.508797
C	-2.744765	4.822519	3.873688
H	-2.96906	3.062336	2.650152
C	-0.478837	5.54229	4.276522
H	1.064711	4.343768	3.378427
C	-1.851783	5.719419	4.461247
H	-3.815793	4.954425	4.005586
H	0.22635	6.232216	4.733162
H	-2.221088	6.550562	5.056166
H	3.878515	3.134383	0.682786
H	2.729857	4.185113	-0.171191
H	2.791457	4.206779	1.58721

Isomer 0010020450



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

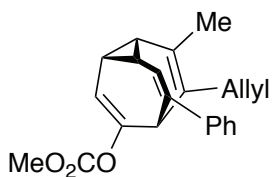
Sum of electronic and thermal Free Energies= -1076.832444 Hartree

Charge = 0 Multiplicity = 1

C	-0.087077	0.038438	0.125024
C	-0.0503	0.073042	1.650456
C	1.266748	0.04048	0.86465
H	-0.352543	-0.932375	-0.284525
H	-0.284068	-0.88515	2.106618
H	1.758492	-0.928418	0.873441
C	2.199592	1.175765	0.816828
C	1.873319	2.485571	0.813154
H	3.25233	0.907516	0.750983
C	-0.497536	1.224111	2.479832
C	-0.290551	2.516958	2.148159
C	-0.551383	1.162229	-0.710802
C	-0.336466	2.444427	-0.390805
H	-1.078424	0.913874	-1.62122
C	0.406246	2.920968	0.841032
H	0.381517	4.010623	0.799824
O	-0.724949	3.562863	-1.147549
C	-1.412929	3.504274	-2.305122
O	-1.832217	2.526156	-2.879963
O	-1.558845	4.773251	-2.720648
C	-2.281545	4.91677	-3.953378

H	-2.309049	5.989485	-4.145802
H	-1.767883	4.393962	-4.764485
H	-3.294725	4.518143	-3.854974
C	2.923456	3.534172	0.763246
C	4.122923	3.389498	1.484217
C	2.758707	4.696793	-0.012568
C	5.122905	4.35833	1.420888
H	4.255709	2.518534	2.119693
C	3.759447	5.665512	-0.075816
H	1.851627	4.831662	-0.595622
C	4.946809	5.50221	0.639975
H	6.036645	4.225367	1.994715
H	3.611467	6.54895	-0.691681
H	5.723561	6.260842	0.594971
C	-1.197918	0.780212	3.761247
H	-1.969398	0.039719	3.508602
H	-1.721901	1.62078	4.226798
C	-0.244366	0.172325	4.762691
C	-0.322558	-1.069888	5.242204
H	0.567285	0.822635	5.091544
H	0.395181	-1.452027	5.963367
H	-1.114746	-1.751653	4.937814
C	-0.687349	3.709379	2.986739
H	0.194069	4.330874	3.197234
H	-1.393603	4.350041	2.4399
H	-1.14248	3.453145	3.944945

Isomer 0010020540



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

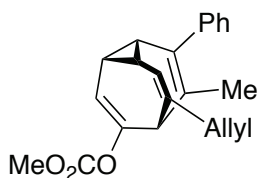
Sum of electronic and thermal Free Energies= -1076.832404 Hartree

Charge = 0 Multiplicity = 1

C	-0.008381	-0.011699	-0.054959
C	-0.008356	-0.009462	1.479912
C	1.320063	-0.009057	0.696997
H	-0.253915	-0.985003	-0.473288
H	-0.253479	-0.97184	1.921119
H	1.821151	-0.973156	0.697703
C	2.25861	1.129	0.705765

C	1.855522	2.405171	0.69453
H	3.314047	0.895136	0.726298
C	-0.464438	1.139365	2.277548
C	-0.312633	2.444576	1.968428
H	-0.945549	0.886351	3.220403
C	-0.518297	1.113046	-0.886027
C	-0.353577	2.415331	-0.566326
C	0.411631	2.861968	0.685317
H	0.449236	3.951261	0.654574
O	2.695855	3.526785	0.769843
C	4.022579	3.496309	0.535522
O	4.703008	2.551431	0.208223
O	4.469894	4.747386	0.73221
C	5.880262	4.91468	0.522274
H	6.078019	5.966599	0.729577
H	6.45012	4.275503	1.201907
C	-0.827014	3.5068	2.869413
C	-2.066706	3.364279	3.518945
C	-0.088795	4.680791	3.109158
C	-2.542926	4.346713	4.38548
H	-2.670667	2.483985	3.317795
C	-0.56517	5.662402	3.977152
H	0.879759	4.814354	2.634935
C	-1.794046	5.501355	4.619981
H	-3.508231	4.215515	4.868054
H	0.029743	6.554743	4.154595
H	-2.167031	6.270411	5.291093
C	-1.245921	0.619774	-2.119789
C	-0.893014	3.579245	-1.386361
H	-1.644617	3.237866	-2.105646
H	-1.406844	4.279619	-0.713439
C	0.199386	4.319022	-2.123527
C	0.521775	5.599376	-1.934664
H	0.759401	3.726089	-2.847846
H	1.323892	6.076409	-2.491616
H	-0.008173	6.222443	-1.21663
H	6.148427	4.669923	-0.508944
H	-0.582465	-0.014316	-2.723629
H	-2.104433	-0.005792	-1.838481
H	-1.613385	1.41679	-2.767172

Isomer 0010040250



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

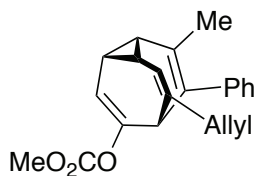
Sum of electronic and thermal Free Energies= -1076.832114 Hartree

Charge = 0 Multiplicity = 1

C	0.006276	0.019206	-0.01438
C	0.002441	0.037512	1.517535
C	1.334889	-0.005593	0.755622
H	-0.267235	-0.94326	-0.43854
H	-0.2617	-0.918347	1.959602
H	1.813531	-0.981041	0.772019
C	2.281965	1.121722	0.753731
C	1.962793	2.426369	0.751329
H	3.336424	0.84647	0.762403
C	-0.444942	1.194877	2.343715
C	-0.244293	2.492	2.010817
C	-0.437383	1.158027	-0.841851
C	-0.218161	2.437357	-0.509855
H	-0.964783	0.923313	-1.755777
C	0.510485	2.895911	0.739169
H	0.518066	3.987667	0.692429
O	-0.645424	3.560813	-1.233559
C	-1.211147	3.513662	-2.454743
O	-1.438712	2.542948	-3.140432
O	-1.487679	4.784323	-2.791949
C	-2.10347	4.93779	-4.079632
H	-1.446005	4.563836	-4.869082
H	-3.053679	4.398633	-4.119875
H	-2.266283	6.00981	-4.193302
C	3.034424	3.500846	0.75123
H	2.891638	4.174261	1.609285
H	4.013633	3.01927	0.884044
C	3.047249	4.321822	-0.516433
C	2.852583	5.639663	-0.578234
H	3.218886	3.760362	-1.43562
H	2.867794	6.177752	-1.522206
H	2.673114	6.233632	0.316127
C	-1.160614	0.793559	3.596573
C	-0.656339	1.123629	4.864272

C	-2.336042	0.026986	3.52962
C	-1.312687	0.715542	6.026517
H	0.26474	1.696082	4.93345
C	-2.994942	-0.379783	4.689624
H	-2.741881	-0.238876	2.556596
C	-2.485573	-0.036364	5.943701
H	-0.902387	0.980435	6.997762
H	-3.908983	-0.963347	4.613731
H	-2.996744	-0.355137	6.848232
C	-0.776433	3.662528	2.801817
H	0.043558	4.286503	3.185995
H	-1.376991	4.311547	2.149261
H	-1.397083	3.361547	3.647039

Isomer 0010040520



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

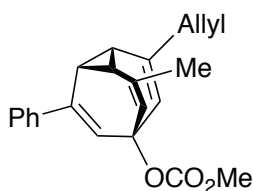
Sum of electronic and thermal Free Energies= -1076.831812 Hartree

Charge = 0 Multiplicity = 1

C	-0.048895	0.003013	0.029269
C	0.003634	-0.010296	1.562085
C	1.305566	0.010734	0.754865
H	-0.305635	-0.959069	-0.405589
H	-0.217376	-0.988354	1.982616
H	1.817767	-0.947567	0.731645
C	2.213402	1.170859	0.72709
C	1.847519	2.462432	0.75851
H	3.274585	0.933244	0.656563
C	-0.471532	1.101586	2.427221
C	-0.295185	2.414871	2.142029
C	-0.564814	1.143879	-0.751304
C	-0.381208	2.420668	-0.389751
H	-1.120575	0.91258	-1.649035
C	0.379876	2.877133	0.839199
H	0.349508	3.967756	0.832736
O	-0.869421	3.54868	-1.071133
C	-1.542481	3.508539	-2.237956
O	-1.833375	2.54178	-2.904414
O	-1.843708	4.781733	-2.542731

C	-2.570164	4.944376	-3.770648
H	-3.523133	4.410302	-3.728656
H	-2.736282	6.017718	-3.864941
H	-1.986917	4.570537	-4.616388
C	2.873956	3.577754	0.68747
H	2.674119	4.20827	-0.191439
H	3.867187	3.130391	0.539624
C	2.892539	4.451573	1.91863
C	2.65258	5.763338	1.927965
H	3.108051	3.938782	2.856677
H	2.672413	6.342768	2.846931
H	2.426466	6.308941	1.01367
C	-1.223221	0.606478	3.645342
C	-0.74644	3.513826	3.045174
C	-0.308441	3.596918	4.377379
C	-1.590716	4.530807	2.564536
C	-0.713627	4.644668	5.205459
H	0.368165	2.837289	4.758958
C	-1.998945	5.576308	3.39127
H	-1.934791	4.496243	1.533894
C	-1.563366	5.637696	4.716822
H	-0.35715	4.687846	6.231645
H	-2.659883	6.345	2.998784
H	-1.878682	6.454978	5.360074
H	-1.706981	1.410187	4.201249
H	-1.997205	-0.110292	3.339163
H	-0.556147	0.068887	4.334059

