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SUPPLEMENTARY MATERIAL

Theoretical Studies for Ozonide Formation during the Ozonolysis of Bicyclic Endoperoxides.

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Contents

Calculated geometrical parameters for both ozone and the bicyclic 1,2-dioxine **13** (starting materials) and for each of the possible primary ozonides (**15a-d**) and ozonides (**19a,b**) and transition states (TS1, TS2 and TS3) as depicted in *Scheme 2*, for both gas (HF/6-31G*, MP2/6-31G*, MP2/6-311G*, DFT(B3LYP)/6-31G*) and dichloromethane (HF/6-31G*, DFT(B3LYP)/6-31G*).

Optimised structures for ozone at all levels reported.

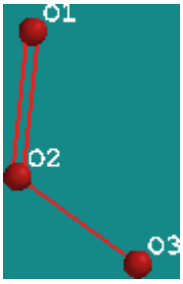

Figure S1: Optimised geometry for ozone

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
1- 2 1.2043; 2- 3 1.2043
Bond Angles
1- 2- 3 119.010
```

HF/6-31G* (DICHLOROMETHANE)

```
Geometry information
Bond Lengths
1- 2 1.2047; 2- 3 1.2047
Bond Angles
1- 2- 3 118.920
```

MP2/6-31G*

```
Geometry information
Bond Lengths
1- 2 1.3002; 2- 3 1.3002
Bond Angles
1- 2- 3 116.303
```

MP2/6-311G*

```
Geometry information
Bond Lengths
1- 2 1.2821; 2- 3 1.2821
Bond Angles
1- 2- 3 116.875
```

DFT/6-31G* (GAS)

```
Geometry information
Bond Lengths
1- 2 1.2643 2- 3 1.2643
Bond Angles
1- 2- 3 117.902
```

DFT/6-31G* (DICHLOROMETHANE)

```
Geometry information
Bond Lengths
1- 2 1.2646; 2- 3 1.2646
Bond Angles
1- 2- 3 117.867
```

Optimised structures for bicyclic endoperoxide 13 at all levels reported.

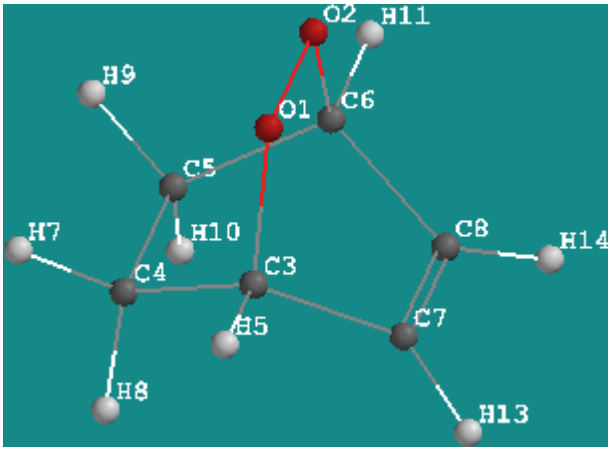

Figure S2: Optimised geometry for bicyclic endoperoxide **13**

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 3 1.5323 1- 8 1.0801 1- 11 1.5086 1- 15 1.4232
5) 2- 3 1.5483 2- 4 1.5323 2- 5 1.0842 2- 9 1.0834
9) 3- 6 1.0834 3- 10 1.0842 4- 7 1.0801 4- 13 1.5086
13) 4- 16 1.4232 11- 12 1.0747 11- 13 1.3177 13- 14 1.0747
17) 15- 16 1.4111
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 3- 6 108.812 1- 3- 10 110.147 1- 11- 12 122.402
4) 1- 11- 13 112.042 1- 15- 16 111.406 2- 3- 6 110.875
7) 2- 3- 10 111.924 2- 4- 7 112.650 2- 4- 13 109.940
10) 2- 4- 16 107.539 3- 1- 8 112.650 3- 1- 11 109.940
13) 3- 1- 15 107.539 3- 2- 4 107.112 3- 2- 5 111.924
16) 3- 2- 9 110.875 4- 2- 3 107.112 4- 2- 5 110.147
19) 4- 2- 9 108.812 4- 13- 14 122.402 5- 2- 3 111.924
22) 5- 2- 4 110.147 5- 2- 9 107.942 6- 3- 10 107.942
25) 7- 4- 13 113.677 7- 4- 16 103.929 8- 1- 3 112.650
28) 8- 1- 11 113.677 8- 1- 15 103.929 9- 2- 3 110.875
31) 9- 2- 4 108.812 9- 2- 5 107.942 10- 3- 6 107.942
34) 11- 1- 3 109.940 11- 1- 8 113.677 11- 1- 15 108.695
37) 11- 13- 14 125.530 12- 11- 13 125.530 13- 4- 7 113.677
40) 13- 4- 16 108.695 13- 11- 12 125.530 15- 1- 3 107.539
43) 15- 1- 8 103.929 15- 1- 11 108.695 16- 4- 7 103.929
46) 16- 4- 13 108.695
Dihedrals
```