Isomer 0200500401



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

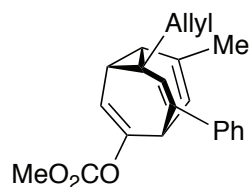
Sum of electronic and thermal Free Energies= -1076.834787 Hartree

Charge = 0 Multiplicity = 1

C	0.017219	0.023453	0.052579
C	0.02277	0.052409	1.589055
C	1.345884	0.05505	0.820155
H	-0.221757	-0.952866	-0.362937
H	-0.195167	-0.908956	2.043237

H	1.852405	-0.905695	0.852472
C	2.280522	1.204013	0.777395
C	1.893458	2.487999	0.760278
H	2.639598	3.275849	0.721395
C	-0.471652	1.206234	2.383236
C	-0.293922	2.491424	2.021497
H	-0.727776	3.279204	2.627443
C	-0.468223	1.152115	-0.776388
C	-0.281427	2.445233	-0.466725
H	-0.665525	3.227623	-1.115692
C	0.444071	2.934107	0.774306
C	-1.211213	0.759293	-2.031296
C	3.758837	0.844299	0.748254
H	3.970099	0.203014	-0.119638
H	4.339549	1.766788	0.613253
C	4.218277	0.141559	2.003156
C	4.769362	-1.072451	2.042874
H	4.065897	0.69382	2.931026
H	5.08407	-1.52813	2.97798
H	4.936543	-1.654871	1.138371
C	-1.213285	0.894614	3.637365
C	-0.994977	1.650873	4.801854
C	-2.152743	-0.14938	3.691237
C	-1.702366	1.382554	5.972978
H	-0.245804	2.437378	4.786672
C	-2.860157	-0.417602	4.862584
H	-2.351652	-0.739603	2.80058
C	-2.638532	0.347436	6.009142
H	-1.511422	1.975953	6.863525
H	-3.590326	-1.222796	4.877305
H	-3.186159	0.135094	6.923477
O	0.372652	4.3881	0.644365
C	0.909333	5.150906	1.607779
O	1.464869	4.778892	2.618589
O	0.719805	6.433321	1.25084
C	1.234966	7.394084	2.184551
H	1.004899	8.367761	1.751086
H	0.751004	7.284263	3.158745
H	2.314749	7.274131	2.306893
H	-0.580712	0.147609	-2.690995
H	-2.098865	0.156924	-1.79417
H	-1.539105	1.638131	-2.594569

Isomer 0014020500



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

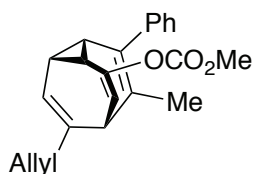
Sum of electronic and thermal Free Energies= -1076.835041 Hartree

Charge = 0 Multiplicity = 1

C	-0.045225	0.02249	-0.056999
C	-0.021823	0.023547	1.484188
C	1.295203	0.024741	0.684197
H	-0.298978	-0.949096	-0.477416
H	1.787348	-0.944792	0.680097
C	2.258223	1.144657	0.667242
C	1.894693	2.433857	0.654148
H	3.3069	0.882447	0.673903
C	-0.435116	1.214092	2.258464
C	-0.251548	2.515646	1.950501
H	-0.923345	0.983369	3.203115
C	-0.531834	1.159464	-0.874236
C	-0.305724	2.445887	-0.563293
H	-0.703552	3.219536	-1.216875
C	0.461082	2.924448	0.658494
H	0.501771	4.013328	0.613299
C	-1.317053	0.779675	-2.106824
O	2.760042	3.538219	0.67413
C	4.104118	3.460126	0.601467
O	4.79263	2.471729	0.492338
O	4.558586	4.721841	0.670423
C	5.987844	4.844664	0.602934
H	6.186846	5.914159	0.673905
H	6.460239	4.310091	1.431277
H	6.364712	4.445893	-0.342618
C	-0.386999	-1.3074	2.154979
H	0.021661	-2.126873	1.546162
H	0.105935	-1.369995	3.134522
C	-1.871045	-1.503833	2.319188
C	-2.489688	-1.737776	3.477515
H	-2.460831	-1.438713	1.403554
H	-3.566156	-1.875865	3.534865
H	-1.940617	-1.807082	4.414808

C	-0.730067	3.58477	2.863833
C	-1.958397	3.462203	3.538508
C	0.032831	4.745417	3.088851
C	-2.39942	4.452202	4.414833
H	-2.580465	2.591861	3.35033
C	-0.40843	5.734709	3.96673
H	0.992849	4.86363	2.593538
C	-1.626342	5.593903	4.634382
H	-3.356623	4.337212	4.917232
H	0.204828	6.616938	4.131806
H	-1.972518	6.36877	5.313147
H	-0.717322	0.156667	-2.784526
H	-2.208602	0.193087	-1.844914
H	-1.645508	1.664211	-2.661258

Isomer 0040100250



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

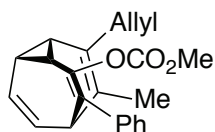
Sum of electronic and thermal Free Energies= -1076.832576 Hartree

Charge = 0 Multiplicity = 1

C	0.091796	0.039439	-0.084274
C	0.070228	0.040651	1.45139
C	1.405679	0.045947	0.698123
H	-0.160423	-0.910051	-0.545256
H	-0.190125	-0.924511	1.877982
H	1.896545	-0.922372	0.688018
C	2.373754	1.180327	0.706821
C	2.011815	2.485089	0.719647
C	-0.407561	1.190017	2.240137
C	-0.220021	2.486671	1.94186
C	-0.361183	1.194331	-0.880844
C	-0.175978	2.485324	-0.581008
C	0.542173	2.918215	0.690229
H	0.542607	4.011947	0.680671
C	-0.777495	3.583817	2.830056
H	-1.407437	4.260235	2.234454
H	-1.428731	3.126549	3.588401
C	0.294063	4.39245	3.522228
C	0.476218	5.7071	3.383004

H	0.957473	3.825928	4.177069
H	1.263319	6.235902	3.914194
H	-0.163766	6.307738	2.73917
H	-0.971107	0.937476	3.137925
O	-1.012387	0.696156	-2.024879
H	-0.552676	3.252145	-1.241976
C	-1.630509	1.458986	-2.945173
O	-1.739293	2.663709	-2.974787
O	-2.126924	0.612722	-3.863308
C	-2.831514	1.248613	-4.940397
H	-3.16019	0.434936	-5.587332
H	-3.690658	1.808968	-4.562034
H	-2.171702	1.929373	-5.48486
C	3.805487	0.741585	0.703007
C	4.673451	1.086737	-0.345109
C	4.302145	-0.077482	1.7311
C	5.996486	0.642655	-0.357957
H	4.299139	1.699473	-1.160602
C	5.624318	-0.521228	1.721196
H	3.646107	-0.356156	2.552306
C	6.477612	-0.162257	0.675706
H	6.649392	0.920251	-1.181645
H	5.989371	-1.145842	2.532644
H	7.507255	-0.50987	0.665433
C	2.990219	3.631882	0.798848
H	4.020819	3.306699	0.949488
H	2.955681	4.240452	-0.116462
H	2.712335	4.300155	1.624373

Isomer 0000120450



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

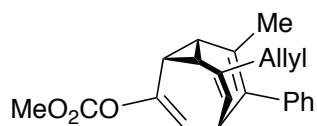
Sum of electronic and thermal Free Energies= -1076.828829 Hartree

Charge = 0 Multiplicity =1

C	0.105302	0.010941	0.089959
C	0.112959	0.079849	1.623617
C	1.43404	0.090906	0.86913
H	-0.104331	-0.976761	-0.311654
H	-0.083067	-0.880358	2.092783
H	1.983598	-0.844259	0.908442

C	2.322761	1.261737	0.798507
C	1.976255	2.559918	0.754911
C	-0.425807	1.221879	2.412045
C	-0.2441	2.517786	2.076162
C	-0.376039	1.125596	-0.741706
C	-0.221497	2.42545	-0.451035
H	-0.890082	0.847252	-1.660043
H	-0.610989	3.171053	-1.14089
C	0.485053	2.936171	0.793548
H	0.450007	4.027251	0.752519
O	3.685726	0.906743	0.684464
C	4.338411	0.631173	1.834812
O	3.874685	0.653573	2.951055
O	5.600937	0.320472	1.510821
C	6.444291	0.011767	2.631813
H	6.50787	0.8658	3.310996
H	6.058432	-0.853256	3.177656
H	7.421694	-0.210398	2.20295
C	2.972659	3.658537	0.629615
C	3.958421	3.646886	-0.372423
C	2.924874	4.762819	1.497785
C	4.864457	4.699345	-0.49618
H	4.006943	2.808656	-1.059131
C	3.834686	5.812507	1.377937
H	2.179952	4.789116	2.288351
C	4.808289	5.786307	0.378073
H	5.614187	4.670873	-1.282747
H	3.783277	6.650164	2.068753
H	5.515118	6.605998	0.2801
C	-1.214865	0.774962	3.631563
H	-1.92454	1.54764	3.949546
H	-1.851489	-0.07496	3.336985
C	-0.392693	0.347964	4.830107
C	0.932641	0.42791	4.955076
H	-0.980273	-0.059107	5.655224
H	1.425839	0.092967	5.864259
H	1.576791	0.81449	4.17046
C	-0.754888	3.684394	2.889353
H	0.068421	4.368577	3.135934
H	-1.484405	4.27347	2.315134
H	-1.221059	3.394515	3.831937

Isomer 0100400520



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

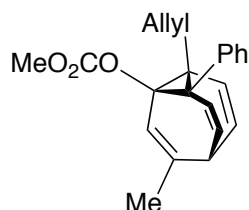
Sum of electronic and thermal Free Energies= -1076.832339 Hartree

Charge = 0 Multiplicity = 1

C	-0.049068	0.022425	-0.03563
C	-0.029922	0.036026	1.497256
C	1.286856	0.016356	0.713293
H	-0.298598	-0.953701	-0.44437
H	-0.282827	-0.9251	1.937117
H	1.80227	-0.938738	0.716476
C	2.218187	1.159553	0.67582
C	1.879195	2.453298	0.644659
H	2.645827	3.213901	0.614462
C	-0.483996	1.193058	2.302627
C	-0.290643	2.468131	1.928888
H	-0.65476	3.26443	2.576087
C	-0.536527	1.138653	-0.889259
C	-0.348679	2.447498	-0.597816
C	0.421921	2.892502	0.656645
H	0.431284	3.984393	0.647424
O	3.528531	0.645981	0.690051
C	4.638933	1.389712	0.530635
O	4.725696	2.583563	0.354328
O	5.675854	0.538305	0.602895
C	6.963998	1.15455	0.454095
H	7.048574	1.641644	-0.520987
H	7.13051	1.895737	1.240326
H	7.682818	0.339173	0.538244
C	-1.200762	0.853623	3.600622
H	-1.400843	1.788525	4.141725
H	-0.544982	0.247902	4.242758
C	-2.497528	0.110892	3.384981
C	-2.777698	-1.099825	3.869619
H	-3.237817	0.628385	2.773374
H	-3.731559	-1.585954	3.682357
H	-2.064693	-1.648638	4.482368
C	-1.231349	0.654387	-2.144248
C	-0.872652	3.556121	-1.448499
C	-2.249922	3.729793	-1.661651
C	0.007653	4.495328	-2.014362

C	-2.730915	4.794467	-2.425497
H	-2.946024	3.027234	-1.211586
C	-0.470926	5.557856	-2.779783
H	1.0781	4.378836	-1.862679
C	-1.843303	5.711873	-2.989172
H	-3.801703	4.909708	-2.573963
H	0.229696	6.265338	-3.216082
H	-2.216733	6.541646	-3.583396
H	-0.583185	-0.046198	-2.688452
H	-2.150992	0.103667	-1.901095
H	-1.493612	1.468017	-2.821432

Isomer 1052004000



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

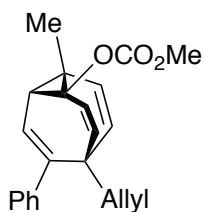
Sum of electronic and thermal Free Energies= -1076.814761 Hartree

Charge = 0 Multiplicity = 1

C	-0.029219	0.001486	-0.044681
C	-0.029763	-0.014718	1.496129
C	1.322414	-0.006343	0.769714
C	2.183144	1.204106	0.810534
C	1.80179	2.486817	0.873777
H	3.249884	0.991511	0.794871
H	2.57219	3.255128	0.89671
C	-0.548185	1.106727	2.316462
C	-0.400631	2.421592	2.0989
H	-1.113901	0.7891	3.188425
C	-0.472717	1.230767	-0.766733
C	-0.328077	2.509654	-0.39364
H	-0.974487	1.030674	-1.710538
H	-0.717891	3.285659	-1.049561
C	0.358065	2.95004	0.885103
H	0.3472	4.043613	0.92473
C	-0.400685	-1.239592	-0.827746
C	-1.552463	-1.987579	-0.546997
C	0.352687	-1.577291	-1.963157
C	-1.921615	-3.05917	-1.361885
H	-2.157871	-1.736225	0.316206

C	-0.015162	-2.647656	-2.778402
H	1.230957	-0.987565	-2.213516
C	-1.153814	-3.396592	-2.47704
H	-2.816183	-3.628987	-1.123937
H	0.586164	-2.892971	-3.650081
H	-1.443164	-4.231873	-3.109343
C	2.137994	-1.311926	0.736859
H	1.459959	-2.167191	0.821898
H	2.615103	-1.403064	-0.246847
C	3.199125	-1.396524	1.806973
C	4.483611	-1.667147	1.567519
H	2.863205	-1.232285	2.829186
H	5.210513	-1.743419	2.372092
H	4.858647	-1.831135	0.558465
O	-0.456562	-1.279222	2.019011
C	-0.011608	-1.645861	3.237008
O	0.738592	-1.028118	3.958402
O	-0.562204	-2.837554	3.513099
C	-0.188036	-3.388289	4.78614
H	0.892125	-3.549498	4.833045
H	-0.486788	-2.72018	5.598102
H	-0.719773	-4.337456	4.855082
C	-0.994619	3.443625	3.031406
H	-0.213978	4.093779	3.450217
H	-1.699908	4.100119	2.502722
H	-1.526527	2.973975	3.864997

Isomer 0021005004



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

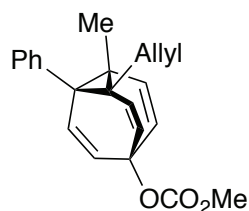
Sum of electronic and thermal Free Energies= -1076.817064 Hartree

Charge = 0 Multiplicity = 1

C	-0.090563	-0.003363	-0.03793
C	-0.007995	-0.030127	1.505365
C	1.268154	-0.052212	0.658229
H	-0.367062	-0.965468	-0.460844
C	2.220167	1.068329	0.553478
C	1.910029	2.370036	0.514088

H	3.260687	0.771437	0.452485
H	2.725771	3.078372	0.379441
C	-0.364002	1.191736	2.263601
C	-0.175698	2.46663	1.89864
H	-0.858186	1.005706	3.216474
H	-0.51617	3.244526	2.578178
C	-0.551122	1.154741	-0.824476
C	-0.323449	2.465258	-0.600603
H	-1.139962	0.895632	-1.702683
C	0.504235	2.951127	0.621677
C	-0.902585	3.448435	-1.569417
C	-2.275544	3.738155	-1.552181
C	-0.101739	4.074214	-2.539133
C	-2.831656	4.62961	-2.472061
H	-2.90643	3.256332	-0.810115
C	-0.655965	4.96411	-3.459058
H	0.959626	3.843189	-2.581834
C	-2.023351	5.246895	-3.427106
H	-3.897931	4.839065	-2.442156
H	-0.020204	5.431302	-4.206815
H	-2.455137	5.939915	-4.144282
O	1.891224	-1.329432	0.488944
C	2.667819	-1.756781	1.50732
O	2.897292	-1.170693	2.539782
O	3.145396	-2.962416	1.16146
C	4.006131	-3.564728	2.140852
H	4.305287	-4.520987	1.711114
H	4.88108	-2.935576	2.32427
H	3.471471	-3.717104	3.082151
C	-0.440677	-1.322133	2.184028
C	0.594515	4.504479	0.669683
H	1.11218	4.846695	-0.236489
H	-0.415033	4.927582	0.624895
C	1.309097	5.046486	1.879378
C	0.814855	5.975759	2.699406
H	2.305988	4.651391	2.076849
H	1.381801	6.350053	3.547724
H	-0.174585	6.404092	2.549536
H	0.049696	-1.426817	3.158232
H	-1.525004	-1.311346	2.345581
H	-0.200653	-2.202965	1.583759

Isomer 2004005001



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

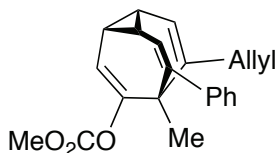
Sum of electronic and thermal Free Energies= -1076.808789 Hartree

Charge = 0 Multiplicity = 1

C	0.016594	0.051149	-0.006822
C	0.013542	0.052429	1.538294
C	1.373214	0.022159	0.763228
C	2.265049	1.218566	0.765255
C	1.93549	2.516337	0.764671
H	3.325912	0.980462	0.767597
H	2.710821	3.277395	0.766524
C	-0.375357	1.261505	2.315224
C	-0.185724	2.553086	2.023103
H	-0.882741	1.040871	3.251924
H	-0.525882	3.316739	2.715341
C	-0.382527	1.262535	-0.77802
C	-0.196458	2.553901	-0.483811
H	-0.891728	1.043069	-1.715451
H	-0.550204	3.31781	-1.168706
C	0.511133	3.026263	0.766848
C	-0.452513	-1.207755	-0.738299
C	2.209524	-1.24002	0.764575
C	2.652229	-1.810352	-0.437996
C	2.686146	-1.781409	1.968011
C	3.51617	-2.906535	-0.438895
H	2.323828	-1.384452	-1.381578
C	3.549693	-2.87761	1.971509
H	2.383326	-1.332798	2.9099
C	3.96426	-3.447947	0.76689
H	3.843461	-3.333162	-1.383564
H	3.902745	-3.281906	2.916704
H	4.63662	-4.301681	0.767785
C	-0.450561	-1.22311	2.267282
H	-0.015547	-1.229522	3.275307
H	-0.060869	-2.11458	1.768845
C	-1.950669	-1.323553	2.380928
C	-2.61976	-1.467507	3.525823
H	-2.507483	-1.276229	1.44503

H	-3.703177	-1.548604	3.549799
H	-2.108129	-1.515249	4.485563
O	0.661803	4.475828	0.766447
C	-0.443269	5.23679	0.770001
O	-1.594137	4.859104	0.767385
O	-0.042464	6.51984	0.776188
C	-1.111556	7.477853	0.780088
H	-0.623434	8.452813	0.785518
H	-1.734432	7.365786	-0.111401
H	-1.736036	7.356616	1.669231
H	-0.122148	-2.138651	-0.279133
H	-1.547709	-1.221158	-0.792129
H	-0.077963	-1.204365	-1.768593

Isomer 0010020045



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

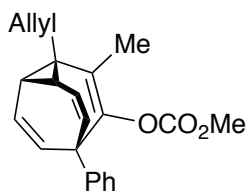
Sum of electronic and thermal Free Energies= -1076.813325 Hartree