I J K L Theta I J K L Theta
1- 3- 2- 4 -0.000 1- 11- 13- 4 -0.000
1- 15- 16- 4 -0.000 1- 3- 2- 5 120.823
1- 3- 2- 9 -118.588 1- 11- 13- 14 178.151
2- 3- 1- 8 174.065 2- 3- 1- 11 -58.035
2- 4- 13- 11 -61.015 2- 4- 13- 14 120.766
2- 3- 1- 15 60.146 2- 4- 16- 15 62.913
3- 2- 4- 7 -174.065 3- 1- 11- 12 -120.766
3- 1- 11- 13 61.015 3- 2- 4- 13 58.035
3- 1- 15- 16 -62.913 3- 2- 4- 16 -60.146
4- 2- 3- 6 118.588 4- 2- 3- 10 -120.823
4- 13- 11- 12 -178.151 5- 2- 3- 6 -120.589
5- 2- 4- 7 63.992 5- 2- 3- 10 -0.000
5- 2- 4- 13 -63.908 5- 2- 4- 16 177.911
6- 3- 1- 8 54.148 6- 3- 2- 9 -0.000
6- 3- 1- 11 -177.952 6- 3- 1- 15 -59.771
7- 4- 2- 9 -54.148 7- 4- 13- 11 171.654
7- 4- 13- 14 -6.564 7- 4- 16- 15 -177.450
8- 1- 3- 10 -63.992 8- 1- 11- 12 6.564
8- 1- 11- 13 -171.654 8- 1- 15- 16 177.450
9- 2- 3- 10 120.589 9- 2- 4- 13 177.952
9- 2- 4- 16 59.771 10- 3- 1- 11 63.908
10- 3- 1- 15 -177.911 11- 1- 15- 16 56.069
11- 13- 4- 16 56.449 12- 11- 13- 14 -0.000
12- 11- 1- 15 121.769 13- 4- 16- 15 -56.069
13- 11- 1- 15 -56.449 14- 13- 4- 16 -121.769

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 3 1.5309 1- 8 1.0797 1- 11 1.5069 1- 15 1.4324
5) 2- 3 1.5474 2- 4 1.5309 2- 5 1.0833 2- 9 1.0833
9) 3- 6 1.0833 3- 10 1.0833 4- 7 1.0797 4- 13 1.5069
13) 4- 16 1.4324 11- 12 1.0744 11- 13 1.3179 13- 14 1.0744
17) 15- 16 1.4123
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 3- 6 108.873 1- 3- 10 109.920 1- 11- 12 122.320
4) 1- 11- 13 112.132 1- 15- 16 111.311 2- 3- 6 110.980
7) 2- 3- 10 111.956 2- 4- 7 112.774 2- 4- 13 110.090
10) 2- 4- 16 107.481 3- 1- 8 112.774 3- 1- 11 110.090
13) 3- 1- 15 107.481 3- 2- 4 107.212 3- 2- 5 111.956
16) 3- 2- 9 110.980 4- 2- 3 107.212 4- 2- 5 109.920
19) 4- 2- 9 108.873 4- 13- 14 122.320 5- 2- 3 111.956
22) 5- 2- 4 109.920 5- 2- 9 107.867 6- 3- 10 107.867
25) 7- 4- 13 113.805 7- 4- 16 103.722 8- 1- 3 112.774
28) 8- 1- 11 113.805 8- 1- 15 103.722 9- 2- 3 110.980
31) 9- 2- 4 108.873 9- 2- 5 107.867 10- 3- 6 107.867
34) 11- 1- 3 110.090 11- 1- 8 113.805 11- 1- 15 108.511
37) 11- 13- 14 125.528 12- 11- 13 125.528 13- 4- 7 113.805
40) 13- 4- 16 108.511 13- 11- 12 125.528 15- 1- 3 107.481
43) 15- 1- 8 103.722 15- 1- 11 108.511 16- 4- 7 103.722
46) 16- 4- 13 108.511
Dihedrals
I J K L Theta I J K L Theta
1- 3- 2- 4 -0.000 1- 11- 13- 4 -0.000
1- 15- 16- 4 -0.000 1- 3- 2- 5 120.628
1- 3- 2- 9 -118.782 1- 11- 13- 14 178.431
2- 3- 1- 8 173.935 2- 3- 1- 11 -57.774
2- 4- 13- 11 -60.732 2- 4- 13- 14 120.779

2- 3- 1- 15 60.235 2- 4- 16- 15 62.880
3- 2- 4- 7 -173.935 3- 1- 11- 12 -120.779
3- 1- 11- 13 60.732 3- 2- 4- 13 57.774
3- 1- 15- 16 -62.880 3- 2- 4- 16 -60.235
4- 2- 3- 6 118.782 4- 2- 3- 10 -120.628
4- 13- 11- 12 -178.431 5- 2- 3- 6 -120.589
5- 2- 4- 7 64.154 5- 2- 3- 10 -0.000
5- 2- 4- 13 -64.137 5- 2- 4- 16 177.854
6- 3- 1- 8 53.800 6- 3- 2- 9 -0.000
6- 3- 1- 11 -177.908 6- 3- 1- 15 -59.900
7- 4- 2- 9 -53.800 7- 4- 13- 11 171.544
7- 4- 13- 14 -6.945 7- 4- 16- 15 -177.472
8- 1- 3- 10 -64.154 8- 1- 11- 12 6.945
8- 1- 11- 13 -171.544 8- 1- 15- 16 177.472
9- 2- 3- 10 120.589 9- 2- 4- 13 177.908
9- 2- 4- 16 59.900 10- 3- 1- 11 64.137
10- 3- 1- 15 -177.854 11- 1- 15- 16 56.147
11- 13- 4- 16 56.639 12- 11- 13- 14 -0.000
12- 11- 1- 15 121.850 13- 4- 16- 15 -56.147
13- 11- 1- 15 -56.639 14- 13- 4- 16 -121.850