Charge = 0 Multiplicity = 1

C	0.026244	0.039351	-0.028399
C	-0.061541	0.000836	1.502071
C	1.303965	-0.018817	0.809429
H	-0.229523	-0.899544	-0.511797
H	-0.367509	-0.958852	1.909236
H	1.789521	-0.990512	0.813399
C	2.23955	1.11069	0.893175
C	1.909708	2.407894	0.887508
H	3.292581	0.85474	0.950477
C	-0.53379	1.157904	2.275696
C	-0.326583	2.468942	2.038865
H	-1.12438	0.904094	3.154331
C	-0.366198	1.23124	-0.793924
C	-0.196476	2.53281	-0.486404
H	-0.864226	1.008632	-1.737099
C	0.493424	3.003412	0.825778
C	-0.708205	3.554729	-1.49054
H	-1.510622	3.085743	-2.079095
H	-1.192698	4.3962	-0.980643
C	0.307757	4.113339	-2.468755

C	1.538621	3.652949	-2.695953
H	-0.053788	4.96346	-3.050351
H	2.178375	4.116303	-3.442741
H	1.957682	2.809593	-2.155046
O	2.923427	3.372567	1.033539
C	3.981051	3.401671	0.193056
O	4.216108	2.653054	-0.72586
O	4.7432	4.437844	0.575909
C	5.925328	4.632014	-0.215751
H	6.56657	3.747506	-0.175725
H	5.662026	4.836904	-1.25677
H	6.429403	5.491132	0.22755
C	-0.942435	3.434249	3.007164
C	-0.176981	4.047027	4.012564
C	-2.317416	3.709198	2.957222
C	-0.767284	4.91129	4.934483
H	0.886225	3.830838	4.077765
C	-2.909962	4.575399	3.878652
H	-2.922128	3.234787	2.188823
C	-2.136211	5.18067	4.869283
H	-0.157946	5.369837	5.709148
H	-3.977402	4.77362	3.822706
H	-2.595942	5.853835	5.588084
C	0.578765	4.544207	0.87935
H	1.09104	4.933845	-0.002304
H	-0.42104	4.980509	0.928505
H	1.125381	4.877508	1.76163

Isomer 0000004512



RB3LYP/6-31G(d) Geometry

Imaginary frequency: none

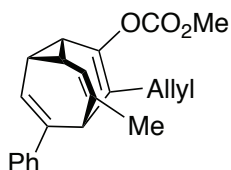
Sum of electronic and thermal Free Energies= -1076.804561 Hartree

Charge = 0 Multiplicity = 1

C	0.008772	0.029954	-0.029978
C	-0.026847	0.021337	1.506984
C	1.324523	0.022566	0.751559
H	-0.298704	-0.940875	1.933292
H	1.815074	-0.947664	0.74423

C	2.264598	1.147712	0.851811
C	1.958164	2.450619	0.900507
H	3.312815	0.867824	0.940441
H	2.765467	3.158298	1.053544
C	-0.419857	1.168582	2.335818
C	-0.181002	2.465389	2.08865
H	-0.910024	0.914779	3.274236
H	-0.465109	3.190269	2.845012
C	-0.461699	1.24165	-0.786142
C	-0.193824	2.509592	-0.417315
C	0.538964	3.009652	0.850096
C	-0.282062	-1.34655	-0.657318
H	-1.344371	-1.458576	-0.900668
H	-0.075848	-2.098711	0.11799
C	0.566683	-1.681915	-1.859486
C	0.127929	-2.269112	-2.973535
H	1.626418	-1.440492	-1.76837
H	0.799898	-2.51853	-3.790313
H	-0.920868	-2.525171	-3.11275
C	-1.326192	0.986165	-2.005433
O	-0.760929	3.538542	-1.199737
C	0.018875	4.079882	-2.160989
O	1.155632	3.770143	-2.429804
O	-0.711354	5.021483	-2.77617
C	-0.013044	5.731472	-3.809626
H	-0.740458	6.433294	-4.21861
H	0.843562	6.26767	-3.392574
H	0.33572	5.043561	-4.584328
C	0.539609	4.555173	0.879344
C	1.61061	5.306082	0.374845
C	-0.570982	5.257716	1.372815
C	1.590428	6.702865	0.40137
H	2.46224	4.807682	-0.073751
C	-0.595946	6.65116	1.400202
H	-1.44098	4.712218	1.724875
C	0.492006	7.383411	0.923464
H	2.440677	7.255534	0.009727
H	-1.47117	7.163508	1.791208
H	0.478132	8.469819	0.949189
H	-0.773006	0.457082	-2.787628
H	-2.187025	0.359351	-1.741988
H	-1.716894	1.913831	-2.419862

Isomer 0020050140



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

Sum of electronic and thermal Free Energies= -1076.448532 Hartree

Charge = 0 Multiplicity =1

C	-0.008522	-0.007262	0.03712
C	0.041016	0.006122	1.566704
C	1.33004	-0.008597	0.765411
H	-0.285044	-0.969307	-0.380745
H	-0.214484	-0.933622	2.044374
H	1.822303	-0.9754	0.764476
C	2.260536	1.136414	0.731829
C	1.92135	2.431881	0.738072
H	3.317678	0.878932	0.703421
C	-0.416778	1.176601	2.333067
C	-0.25791	2.469935	2.039976
C	-0.505935	1.144712	-0.734034
C	-0.328235	2.446652	-0.44472
H	-1.083805	0.893778	-1.62095
C	0.474376	2.890596	0.772999
H	0.475921	3.98502	0.777819
C	-0.970434	3.497659	-1.274602
C	-2.299228	3.36107	-1.695086
C	-0.277142	4.662119	-1.628445
C	-2.912123	4.353398	-2.456918
H	-2.86336	2.48545	-1.386072
C	-0.886547	5.654345	-2.390676
H	0.755407	4.788724	-1.312412
C	-2.209084	5.504791	-2.807288
H	-3.947176	4.233685	-2.762942
H	-0.32799	6.54551	-2.660619
H	-2.688678	6.282076	-3.39402
C	2.958566	3.520311	0.714225
O	-1.112604	0.807732	3.50052
C	-2.449485	0.755539	3.399681
O	-3.103576	1.020813	2.422336
O	-2.934125	0.366171	4.577758
C	-4.360334	0.282884	4.636066
H	-4.589311	-0.037411	5.650628

H	-4.805255	1.258452	4.429873
H	-4.728145	-0.443491	3.908875
C	-0.907415	3.583217	2.830217
H	-0.154028	4.344015	3.073204
H	-1.305842	3.199511	3.774116
C	-1.999748	4.207443	1.996758
C	-1.943087	5.437548	1.488813
H	-2.837039	3.551858	1.756876
H	-2.723742	5.82007	0.838169
H	-1.10168	6.096732	1.695114
H	3.971088	3.109181	0.704093
H	2.839114	4.156937	-0.170987
H	2.857371	4.170286	1.591994

Transition state 0020050140–0415002000

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -350.25 cm⁻¹

Sum of electronic and thermal Free Energies= -1076.421569 Hartree

Charge = 0 Multiplicity = 1

C	-0.00656	0.017129	0.102793
C	-0.036704	0.034533	1.598061
C	1.459822	0.003728	1.579177
H	-0.14613	-0.953621	-0.361482
H	-0.436209	-0.90331	1.981155
H	1.911408	-0.9788	1.67519
C	2.298978	1.089209	1.406
C	1.941562	2.40966	1.107013
H	3.363758	0.869109	1.36732
C	-0.727012	1.174561	2.278345
C	-0.49955	2.467485	2.066891
C	0.206867	1.105403	-0.718497
C	0.537555	2.419867	-0.346018
H	0.225346	0.90136	-1.786064
C	0.531129	2.923693	1.071918
H	0.549778	4.015477	1.078559
C	0.845197	3.392223	-1.42805
C	0.292001	4.679513	-1.424564
C	1.698185	3.037299	-2.483112
C	0.570999	5.578159	-2.451832
H	-0.381581	4.970167	-0.622673
C	1.978314	3.934943	-3.509659
H	2.162351	2.054356	-2.47797
C	1.414932	5.210473	-3.498348

H	0.123121	6.567354	-2.435996
H	2.647162	3.642376	-4.313461
H	1.635273	5.913122	-4.29595
C	3.024318	3.440394	0.912784
O	-1.636103	0.807687	3.282917
C	-2.713943	0.117029	2.881304
O	-2.976654	-0.187781	1.745209
O	-3.441595	-0.173684	3.95757
C	-4.63893	-0.907004	3.684014
H	-5.107608	-1.065401	4.653159
H	-5.293196	-0.330231	3.027407
H	-4.399061	-1.860387	3.209243
C	-1.258805	3.562625	2.780679
H	-0.54578	4.256364	3.244708
H	-1.867269	3.128237	3.578582
C	-2.135687	4.321808	1.818277
C	-2.028746	5.625953	1.565936
H	-2.886481	3.729683	1.294084
H	-2.685271	6.123763	0.858999
H	-1.282288	6.238088	2.068203
H	3.99731	2.968224	0.754602
H	2.818049	4.088625	0.054873
H	3.092475	4.083789	1.799106

Transition state 0020050140–0204105000

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -384.22 cm^{-1}

Sum of electronic and thermal Free Energies= -1076.415646 Hartree

Charge = 0 Multiplicity = 1

C	-0.418358	0.001447	-0.047267
C	-0.33988	-0.023442	1.448931
C	1.063509	-0.214872	-0.039917
H	-0.928965	-0.893689	-0.400565
H	-0.538946	-0.968065	1.944428
H	1.395685	-1.2453	-0.123607
C	2.028541	0.761369	0.117988
C	1.841434	2.116185	0.427294
H	3.056929	0.410836	0.155461
C	0.015912	1.036591	2.252261
C	0.498337	2.298728	1.889937
C	-0.986859	1.208446	-0.72306
C	-0.586755	2.465204	-0.502326
H	-1.806648	1.035467	-1.41704

C	0.505047	2.803999	0.475606
H	0.654763	3.885449	0.484859
C	-1.229923	3.599996	-1.216651
C	-1.591239	4.764739	-0.525196
C	-1.502584	3.522992	-2.587947
C	-2.222236	5.815438	-1.185568
H	-1.402643	4.834774	0.543802
C	-2.132009	4.575561	-3.248989
H	-1.197004	2.638752	-3.140069
C	-2.494318	5.725581	-2.550402
H	-2.506784	6.704597	-0.631058
H	-2.328227	4.501131	-4.31434
H	-2.981683	6.547404	-3.06557
C	3.065628	2.990059	0.553983
O	0.026539	0.746374	3.637434
C	1.194951	0.314168	4.135931
O	2.224138	0.17307	3.525724
O	1.022963	0.078527	5.437605
C	2.192499	-0.386503	6.114728
H	1.891926	-0.52265	7.151848
H	2.530557	-1.330788	5.683221
H	2.993283	0.351751	6.037912
C	0.819621	3.305863	2.975928
H	1.458498	4.096814	2.574564
H	1.366882	2.837757	3.80133
C	-0.456916	3.928918	3.481631
C	-0.753997	5.222496	3.360657
H	-1.167048	3.24439	3.944196
H	-1.69459	5.62537	3.72282
H	-0.057952	5.921528	2.900929
H	3.97036	2.380905	0.613757
H	3.146653	3.64857	-0.319578
H	3.042612	3.630313	1.439395

Transition state 0020050140–0502004100

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -357.1 cm^{-1}

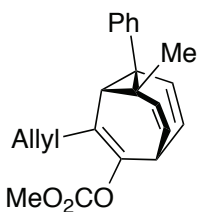
Sum of electronic and thermal Free Energies= -1076.417745 Hartree

Charge = 0 Multiplicity = 1

C	0.007379	-0.040122	0.023294
C	0.054102	-0.023816	2.074524
C	1.121502	-0.03301	1.027421
H	-0.283275	-1.012934	-0.361645

H	-0.243156	-0.979846	2.493304
H	1.628139	-0.997401	1.031254
C	2.129847	1.072018	0.990486
C	1.829338	2.370382	0.990033
H	3.17605	0.774202	0.963812
C	-0.616171	1.089569	2.53384
C	-0.582638	2.39769	2.043882
C	-0.693879	1.063475	-0.428534
C	-0.61446	2.384964	0.041557
H	-1.489023	0.867977	-1.143797
C	0.414959	2.875476	1.025467
H	0.428859	3.966534	1.042782
C	-1.56919	3.382642	-0.514391
C	-2.937432	3.091581	-0.596794
C	-1.123768	4.628102	-0.975813
C	-3.831818	4.013929	-1.134049
H	-3.299094	2.141897	-0.210914
C	-2.016236	5.551181	-1.515254
H	-0.064274	4.868105	-0.931578
C	-3.374563	5.247722	-1.595277
H	-4.889724	3.773848	-1.180074
H	-1.649237	6.506494	-1.877786
H	-4.072114	5.968766	-2.009534
C	2.887724	3.437849	0.952406
O	-1.658306	0.836314	3.449181
C	-1.30197	0.721992	4.739707
O	-0.182224	0.694649	5.17815
O	-2.422992	0.622289	5.457725
C	-2.209875	0.533971	6.867015
H	-3.201823	0.446193	7.306597
H	-1.601757	-0.340307	7.107496
H	-1.70547	1.434098	7.226861
C	-1.528867	3.427235	2.630756
H	-2.54582	3.026666	2.696171
H	-1.56383	4.294216	1.960747
C	-1.071301	3.867012	3.998131
C	-1.830045	3.820184	5.092213
H	-0.044689	4.228135	4.06922
H	-1.45358	4.15086	6.055296
H	-2.849525	3.44233	5.053089
H	3.889771	3.004289	0.914701
H	2.757617	4.083415	0.075144
H	2.82139	4.080015	1.838885

Isomer 0415002000



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

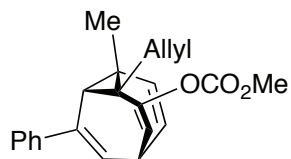
Sum of electronic and thermal Free Energies= -1076.441543 Hartree

Charge = 0 Multiplicity = 1

C	0.085698	-0.006576	-0.106243
C	0.069828	0.027233	1.443328
C	1.388588	-0.033511	0.686065
H	1.832522	-1.026626	0.723183
C	2.423946	1.029078	0.666052
C	2.12631	2.331354	0.634264
C	-0.340655	1.25354	2.16511
C	-0.054929	2.520015	1.843869
H	-0.935073	1.075074	3.060252
H	-0.425828	3.320036	2.479074
C	-0.288396	1.191714	-0.904789
C	-0.007327	2.470109	-0.632143
H	-0.828378	0.970352	-1.822414
H	-0.313768	3.240674	-1.333072
C	0.731406	2.913929	0.611675
H	0.829172	4.000501	0.590006
C	3.852559	0.524802	0.6538
H	3.992465	-0.188054	1.476035
H	4.539737	1.359193	0.815721
C	4.164362	-0.156234	-0.653553
C	4.490391	-1.442429	-0.77792
H	4.084819	0.469284	-1.543327
H	4.69656	-1.885892	-1.747117
H	4.566953	-2.091361	0.092196
O	3.179274	3.257149	0.702262
C	3.297307	4.104301	-0.329731
O	2.598105	4.129071	-1.31208
O	4.322332	4.916837	-0.081173
C	4.579112	5.87944	-1.107336
H	3.720303	6.543114	-1.226528
H	5.451305	6.435843	-0.770005
C	-0.335416	-1.243904	2.169278

C	-0.358766	-1.287451	-0.758629
C	-1.724577	-1.589191	-0.800043
C	0.544269	-2.162064	-1.365055
C	-2.178562	-2.748129	-1.422955
H	-2.430363	-0.9046	-0.334045
C	0.091757	-3.324062	-1.991306
H	1.605875	-1.927168	-1.351489
C	-1.26867	-3.621876	-2.01948
H	-3.240942	-2.97186	-1.441569
H	0.805067	-3.995285	-2.46028
H	-1.619681	-4.527599	-2.504294
H	4.782082	5.377313	-2.055166
H	0.091177	-1.24169	3.177962
H	-1.425733	-1.310923	2.257004
H	0.0109	-2.139599	1.65

Isomer 0204105000



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

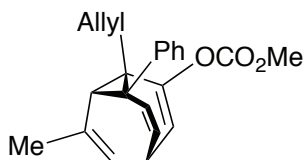
Sum of electronic and thermal Free Energies= -1076.435492 Hartree

Charge = 0 Multiplicity = 1

C	0.05961	0.145794	-0.105843
C	0.251365	0.214671	1.40675
C	1.477364	0.225803	0.467315
H	-0.185043	-0.861931	-0.432448
C	2.25483	1.483696	0.303799
C	1.810399	2.736928	0.229215
H	2.547985	3.524293	0.104394
C	-0.145768	1.427886	2.164159
C	-0.135386	2.696817	1.743864
H	-0.493557	1.230129	3.176753
H	-0.465353	3.477006	2.424782
C	-0.608922	1.183435	-0.929879
C	-0.485617	2.50523	-0.726111
H	-0.987985	3.186431	-1.408936
C	0.352695	3.113458	0.374568
H	0.279653	4.199885	0.295414
C	-1.453774	0.686286	-2.051657
C	-0.99736	-0.329458	-2.902251

C	-2.717987	1.239002	-2.290508
C	-1.774333	-0.764788	-3.972532
H	-0.013415	-0.763058	-2.740419
C	-3.496536	0.803768	-3.360182
H	-3.096727	2.001611	-1.616129
C	-3.027022	-0.198751	-4.206589
H	-1.397766	-1.542659	-4.629829
H	-4.476632	1.241158	-3.524943
H	-3.633691	-0.539707	-5.039621
C	2.309419	-1.050645	0.335002
H	2.928738	-0.980615	-0.566028
H	1.627233	-1.891913	0.174339
C	3.180486	-1.358616	1.524064
C	4.458412	-1.725803	1.440364
H	2.709968	-1.276723	2.503552
H	5.035845	-1.968913	2.327264
H	4.96772	-1.786335	0.481124
O	3.639546	1.288998	0.163233
C	4.368521	1.394727	1.288997
O	3.951822	1.653208	2.387724
O	5.641805	1.17281	0.966583
C	6.541202	1.200222	2.076071
H	7.527771	1.015527	1.654929
H	6.506845	2.173427	2.569943
C	-0.074948	-1.051393	2.186243
H	6.273413	0.421141	2.793845
H	0.423313	-1.042686	3.161207
H	-1.155067	-1.096155	2.359966
H	0.213527	-1.964141	1.663597