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 3 1.5315 1- 8 1.0941 1- 11 1.4978 1- 15 1.4538
5) 2- 3 1.5444 2- 4 1.5315 2- 5 1.0949 2- 9 1.0937
9) 3- 6 1.0937 3- 10 1.0949 4- 7 1.0941 4- 13 1.4978
13) 4- 16 1.4538 11- 12 1.0863 11- 13 1.3436 13- 14 1.0863
17) 15- 16 1.4980
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 3- 6 108.329 1- 3- 10 109.824 1- 11- 12 122.819
4) 1- 11- 13 112.076 1- 15- 16 109.517 2- 3- 6 111.027
7) 2- 3- 10 112.011 2- 4- 7 112.616 2- 4- 13 110.641
10) 2- 4- 16 107.902 3- 1- 8 112.616 3- 1- 11 110.641
13) 3- 1- 15 107.902 3- 2- 4 107.577 3- 2- 5 112.011
16) 3- 2- 9 111.027 4- 2- 3 107.577 4- 2- 5 109.824
19) 4- 2- 9 108.329 4- 13- 14 122.819 5- 2- 3 112.011
22) 5- 2- 4 109.824 5- 2- 9 108.013 6- 3- 10 108.013
25) 7- 4- 13 113.832 7- 4- 16 102.290 8- 1- 3 112.616
28) 8- 1- 11 113.832 8- 1- 15 102.290 9- 2- 3 111.027
31) 9- 2- 4 108.329 9- 2- 5 108.013 10- 3- 6 108.013
34) 11- 1- 3 110.641 11- 1- 8 113.832 11- 1- 15 109.031
37) 11- 13- 14 125.022 12- 11- 13 125.022 13- 4- 7 113.832
40) 13- 4- 16 109.031 13- 11- 12 125.022 15- 1- 3 107.902
43) 15- 1- 8 102.290 15- 1- 11 109.031 16- 4- 7 102.290
46) 16- 4- 13 109.031
Dihedrals
I J K L Theta I J K L Theta
1- 3- 2- 4 -0.000 1- 11- 13- 4 -0.000
1- 15- 16- 4 -0.000 1- 3- 2- 5 120.782
1- 3- 2- 9 -118.371 1- 11- 13- 14 176.779
2- 3- 1- 8 174.068 2- 3- 1- 11 -57.274
2- 4- 13- 11 -59.932 2- 4- 13- 14 123.206
2- 3- 1- 15 61.926 2- 4- 16- 15 63.179
3- 2- 4- 7 -174.068 3- 1- 11- 12 -123.206
3- 1- 11- 13 59.932 3- 2- 4- 13 57.274
3- 1- 15- 16 -63.179 3- 2- 4- 16 -61.926
4- 2- 3- 6 118.371 4- 2- 3- 10 -120.782
4- 13- 11- 12 -176.779 5- 2- 3- 6 -120.847

5- 2- 4- 7 63.784 5- 2- 3- 10 -0.000
5- 2- 4- 13 -64.874 5- 2- 4- 16 175.926
6- 3- 1- 8 53.973 6- 3- 2- 9 -0.000
6- 3- 1- 11 -177.369 6- 3- 1- 15 -58.169
7- 4- 2- 9 -53.973 7- 4- 13- 11 172.069
7- 4- 13- 14 -4.792 7- 4- 16- 15 -177.875
8- 1- 3- 10 -63.784 8- 1- 11- 12 4.792
8- 1- 11- 13 -172.069 8- 1- 15- 16 177.875
9- 2- 3- 10 120.847 9- 2- 4- 13 177.369
9- 2- 4- 16 58.169 10- 3- 1- 11 64.874
10- 3- 1- 15 -175.926 11- 1- 15- 16 57.039
11- 13- 4- 16 58.583 12- 11- 13- 14 -0.000
12- 11- 1- 15 118.278 13- 4- 16- 15 -57.039
13- 11- 1- 15 -58.583 14- 13- 4- 16 -118.278