Isomer 0502004100



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

Sum of electronic and thermal Free Energies= -1076.438110 Hartree

Charge = 0 Multiplicity =1

C	0.008674	0.141164	0.106538
C	0.157441	0.152435	1.623758
C	1.40884	0.069023	0.710094
H	-0.343384	-0.828814	-0.242033

C	2.34786	1.215083	0.577898
C	2.039476	2.516359	0.532019
H	3.394028	0.930076	0.495359
H	2.844935	3.237696	0.419836
C	-0.096356	1.396493	2.396386
C	0.082173	2.659366	2.012858
H	-0.140939	3.444258	2.729392
C	-0.507317	1.261535	-0.719283
C	-0.244458	2.5523	-0.480213
H	-0.675516	3.303029	-1.138892
C	0.626945	3.043917	0.655046
H	0.659909	4.134177	0.608312
C	-1.379469	0.837139	-1.872276
C	2.131281	-1.251024	0.664884
C	2.098094	-2.074526	-0.461068
C	2.906959	-1.637949	1.763519
C	2.817385	-3.269992	-0.486801
H	1.510456	-1.774822	-1.325329
C	3.623484	-2.830643	1.742276
H	2.935673	-0.995938	2.641298
C	3.578816	-3.652338	0.615055
H	2.784954	-3.899717	-1.370664
H	4.214713	-3.121451	2.60521
H	4.136587	-4.583304	0.596537
C	-0.304883	-1.134282	2.304076
H	0.031714	-1.979309	1.693332
H	0.16471	-1.245268	3.2873
C	-1.802633	-1.203554	2.433797
C	-2.450679	-1.58387	3.533839
H	-2.372444	-0.926201	1.545242
H	-3.534726	-1.639196	3.55929
H	-1.91414	-1.843842	4.443585
O	-0.490591	1.147691	3.719344
C	-1.761465	1.422608	4.064268
O	-2.600204	1.942401	3.37723
O	-1.922554	1.02556	5.327116
C	-3.245643	1.20492	5.834315
H	-3.524356	2.260245	5.8087
H	-3.956787	0.628754	5.237667
H	-3.21605	0.838836	6.858976
H	-0.831878	0.170853	-2.549536
H	-2.257397	0.28684	-1.514081
H	-1.725295	1.700621	-2.445005

Transition state 0415002000–0000051402

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -416.37 cm⁻¹

Sum of electronic and thermal Free Energies= -1076.403704 Hartree

Charge = 0 Multiplicity =1

C	-0.200815	-0.058528	-0.121166
C	0.101105	-0.024575	1.368018
C	1.293734	-0.077932	-0.262075
H	1.715309	-1.078562	-0.316587
C	2.220254	0.962316	-0.295526
C	1.888937	2.289641	0.008227
C	0.417638	1.136479	2.069523
C	0.716197	2.402654	1.566215
H	0.673651	0.991226	3.116527
H	1.132749	3.124932	2.261298
C	-0.954431	1.099352	-0.733138
C	-0.624428	2.382349	-0.631214
H	-1.827358	0.829755	-1.321534
H	-1.237228	3.126822	-1.132361
C	0.527566	2.886925	0.16417
H	0.611462	3.970341	0.104323
C	3.681123	0.540196	-0.397401
H	3.692318	-0.462065	-0.841976
H	4.113361	0.453203	0.60715
C	4.563397	1.42014	-1.243306
C	5.809317	1.756427	-0.911861
H	4.141335	1.771035	-2.185194
H	6.427609	2.366034	-1.562883
H	6.244204	1.425594	0.029899
O	2.868962	3.286612	0.02919
C	3.825589	3.276023	0.973545
O	3.941635	2.48409	1.87326
O	4.610758	4.32751	0.751475
C	5.720578	4.434823	1.643589
H	6.376442	3.568127	1.530402
H	6.23841	5.347259	1.354194
C	0.072187	-1.32851	2.1368
C	-0.888499	-1.338615	-0.573267
C	-2.150173	-1.635474	-0.044757
C	-0.355394	-2.182105	-1.546527
C	-2.850007	-2.764189	-0.45585
H	-2.581299	-0.966996	0.698133

C	-1.056929	-3.315548	-1.965127
H	0.607598	-1.952354	-1.993147
C	-2.300192	-3.614291	-1.41734
H	-3.8238	-2.981876	-0.027663
H	-0.627218	-3.962704	-2.723766
H	-2.842197	-4.498098	-1.738972
H	5.37513	4.495786	2.677472
H	0.687456	-1.251645	3.036247
H	-0.948823	-1.587109	2.44001
H	0.441655	-2.164969	1.538357

Transition state 0415002000–0001400025

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -390.99 cm⁻¹

Sum of electronic and thermal Free Energies= -1076.409457 Hartree

Charge = 0 Multiplicity =1

C	3.706012	-2.173098	-0.544283
C	4.429625	-2.115726	-1.878168
C	3.431018	-1.041349	-2.194668
H	2.551947	-1.409707	-2.719312
C	3.453655	0.327575	-1.939318
C	4.401114	0.9308	-1.109585
C	5.891197	-1.761772	-1.862227
C	6.425594	-0.681623	-1.300718
H	6.550063	-2.465726	-2.367926
H	7.500075	-0.528537	-1.356117
C	3.937115	-1.296187	0.518781
C	4.707913	-0.137592	0.532872
H	3.295095	-1.43841	1.384878
H	4.61581	0.509465	1.399438
C	5.643768	0.333549	-0.537047
H	6.284205	1.135643	-0.173924
C	2.250869	1.148467	-2.393847
H	2.565653	2.192252	-2.520202
H	1.481916	1.139204	-1.610539
C	1.658822	0.679851	-3.692347
C	0.392836	0.293166	-3.843736
H	2.331266	0.667487	-4.550406
H	0.005076	-0.022589	-4.807019
H	-0.296029	0.283177	-3.002057
O	4.308834	2.299058	-0.830015
C	3.296697	2.756313	-0.069267
O	2.463233	2.097359	0.495206

O	3.392073	4.084626	-0.040748
C	2.393013	4.734266	0.750223
H	2.432927	4.375902	1.78051
H	2.630408	5.795049	0.700541
C	4.224799	-3.324477	-2.790862
C	2.661778	-3.221189	-0.326925
C	3.026972	-4.55973	-0.139123
C	1.307575	-2.87867	-0.254879
C	2.060806	-5.533042	0.104083
H	4.078361	-4.832794	-0.170566
C	0.33852	-3.851074	-0.012185
H	1.022883	-1.838834	-0.397101
C	0.712512	-5.181514	0.164605
H	2.361188	-6.565958	0.251981
H	-0.708681	-3.568173	0.036517
H	-0.041075	-5.940342	0.351027
H	1.400718	4.541228	0.337504
H	4.574626	-3.065837	-3.79561
H	4.799386	-4.186373	-2.436807
H	3.174853	-3.617418	-2.853062

Transition state 0204105000-0010200054

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -401.63 cm⁻¹

Sum of electronic and thermal Free Energies= -1076.409898 Hartree

Charge = 0 Multiplicity = 1

C	0.166839	0.17072	-0.065075
C	0.221199	0.321514	1.914446
C	1.324949	0.31706	0.874652
H	-0.049188	-0.866325	-0.310721
C	2.166438	1.566554	0.825201
C	1.742348	2.808881	0.647651
H	2.480729	3.605097	0.673524
C	-0.52654	1.457072	2.262986
C	-0.596518	2.69784	1.639833
H	-1.275891	1.290078	3.032935
H	-1.356191	3.391135	1.987257
C	-0.650117	1.127521	-0.671588
C	-0.647362	2.482297	-0.357588
H	-1.41133	3.108249	-0.808382
C	0.303728	3.188729	0.549677
H	0.211656	4.26625	0.42319
C	-1.749276	0.610529	-1.53795

C	-1.475064	-0.313142	-2.554447
C	-3.074821	1.020307	-1.346952
C	-2.497163	-0.814136	-3.357287
H	-0.446411	-0.622918	-2.722812
C	-4.097066	0.522353	-2.15137
H	-3.305673	1.715423	-0.544048
C	-3.812371	-0.396485	-3.160411
H	-2.264449	-1.524075	-4.145459
H	-5.120238	0.844896	-1.982435
H	-4.60894	-0.784375	-3.787659
C	2.189373	-0.959854	0.819811
H	1.538604	-1.829386	0.937389
H	2.887206	-0.978669	1.663564
C	2.921332	-1.084657	-0.488935
C	2.705745	-2.066043	-1.363951
H	3.652851	-0.311594	-0.716796
H	3.248338	-2.117356	-2.302556
H	1.981099	-2.85374	-1.167363
O	3.552102	1.398455	0.998439
C	3.955838	1.160018	2.256438
O	3.239369	1.032676	3.217053
O	5.283541	1.070081	2.252724
C	5.862643	0.798523	3.532458
H	6.936135	0.756076	3.360116
H	5.613907	1.595549	4.235761
C	-0.013223	-0.940261	2.715538
H	5.49448	-0.153555	3.91939
H	0.891094	-1.216084	3.269699
H	-0.817571	-0.780238	3.436381
H	-0.299925	-1.791612	2.092103

Transition state 0204105000-0000140205

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -414.14 cm⁻¹

Sum of electronic and thermal Free Energies= -1076.409249 Hartree

Charge = 0 Multiplicity = 1

C	0.032664	0.062396	0.146073
C	-0.19467	0.021547	1.629058
C	1.320251	0.105238	1.675329
H	0.072752	-0.918382	-0.323117
C	2.005948	1.323061	1.609442
C	1.549254	2.586322	1.266115
H	2.310287	3.343397	1.109283

C	-0.989635	1.119205	2.284049
C	-0.878657	2.422107	2.046195
H	-1.726115	0.786499	3.01307
H	-1.521904	3.115208	2.582159
C	0.175534	1.162535	-0.700843
C	0.29704	2.486891	-0.27375
H	0.581124	3.223459	-1.019893
C	0.125062	3.012085	1.116695
H	0.054131	4.098458	1.106888
C	0.410874	0.891587	-2.149379
C	1.318908	-0.089635	-2.566761
C	-0.282476	1.62129	-3.122085
C	1.519214	-0.337373	-3.921981
H	1.899807	-0.623971	-1.820527
C	-0.077149	1.378332	-4.478863
H	-1.004184	2.37054	-2.806753
C	0.822124	0.394224	-4.883453
H	2.234356	-1.094525	-4.229876
H	-0.629034	1.950062	-5.219002
H	0.981466	0.199984	-5.939656
C	2.139306	-1.157807	1.886581
H	3.056751	-1.130348	1.292737
H	1.580063	-2.025738	1.530917
C	2.488921	-1.342734	3.342014
C	3.728634	-1.283863	3.823401
H	1.653132	-1.511689	4.021105
H	3.933258	-1.411829	4.881499
H	4.575642	-1.085546	3.170584
O	3.414704	1.246411	1.716028
C	4.078639	0.986471	0.583179
O	3.592321	0.795666	-0.503703
O	5.382084	0.956845	0.866187
C	6.226174	0.691565	-0.256937
H	7.242248	0.719774	0.132034
H	6.001061	-0.290776	-0.677559
C	-0.803082	-1.311214	2.073848
H	6.084647	1.453326	-1.025851
H	-0.667533	-1.460787	3.150154
H	-1.876769	-1.286527	1.8649
H	-0.389933	-2.170709	1.545753