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 3 1.5331 1- 8 1.0929 1- 11 1.5007 1- 15 1.4460
5) 2- 3 1.5464 2- 4 1.5331 2- 5 1.0939 2- 9 1.0932
9) 3- 6 1.0932 3- 10 1.0939 4- 7 1.0929 4- 13 1.5007
13) 4- 16 1.4460 11- 12 1.0861 11- 13 1.3450 13- 14 1.0861
17) 15- 16 1.4789
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 3- 6 108.241 1- 3- 10 109.952 1- 11- 12 123.069
4) 1- 11- 13 111.899 1- 15- 16 109.926 2- 3- 6 110.904
7) 2- 3- 10 112.106 2- 4- 7 112.708 2- 4- 13 110.309
10) 2- 4- 16 108.024 3- 1- 8 112.708 3- 1- 11 110.309
13) 3- 1- 15 108.024 3- 2- 4 107.422 3- 2- 5 112.106
16) 3- 2- 9 110.904 4- 2- 3 107.422 4- 2- 5 109.952
19) 4- 2- 9 108.241 4- 13- 14 123.069 5- 2- 3 112.106
22) 5- 2- 4 109.952 5- 2- 9 108.151 6- 3- 10 108.151
25) 7- 4- 13 113.775 7- 4- 16 102.375 8- 1- 3 112.708
28) 8- 1- 11 113.775 8- 1- 15 102.375 9- 2- 3 110.904
31) 9- 2- 4 108.241 9- 2- 5 108.151 10- 3- 6 108.151
34) 11- 1- 3 110.309 11- 1- 8 113.775 11- 1- 15 109.177
37) 11- 13- 14 124.955 12- 11- 13 124.955 13- 4- 7 113.775
40) 13- 4- 16 109.177 13- 11- 12 124.955 15- 1- 3 108.024
43) 15- 1- 8 102.375 15- 1- 11 109.177 16- 4- 7 102.375
46) 16- 4- 13 109.177
Dihedrals
I J K L Theta I J K L Theta
1- 3- 2- 4 -0.000 1- 11- 13- 4 -0.000
1- 15- 16- 4 -0.000 1- 3- 2- 5 120.896
1- 3- 2- 9 -118.102 1- 11- 13- 14 176.886
2- 3- 1- 8 173.826 2- 3- 1- 11 -57.796
2- 4- 13- 11 -60.472 2- 4- 13- 14 122.573
2- 3- 1- 15 61.463 2- 4- 16- 15 63.073
3- 2- 4- 7 -173.826 3- 1- 11- 12 -122.573
3- 1- 11- 13 60.472 3- 2- 4- 13 57.796
3- 1- 15- 16 -63.073 3- 2- 4- 16 -61.463
4- 2- 3- 6 118.102 4- 2- 3- 10 -120.896
4- 13- 11- 12 -176.886 5- 2- 3- 6 -121.002
5- 2- 4- 7 63.930 5- 2- 3- 10 -0.000
5- 2- 4- 13 -64.448 5- 2- 4- 16 176.293
6- 3- 1- 8 54.013 6- 3- 2- 9 -0.000
6- 3- 1- 11 -177.609 6- 3- 1- 15 -58.350
7- 4- 2- 9 -54.013 7- 4- 13- 11 171.734
7- 4- 13- 14 -5.221 7- 4- 16- 15 -177.784

8- 1- 3- 10 -63.930 8- 1- 11- 12 5.221
8- 1- 11- 13 -171.734 8- 1- 15- 16 177.784
9- 2- 3- 10 121.002 9- 2- 4- 13 177.609
9- 2- 4- 16 58.350 10- 3- 1- 11 64.448
10- 3- 1- 15 -176.293 11- 1- 15- 16 56.901
11- 13- 4- 16 58.084 12- 11- 13- 14 -0.000
12- 11- 1- 15 118.871 13- 4- 16- 15 -56.901
13- 11- 1- 15 -58.084 14- 13- 4- 16 -118.871

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 3 1.5415 1- 8 1.0934 1- 11 1.5079 1- 15 1.4506
5) 2- 3 1.5535 2- 4 1.5415 2- 5 1.0954 2- 9 1.0945
9) 3- 6 1.0945 3- 10 1.0954 4- 7 1.0934 4- 13 1.5079
13) 4- 16 1.4506 11- 12 1.0862 11- 13 1.3365 13- 14 1.0862
17) 15- 16 1.4806
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 3- 6 108.538 1- 3- 10 110.027 1- 11- 12 122.404
4) 1- 11- 13 112.196 1- 15- 16 110.060 2- 3- 6 110.957
7) 2- 3- 10 111.988 2- 4- 7 112.572 2- 4- 13 110.413
10) 2- 4- 16 107.819 3- 1- 8 112.572 3- 1- 11 110.413
13) 3- 1- 15 107.819 3- 2- 4 107.406 3- 2- 5 111.988
16) 3- 2- 9 110.957 4- 2- 3 107.406 4- 2- 5 110.027
19) 4- 2- 9 108.538 4- 13- 14 122.404 5- 2- 3 111.988
22) 5- 2- 4 110.027 5- 2- 9 107.882 6- 3- 10 107.882
25) 7- 4- 13 113.862 7- 4- 16 102.836 8- 1- 3 112.572
28) 8- 1- 11 113.862 8- 1- 15 102.836 9- 2- 3 110.957
31) 9- 2- 4 108.538 9- 2- 5 107.882 10- 3- 6 107.882
34) 11- 1- 3 110.413 11- 1- 8 113.862 11- 1- 15 108.852
37) 11- 13- 14 125.323 12- 11- 13 125.323 13- 4- 7 113.862
40) 13- 4- 16 108.852 13- 11- 12 125.323 15- 1- 3 107.819
43) 15- 1- 8 102.836 15- 1- 11 108.852 16- 4- 7 102.836
46) 16- 4- 13 108.852
Dihedrals
I J K L Theta I J K L Theta
1- 3- 2- 4 -0.000 1- 11- 13- 4 -0.000
1- 15- 16- 4 -0.000 1- 3- 2- 5 120.906
1- 3- 2- 9 -118.481 1- 11- 13- 14 176.857
2- 3- 1- 8 174.149 2- 3- 1- 11 -57.377
2- 4- 13- 11 -60.226 2- 4- 13- 14 122.811
2- 3- 1- 15 61.423 2- 4- 16- 15 63.136
3- 2- 4- 7 -174.149 3- 1- 11- 12 -122.811
3- 1- 11- 13 60.226 3- 2- 4- 13 57.377
3- 1- 15- 16 -63.136 3- 2- 4- 16 -61.423
4- 2- 3- 6 118.481 4- 2- 3- 10 -120.906
4- 13- 11- 12 -176.857 5- 2- 3- 6 -120.613
5- 2- 4- 7 63.717 5- 2- 3- 10 -0.000
5- 2- 4- 13 -64.757 5- 2- 4- 16 176.443
6- 3- 1- 8 54.118 6- 3- 2- 9 -0.000
6- 3- 1- 11 -177.408 6- 3- 1- 15 -58.608
7- 4- 2- 9 -54.118 7- 4- 13- 11 172.005
7- 4- 13- 14 -4.957 7- 4- 16- 15 -177.737
8- 1- 3- 10 -63.717 8- 1- 11- 12 4.957
8- 1- 11- 13 -172.005 8- 1- 15- 16 177.737
9- 2- 3- 10 120.613 9- 2- 4- 13 177.408
9- 2- 4- 16 58.608 10- 3- 1- 11 64.757
10- 3- 1- 15 -176.443 11- 1- 15- 16 56.658
11- 13- 4- 16 57.944 12- 11- 13- 14 -0.000

12- 11- 1- 15 119.019 13- 4- 16- 15 -56.658
13- 11- 1- 15 -57.944 14- 13- 4- 16 -119.019

DFT/6-31G* (DICHLOROMETHANE)

Bond Lengths
I J R I J R I J R I J R
1) 1- 3 1.5394 1- 8 1.0929 1- 11 1.5061 1- 15 1.4611
5) 2- 3 1.5523 2- 4 1.5394 2- 5 1.0944 2- 9 1.0943
9) 3- 6 1.0943 3- 10 1.0944 4- 7 1.0929 4- 13 1.5061
13) 4- 16 1.4611 11- 12 1.0856 11- 13 1.3364 13- 14 1.0856
17) 15- 16 1.4823
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 3- 6 108.663 1- 3- 10 109.723 1- 11- 12 122.312
4) 1- 11- 13 112.293 1- 15- 16 109.945 2- 3- 6 111.107
7) 2- 3- 10 112.032 2- 4- 7 112.710 2- 4- 13 110.541
10) 2- 4- 16 107.787 3- 1- 8 112.710 3- 1- 11 110.541
13) 3- 1- 15 107.787 3- 2- 4 107.518 3- 2- 5 112.032
16) 3- 2- 9 111.107 4- 2- 3 107.518 4- 2- 5 109.723
19) 4- 2- 9 108.663 4- 13- 14 122.312 5- 2- 3 112.032
22) 5- 2- 4 109.723 5- 2- 9 107.753 6- 3- 10 107.753
25) 7- 4- 13 113.979 7- 4- 16 102.627 8- 1- 3 112.710
28) 8- 1- 11 113.979 8- 1- 15 102.627 9- 2- 3 111.107
31) 9- 2- 4 108.663 9- 2- 5 107.753 10- 3- 6 107.753
34) 11- 1- 3 110.541 11- 1- 8 113.979 11- 1- 15 108.659
37) 11- 13- 14 125.341 12- 11- 13 125.341 13- 4- 7 113.979
40) 13- 4- 16 108.659 13- 11- 12 125.341 15- 1- 3 107.787
43) 15- 1- 8 102.627 15- 1- 11 108.659 16- 4- 7 102.627
46) 16- 4- 13 108.659
Dihedrals
I J K L Theta I J K L Theta
1- 3- 2- 4 -0.000 1- 11- 13- 4 -0.000
1- 15- 16- 4 -0.000 1- 3- 2- 5 120.630
1- 3- 2- 9 -118.786 1- 11- 13- 14 177.360
2- 3- 1- 8 174.043 2- 3- 1- 11 -57.107
2- 4- 13- 11 -59.932 2- 4- 13- 14 122.616
2- 3- 1- 15 61.515 2- 4- 16- 15 63.083
3- 2- 4- 7 -174.043 3- 1- 11- 12 -122.616
3- 1- 11- 13 59.932 3- 2- 4- 13 57.107
3- 1- 15- 16 -63.083 3- 2- 4- 16 -61.515
4- 2- 3- 6 118.786 4- 2- 3- 10 -120.630
4- 13- 11- 12 -177.360 5- 2- 3- 6 -120.583
5- 2- 4- 7 63.881 5- 2- 3- 10 -0.000
5- 2- 4- 13 -64.969 5- 2- 4- 16 176.409
6- 3- 1- 8 53.699 6- 3- 2- 9 -0.000
6- 3- 1- 11 -177.451 6- 3- 1- 15 -58.829
7- 4- 2- 9 -53.699 7- 4- 13- 11 171.907
7- 4- 13- 14 -5.545 7- 4- 16- 15 -177.750
8- 1- 3- 10 -63.881 8- 1- 11- 12 5.545
8- 1- 11- 13 -171.907 8- 1- 15- 16 177.750
9- 2- 3- 10 120.583 9- 2- 4- 13 177.451
9- 2- 4- 16 58.829 10- 3- 1- 11 64.969
10- 3- 1- 15 -176.409 11- 1- 15- 16 56.737
11- 13- 4- 16 58.158 12- 11- 13- 14 -0.000
12- 11- 1- 15 119.294 13- 4- 16- 15 -56.737
13- 11- 1- 15 -58.158 14- 13- 4- 16 -119.294

Optimised structures for primary ozonide (15a) *endo-exo* at all levels reported.