Transition state 0502004100-0000500142
RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -422.71 cm⁻¹

Sum of electronic and thermal Free Energies= -1076.405722 Hartree

Charge = 0 Multiplicity =1

C	0.065504	0.027023	0.138612
C	0.13013	0.011316	2.135978
C	1.23327	0.039061	1.082747
H	-0.238699	-0.969506	-0.175079
C	2.185289	1.212676	1.040099
C	1.848273	2.496727	0.98203
H	3.239816	0.951305	1.03131
H	2.635025	3.24502	0.930983
C	-0.492	1.173675	2.596358
C	-0.463977	2.461949	2.077932
H	-1.182371	3.159689	2.495376
C	-0.70582	1.088169	-0.329183
C	-0.595276	2.407524	0.111413
H	-1.365568	3.102322	-0.21215
C	0.445266	2.988169	1.018638
H	0.411328	4.075948	0.993764
C	-1.949362	0.738797	-1.122147
C	2.09033	-1.217084	1.030838
C	2.239525	-1.957485	-0.139499
C	2.829699	-1.584731	2.161657
C	3.09632	-3.060324	-0.177819
H	1.694421	-1.667788	-1.033161
C	3.680012	-2.684305	2.128429
H	2.723166	-1.003192	3.075769
C	3.813646	-3.429936	0.95516
H	3.200856	-3.62661	-1.098296
H	4.238629	-2.962305	3.016932
H	4.474754	-4.290324	0.927762
C	-0.328874	-1.326057	2.704548
H	0.316727	-2.116006	2.311273
H	-0.189192	-1.318077	3.792568
C	-1.754546	-1.707703	2.394018
C	-2.627003	-2.157322	3.294386
H	-2.05727	-1.615768	1.350288
H	-3.628917	-2.460599	3.00551
H	-2.368158	-2.229195	4.348258
O	-1.467675	0.971314	3.599245
C	-2.748341	0.944882	3.199582
O	-3.154024	1.089855	2.073231
O	-3.505895	0.746431	4.277793

C	-4.902305	0.630009	4.003802
H	-5.278812	1.546121	3.543978
H	-5.083746	-0.212612	3.332379
H	-5.374942	0.461811	4.969812
H	-1.828617	-0.208927	-1.653648
H	-2.80412	0.651343	-0.440481
H	-2.179092	1.509625	-1.862745

Transition state 0502004100–0010020504

RM062X/6-31+G(d,p) Geometry

Imaginary frequency: -402.13 cm⁻¹

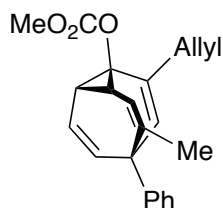
Sum of electronic and thermal Free Energies= -1076.407799 Hartree

Charge = 0 Multiplicity = 1

C	0.090446	-0.002289	0.138452
C	-0.066736	0.081233	1.628505
C	1.452446	0.045621	1.603293
H	0.018634	-1.024632	-0.228164
C	2.275529	1.157804	1.372039
C	1.922922	2.431749	0.93884
H	3.341435	0.942784	1.378852
H	2.727231	3.110265	0.672569
C	-0.675725	1.320316	2.238252
C	-0.440694	2.575889	1.886436
H	-0.926108	3.370052	2.445424
C	0.294114	0.990335	-0.816151
C	0.552034	2.323393	-0.518091
H	0.834482	2.976234	-1.339723
C	0.53113	2.97286	0.826519
H	0.541329	4.056428	0.721197
C	0.528833	0.535178	-2.241772
C	2.152127	-1.243271	1.896982
C	2.831569	-1.939698	0.893147
C	2.17466	-1.750107	3.202234
C	3.51088	-3.122795	1.18163
H	2.814186	-1.547	-0.12055
C	2.853603	-2.930597	3.493075
H	1.660849	-1.20762	3.991773
C	3.521176	-3.622424	2.482057
H	4.029906	-3.653671	0.389345
H	2.864413	-3.309489	4.510482
H	4.048544	-4.543772	2.70862
C	-0.766945	-1.193264	2.134226
H	-0.202599	-2.070327	1.806422

H	-0.772977	-1.202049	3.228988
C	-2.17215	-1.288132	1.599086
C	-2.698035	-2.402822	1.093587
H	-2.778445	-0.381475	1.610934
H	-3.71685	-2.430428	0.720825
H	-2.124162	-3.325511	1.040918
O	-1.450983	1.057058	3.375726
C	-2.735083	1.449378	3.413941
O	-3.341104	2.026431	2.548652
O	-3.229863	1.070545	4.591338
C	-4.608163	1.398112	4.786906
H	-4.754539	2.477678	4.716733
H	-5.224613	0.899467	4.036338
H	-4.851178	1.039235	5.7851
H	1.583553	0.269853	-2.391636
H	-0.076331	-0.341855	-2.484316
H	0.278265	1.322954	-2.95671

Isomer 0000051402



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

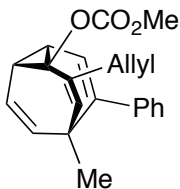
Sum of electronic and thermal Free Energies= -1076.429081 Hartree

Charge = 0 Multiplicity = 1

C	-0.098896	0.009738	-0.064522
C	-0.050924	-0.029363	1.459557
C	1.233102	-0.01124	0.679313
H	-0.38545	-0.944823	-0.492838
H	1.712854	-0.984401	0.665192
C	2.173618	1.121719	0.688061
C	1.891316	2.431033	0.721085
H	3.222275	0.833898	0.66203
C	-0.545618	1.104645	2.274841
C	-0.31717	2.392919	1.975402
H	-0.821973	3.125546	2.599835
C	-0.574602	1.200011	-0.784713
C	-0.347977	2.478962	-0.455283
H	-1.193532	1.002168	-1.656063
H	-0.827565	3.241301	-1.061047

C	0.43294	2.951651	0.769215
C	3.026844	3.423317	0.712947
O	-0.405256	-1.314508	1.946428
C	0.323891	-1.766493	2.975843
O	1.254592	-1.204927	3.496466
O	-0.171276	-2.951359	3.337843
C	0.50563	-3.563842	4.438792
H	0.451933	-2.922453	5.320696
H	-0.015087	-4.503534	4.612292
H	1.552765	-3.743702	4.187406
C	-1.504223	0.766522	3.401663
H	-1.112952	-0.032725	4.039764
H	-1.601533	1.655409	4.034336
C	-2.860147	0.381972	2.864153
C	-3.411344	-0.823463	2.985598
H	-3.388166	1.169437	2.325869
H	-4.390159	-1.043103	2.570963
H	-2.889682	-1.633782	3.489873
C	0.453009	4.486431	0.836428
C	0.479527	5.267414	-0.324242
C	0.560363	5.147372	2.065563
C	0.573764	6.65678	-0.260147
H	0.452231	4.793112	-1.300518
C	0.655928	6.535416	2.136419
H	0.596907	4.573678	2.986985
C	0.653451	7.299839	0.972061
H	0.589349	7.234806	-1.179132
H	0.738533	7.017411	3.10587
H	0.723144	8.381774	1.024353
H	3.982299	2.895752	0.668021
H	2.963857	4.100816	-0.14482
H	3.01969	4.052168	1.60881

Isomer 0001400025



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

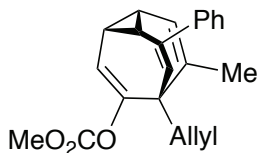
Sum of electronic and thermal Free Energies= -1076.437790 Hartree

Charge = 0 Multiplicity =1

C	0.125753	-0.073692	-0.032969
C	0.137373	-0.11235	1.476332
C	1.45465	-0.046516	0.69836
H	-0.084123	-1.101659	1.862775
H	1.971476	-0.99884	0.643809
C	2.334865	1.13517	0.719725
C	1.968755	2.426444	0.787051
H	3.400168	0.915708	0.69514
C	-0.348443	0.997318	2.313735
C	-0.194356	2.297494	2.045932
H	-0.866105	0.707886	3.224214
H	-0.594085	3.024897	2.75068
C	-0.346312	1.079245	-0.838952
C	-0.173479	2.35303	-0.458747
H	-0.515696	3.12543	-1.147435
C	0.490004	2.861817	0.81234
O	-0.099897	-1.344207	-0.63014
C	-1.335102	-1.849813	-0.486052
O	-2.256833	-1.327993	0.088528
O	-1.366415	-3.032287	-1.099127
C	-2.635002	-3.691403	-1.05048
H	-2.496241	-4.625264	-1.591598
H	-2.922171	-3.883579	-0.014849
H	-3.399308	-3.076272	-1.529456
C	-0.949762	0.777827	-2.198265
H	-1.760818	0.046088	-2.097156
H	-1.402327	1.696912	-2.582682
C	0.076082	0.279454	-3.185401
C	0.405608	0.931439	-4.299174
H	0.565804	-0.662851	-2.944369
H	1.153031	0.543651	-4.983951
H	-0.065656	1.875952	-4.561977
C	3.039538	3.465988	0.79932
C	3.737911	3.775057	-0.372377
C	3.370323	4.141811	1.980273
C	4.743472	4.741477	-0.36578
H	3.483284	3.251043	-1.289875
C	4.374863	5.10574	1.988637
H	2.841549	3.894328	2.897622
C	5.062589	5.410434	0.813594
H	5.277437	4.97032	-1.283113
H	4.625753	5.616172	2.913574
H	5.845968	6.162126	0.820038