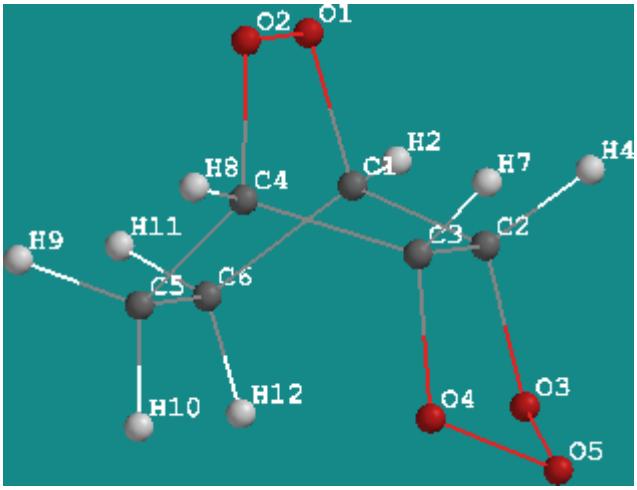

Figure S3: Optimised geometry for *endo-exo* primary ozonide **15a**

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5226 1- 7 1.0806 1- 11 1.4153 1- 13 1.5259
5) 2- 3 1.5227 2- 4 1.5457 2- 5 1.0816 2- 8 1.0829
9) 3- 9 1.0806 3- 12 1.4153 3- 14 1.5259 4- 6 1.0829
13) 4- 10 1.0816 11- 12 1.4169 13- 14 1.5414 13- 15 1.0812
17) 13- 17 1.4058 14- 16 1.0812 14- 18 1.4058 17- 19 1.3833
21) 18- 19 1.3834
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.075 1- 4- 10 109.938 1- 11- 12 112.295
4) 1- 13- 14 108.121 1- 13- 15 111.151 1- 13- 17 111.443
7) 2- 3- 9 112.215 2- 3- 12 109.874 2- 3- 14 112.769
10) 2- 4- 6 110.901 2- 4- 10 111.824 3- 2- 4 108.073
13) 3- 2- 5 109.939 3- 2- 8 108.095 3- 14- 16 111.148
16) 3- 14- 18 111.417 4- 1- 7 112.214 4- 1- 11 109.895
19) 4- 1- 13 112.781 4- 2- 3 108.073 4- 2- 5 111.818
22) 4- 2- 8 110.899 5- 2- 3 109.939 5- 2- 4 111.818
25) 5- 2- 8 107.955 6- 4- 10 107.956 7- 1- 4 112.214
28) 7- 1- 11 103.930 7- 1- 13 111.711 8- 2- 3 108.095
31) 8- 2- 4 110.899 8- 2- 5 107.955 9- 3- 12 103.932
34) 9- 3- 14 111.707 10- 4- 6 107.956 11- 1- 4 109.895
37) 11- 1- 7 103.930 11- 1- 13 105.714 12- 3- 9 103.932
40) 12- 3- 14 105.751 13- 1- 4 112.781 13- 1- 7 111.711
43) 13- 1- 11 105.714 13- 14- 16 112.245 13- 14- 18 102.878
46) 13- 17- 19 103.760 14- 3- 9 111.707 14- 3- 12 105.751
49) 14- 13- 15 112.239 14- 13- 17 102.865 14- 18- 19 103.787
52) 15- 13- 14 112.239 15- 13- 17 110.731 16- 14- 18 110.736
```

55) 17- 13- 14 102.865 17- 13- 15 110.731 18- 14- 16 110.736
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 0.171 1- 11- 12- 3 0.238
1- 13- 14- 3 0.145 1- 4- 2- 5 -120.963
1- 4- 2- 8 118.486 1- 13- 14- 16 -122.814
1- 13- 14- 18 118.113 1- 13- 17- 19 -143.659
2- 4- 1- 7 -172.355 2- 3- 12- 11 -59.818
2- 4- 1- 11 -57.247 2- 3- 14- 13 60.475
2- 4- 1- 13 60.423 2- 3- 14- 16 -175.901
2- 3- 14- 18 -51.878 3- 2- 4- 6 -118.128
3- 2- 4- 10 121.314 3- 14- 13- 15 123.101
3- 14- 13- 17 -117.844 3- 14- 18- 19 143.456
4- 2- 3- 9 172.153 4- 1- 11- 12 59.526
4- 2- 3- 12 57.055 4- 1- 13- 14 -60.641
4- 2- 3- 14 -60.640 4- 1- 13- 15 175.745
4- 1- 13- 17 51.707 5- 2- 4- 6 120.738
5- 2- 3- 9 -65.554 5- 2- 4- 10 0.180
5- 2- 3- 12 179.348 5- 2- 3- 14 61.653
6- 4- 1- 7 -52.266 6- 4- 2- 8 0.187
6- 4- 1- 11 62.842 6- 4- 1- 13 -179.487
7- 1- 4- 10 65.338 7- 1- 11- 12 179.791
7- 1- 13- 14 171.873 7- 1- 13- 15 48.258
7- 1- 13- 17 -75.780 8- 2- 3- 9 52.061
8- 2- 4- 10 -120.371 8- 2- 3- 12 -63.037
8- 2- 3- 14 179.268 9- 3- 12- 11 179.925
9- 3- 14- 13 -172.049 9- 3- 14- 16 -48.425
9- 3- 14- 18 75.598 10- 4- 1- 11 -179.554
10- 4- 1- 13 -61.884 11- 1- 13- 14 59.464
11- 12- 3- 14 62.156 11- 1- 13- 15 -64.151
11- 1- 13- 17 171.811 12- 3- 14- 13 -59.620
12- 11- 1- 13 -62.451 12- 3- 14- 16 64.003
12- 3- 14- 18 -171.973 13- 17- 19- 18 47.342
13- 14- 18- 19 27.831 14- 18- 19- 17 -47.256
14- 13- 17- 19 -28.035 15- 13- 14- 16 0.142
15- 13- 14- 18 -118.931 15- 13- 17- 19 92.066
16- 14- 13- 17 119.197 16- 14- 18- 19 -92.288
17- 13- 14- 18 0.125

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5217 1- 7 1.0800 1- 11 1.4207 1- 13 1.5262
5) 2- 3 1.5217 2- 4 1.5448 2- 5 1.0813 2- 8 1.0824
9) 3- 9 1.0800 3- 12 1.4207 3- 14 1.5262 4- 6 1.0824
13) 4- 10 1.0813 11- 12 1.4176 13- 14 1.5405 13- 15 1.0804
17) 13- 17 1.4108 14- 16 1.0804 14- 18 1.4108 17- 19 1.3836
21) 18- 19 1.3837
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.044 1- 4- 10 109.876 1- 11- 12 112.262
4) 1- 13- 14 108.202 1- 13- 15 111.257 1- 13- 17 111.400
7) 2- 3- 9 112.356 2- 3- 12 109.795 2- 3- 14 112.995
10) 2- 4- 6 110.967 2- 4- 10 111.890 3- 2- 4 108.170
13) 3- 2- 5 109.878 3- 2- 8 108.055 3- 14- 16 111.256
16) 3- 14- 18 111.385 4- 1- 7 112.355 4- 1- 11 109.808
19) 4- 1- 13 113.002 4- 2- 3 108.170 4- 2- 5 111.886
22) 4- 2- 8 110.966 5- 2- 3 109.878 5- 2- 4 111.886
25) 5- 2- 8 107.819 6- 4- 10 107.820 7- 1- 4 112.355

28) 7- 1- 11 103.860 7- 1- 13 111.724 8- 2- 3 108.055
31) 8- 2- 4 110.966 8- 2- 5 107.819 9- 3- 12 103.860
34) 9- 3- 14 111.723 10- 4- 6 107.820 11- 1- 4 109.808
37) 11- 1- 7 103.860 11- 1- 13 105.438 12- 3- 9 103.860
40) 12- 3- 14 105.459 13- 1- 4 113.002 13- 1- 7 111.724
43) 13- 1- 11 105.438 13- 14- 16 112.326 13- 14- 18 102.886
46) 13- 17- 19 103.757 14- 3- 9 111.723 14- 3- 12 105.459
49) 14- 13- 15 112.322 14- 13- 17 102.878 14- 18- 19 103.772
52) 15- 13- 14 112.322 15- 13- 17 110.489 16- 14- 18 110.491
55) 17- 13- 14 102.878 17- 13- 15 110.489 18- 14- 16 110.491
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 0.096 1- 11- 12- 3 0.137
1- 13- 14- 3 0.083 1- 4- 2- 5 -121.069
1- 4- 2- 8 118.461 1- 13- 14- 16 -123.121
1- 13- 14- 18 118.052 1- 13- 17- 19 -143.632
2- 4- 1- 7 -172.286 2- 3- 12- 11 -59.714
2- 4- 1- 11 -57.235 2- 3- 14- 13 60.200
2- 4- 1- 13 60.170 2- 3- 14- 16 -175.951
2- 3- 14- 18 -52.190 3- 2- 4- 6 -118.260
3- 2- 4- 10 121.265 3- 14- 13- 15 123.284
3- 14- 13- 17 -117.899 3- 14- 18- 19 143.517
4- 2- 3- 9 172.171 4- 1- 11- 12 59.546
4- 2- 3- 12 57.127 4- 1- 13- 14 -60.295
4- 2- 3- 14 -60.292 4- 1- 13- 15 175.861
4- 1- 13- 17 52.091 5- 2- 4- 6 120.575
5- 2- 3- 9 -65.427 5- 2- 4- 10 0.100
5- 2- 3- 12 179.529 5- 2- 3- 14 62.110
6- 4- 1- 7 -52.083 6- 4- 2- 8 0.105
6- 4- 1- 11 62.968 6- 4- 1- 13 -179.627
7- 1- 4- 10 65.305 7- 1- 11- 12 179.895
7- 1- 13- 14 171.830 7- 1- 13- 15 47.986
7- 1- 13- 17 -75.783 8- 2- 3- 9 51.967
8- 2- 4- 10 -120.370 8- 2- 3- 12 -63.077
8- 2- 3- 14 179.504 9- 3- 12- 11 179.943
9- 3- 14- 13 -171.931 9- 3- 14- 16 -48.082
9- 3- 14- 18 75.679 10- 4- 1- 11 -179.644