C	0.338663	4.388223	0.833137
H	0.841881	4.847125	-0.022962
H	-0.72571	4.641444	0.791279
H	0.759988	4.820867	1.744002

Isomer 0010200054



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

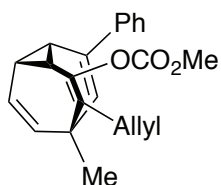
Sum of electronic and thermal Free Energies= -1076.438088 Hartree

Charge = 0 Multiplicity =1

C	0.240479	-0.148162	-0.314718
C	0.067922	-0.074034	1.200615
C	1.46027	-0.063311	0.585419
H	0.07995	-1.134384	-0.736114
H	-0.205061	-1.018695	1.659336
H	1.994485	-1.003883	0.665548
C	2.326925	1.132242	0.649986
C	1.879006	2.395053	0.561951
H	2.610804	3.191044	0.678129
C	-0.527836	1.100281	1.865968
C	-0.416758	2.40249	1.549132
H	-1.165401	0.853064	2.712455
C	-0.211081	0.946167	-1.185934
C	-0.150682	2.246817	-0.901858
H	-0.683043	0.666309	-2.123719
C	0.44596	2.865443	0.358149
O	-0.675698	3.1185	-1.872911
C	-1.884519	3.638923	-1.620306
O	-2.5563	3.434735	-0.639809
O	-2.209474	4.434041	-2.637038
C	-3.483777	5.071582	-2.511274
H	-3.601552	5.661524	-3.418077
H	-4.274344	4.323276	-2.42983
H	-3.499828	5.713268	-1.628144
C	3.780021	0.890494	0.870608
C	4.742087	1.635486	0.176536
C	4.216659	-0.074987	1.787478
C	6.100858	1.432269	0.404353
H	4.415115	2.364976	-0.559348

C	5.575119	-0.278103	2.016304
H	3.485582	-0.653201	2.346499
C	6.523056	0.475197	1.325435
H	6.831656	2.014974	-0.148343
H	5.894322	-1.022283	2.739825
H	7.582142	0.313692	1.500305
C	-1.182439	3.426142	2.347054
C	0.50335	4.412154	0.254196
H	-0.508501	4.812591	0.12991
H	0.873647	4.793067	1.212051
C	1.396641	4.930265	-0.841697
C	2.432035	5.742135	-0.6285
H	1.160288	4.621992	-1.858275
H	3.042693	6.10821	-1.447777
H	2.699953	6.069939	0.373924
H	-0.523069	4.170391	2.805395
H	-1.89907	3.954126	1.709769
H	-1.73933	2.933495	3.147445

Isomer 0000140205



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

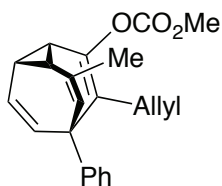
Sum of electronic and thermal Free Energies= -1076.441922 Hartree

Charge = 0 Multiplicity = 1

C	0.022297	0.015429	-0.018955
C	0.011285	0.03615	1.507417
C	1.328927	0.056119	0.753963
H	-0.201491	-0.960248	-0.436936
H	-0.228908	-0.923129	1.952998
H	1.878263	-0.878506	0.77511
C	2.209015	1.236374	0.777268
C	1.90263	2.539247	0.724946
C	-0.458003	1.199052	2.293799
C	-0.27137	2.482135	1.939005
H	-0.612413	3.252065	2.630734
C	-0.440221	1.146704	-0.839455
C	-0.261816	2.441223	-0.556947
H	-0.9632	0.883217	-1.755395

H	-0.648104	3.182306	-1.254757
C	0.427237	2.983266	0.684047
O	3.57577	0.902664	0.847614
C	3.987342	0.374536	2.009889
O	3.286471	0.079101	2.946194
O	5.307705	0.217657	1.944489
C	5.89958	-0.328349	3.125951
H	5.701768	0.321327	3.980807
H	5.497429	-1.323576	3.32591
H	6.966501	-0.378794	2.917625
C	3.012067	3.561977	0.804973
H	3.913747	3.157096	0.333286
H	2.747211	4.452781	0.226992
C	3.371858	3.991336	2.210076
C	2.910936	3.457872	3.341487
H	4.09233	4.807803	2.264764
H	3.246392	3.830448	4.304427
H	2.201073	2.63406	3.344108
C	-1.136887	0.885814	3.581558
C	-2.332585	1.521461	3.93401
C	-0.577943	-0.041415	4.471723
C	-2.952529	1.246086	5.150861
H	-2.783907	2.221171	3.236229
C	-1.197915	-0.316122	5.688049
H	0.364475	-0.522121	4.21938
C	-2.387739	0.325437	6.031392
H	-3.883422	1.743607	5.405746
H	-0.747015	-1.02754	6.373363
H	-2.872053	0.10759	6.978213
C	0.293551	4.512277	0.663058
H	0.703357	4.937478	-0.257588
H	-0.768334	4.773919	0.707771
H	0.797002	4.967159	1.521426

Isomer 0000500142



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

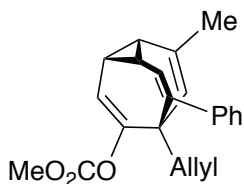
Sum of electronic and thermal Free Energies= -1076.432597 Hartree

Charge = 0 Multiplicity =1

C	0.04166	0.036777	-0.009363
C	0.012098	0.026164	1.526233
C	1.328643	0.066364	0.782138
H	-0.170299	-0.926338	-0.463923
H	-0.219828	-0.941978	1.95694
H	1.878084	-0.868129	0.780061
C	2.209744	1.244948	0.77864
C	1.90928	2.54874	0.800418
C	-0.508059	1.174141	2.28231
C	-0.336988	2.468943	1.988804
H	-1.126035	0.927282	3.141956
H	-0.856833	3.191173	2.609452
C	-0.45013	1.191112	-0.789898
C	-0.284058	2.480841	-0.455081
H	-0.758427	3.219429	-1.094837
C	0.427503	3.013563	0.786969
C	-1.222059	0.816387	-2.029813
O	3.577121	0.908638	0.777884
C	4.048746	0.368347	-0.355943
O	3.394549	0.035507	-1.3128
O	5.368881	0.245607	-0.233818
C	6.020152	-0.299087	-1.383697
H	7.079056	-0.320331	-1.133596
H	5.650722	-1.306111	-1.588038
H	5.839762	0.336386	-2.253171
C	3.049313	3.544597	0.750226
H	2.752948	4.493138	1.207325
H	3.883624	3.165021	1.350421
C	3.573294	3.829207	-0.638854
C	3.16557	3.260146	-1.773288
H	4.368781	4.573778	-0.676371
H	3.618107	3.53159	-2.722321
H	2.381077	2.506505	-1.789599
C	0.396424	4.550522	0.794388
C	0.496487	5.278001	-0.396376
C	0.388678	5.269201	1.99603
C	0.551595	6.670834	-0.390303
H	0.568186	4.758223	-1.345932
C	0.442826	6.661609	2.007943
H	0.372228	4.743497	2.945344
C	0.516864	7.371694	0.812126
H	0.630486	7.205487	-1.332067

H	0.434288	7.189343	2.956846
H	0.556883	8.456404	0.818237
H	-0.593978	0.230706	-2.710471
H	-2.090449	0.198535	-1.773304
H	-1.575012	1.702931	-2.561659

Isomer 0010020504



RM062X/6-31+G(d,p) Geometry

Imaginary frequency: none

Sum of electronic and thermal Free Energies= -1076.437702 Hartree

Charge = 0 Multiplicity = 1

C	-0.124794	-0.040621	-0.095303
C	0.08626	-0.081859	1.416994
C	1.279107	-0.145483	0.477308
H	-0.495862	-0.972232	-0.512996
H	-0.167503	-1.033389	1.871804
H	1.719314	-1.132275	0.384614
C	2.257355	0.949313	0.397268
C	1.98358	2.248379	0.501465
H	3.299259	0.671811	0.26418
C	-0.202	1.080821	2.275802
C	-0.001508	2.383606	2.015636
H	-0.65552	0.836606	3.234354
C	-0.633152	1.166346	-0.781188
C	-0.319153	2.426497	-0.44585
H	-0.766046	3.231521	-1.02624
C	0.60311	2.87428	0.681444
O	3.074464	3.125434	0.365206
C	3.619483	3.597228	1.49318
O	3.297179	3.303526	2.617663
O	4.580049	4.455115	1.158013
C	5.264377	5.045085	2.266904
H	5.75151	4.272346	2.864747
H	6.000965	5.715269	1.828273
H	4.562352	5.600127	2.892311
C	-0.47574	3.378961	3.026363
C	0.408252	3.989868	3.923359
C	-1.836235	3.701209	3.091102

C	-0.06416	4.904732	4.863147
H	1.462745	3.735079	3.879973
C	-2.30694	4.618397	4.029882
H	-2.523452	3.225099	2.3962
C	-1.420387	5.224444	4.91773
H	0.630573	5.364484	5.559937
H	-3.365736	4.856764	4.067781
H	-1.78516	5.937639	5.650593
C	-1.580418	0.887481	-1.92025
C	0.679535	4.422233	0.643863
H	-0.311803	4.80888	0.904053
H	1.354025	4.76756	1.437546
C	1.095901	5.005481	-0.679741
C	0.364432	5.891888	-1.355081
H	2.054373	4.687535	-1.084574
H	0.707265	6.306153	-2.29802
H	-0.598186	6.235935	-0.982447
H	-1.090077	0.284225	-2.693052
H	-2.451388	0.321027	-1.570636
H	-1.932363	1.814251	-2.378831