10- 4- 1- 13 -62.239 11- 1- 13- 14 59.649
11- 12- 3- 14 62.313 11- 1- 13- 15 -64.195
11- 1- 13- 17 172.035 12- 3- 14- 13 -59.738
12- 11- 1- 13 -62.483 12- 3- 14- 16 64.111
12- 3- 14- 18 -172.128 13- 17- 19- 18 47.250
13- 14- 18- 19 27.810 14- 18- 19- 17 -47.201
14- 13- 17- 19 -27.927 15- 13- 14- 16 0.080
15- 13- 14- 18 -118.746 15- 13- 17- 19 92.163
16- 14- 13- 17 118.897 16- 14- 18- 19 -92.289
17- 13- 14- 18 0.071

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5197 1- 7 1.0950 1- 11 1.4401 1- 13 1.5257
5) 2- 3 1.5224 2- 4 1.5409 2- 5 1.0929 2- 8 1.0933
9) 3- 9 1.0954 3- 12 1.4397 3- 14 1.5256 4- 6 1.0937
13) 4- 10 1.0933 11- 12 1.5081 13- 14 1.5499 13- 15 1.0952
17) 13- 17 1.4257 14- 16 1.0953 14- 18 1.4295 17- 19 1.4574
21) 18- 19 1.4753
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.216 1- 4- 10 109.983 1- 11- 12 109.578

4) 1- 13- 14 107.788 1- 13- 15 112.071 1- 13- 17 110.694
7) 2- 3- 9 112.830 2- 3- 12 110.013 2- 3- 14 111.793
10) 2- 4- 6 111.225 2- 4- 10 111.735 3- 2- 4 107.487
13) 3- 2- 5 109.276 3- 2- 8 109.136 3- 14- 16 111.446
16) 3- 14- 18 109.402 4- 1- 7 112.483 4- 1- 11 111.002
19) 4- 1- 13 112.741 4- 2- 3 107.487 4- 2- 5 111.741
22) 4- 2- 8 111.018 5- 2- 3 109.276 5- 2- 4 111.741
25) 5- 2- 8 108.146 6- 4- 10 108.131 7- 1- 4 112.483
28) 7- 1- 11 102.793 7- 1- 13 112.133 8- 2- 3 109.136
31) 8- 2- 4 111.018 8- 2- 5 108.146 9- 3- 12 102.863
34) 9- 3- 14 111.462 10- 4- 6 108.131 11- 1- 4 111.002
37) 11- 1- 7 102.793 11- 1- 13 104.972 12- 3- 9 102.863
40) 12- 3- 14 107.370 13- 1- 4 112.741 13- 1- 7 112.133
43) 13- 1- 11 104.972 13- 14- 16 111.665 13- 14- 18 104.763
46) 13- 17- 19 100.574 14- 3- 9 111.462 14- 3- 12 107.370
49) 14- 13- 15 111.390 14- 13- 17 103.567 14- 18- 19 102.880
52) 15- 13- 14 111.390 15- 13- 17 110.969 16- 14- 18 111.324
55) 17- 13- 14 103.567 17- 13- 15 110.969 18- 14- 16 111.324
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 14.004 1- 11- 12- 3 16.860
1- 13- 14- 3 11.710 1- 4- 2- 5 -105.881
1- 4- 2- 8 133.295 1- 13- 14- 16 -111.142
1- 13- 14- 18 128.240 1- 13- 17- 19 -153.491
2- 4- 1- 7 179.051 2- 3- 12- 11 -69.762
2- 4- 1- 11 -66.394 2- 3- 14- 13 53.218
2- 4- 1- 13 51.056 2- 3- 14- 16 176.203
2- 3- 14- 18 -60.254 3- 2- 4- 6 -103.662
3- 2- 4- 10 135.394 3- 14- 13- 15 135.041
3- 14- 13- 17 -105.626 3- 14- 18- 19 136.258
4- 2- 3- 9 164.611 4- 1- 11- 12 49.158
4- 2- 3- 12 50.381 4- 1- 13- 14 -66.353
4- 2- 3- 14 -68.816 4- 1- 13- 15 170.731
4- 1- 13- 17 46.263 5- 2- 4- 6 136.453
5- 2- 3- 9 -73.949 5- 2- 4- 10 15.509
5- 2- 3- 12 171.821 5- 2- 3- 14 52.625
6- 4- 1- 7 -60.754 6- 4- 2- 8 15.629
6- 4- 1- 11 53.801 6- 4- 1- 13 171.251
7- 1- 4- 10 56.590 7- 1- 11- 12 169.636
7- 1- 13- 14 165.469 7- 1- 13- 15 42.553
7- 1- 13- 17 -81.915 8- 2- 3- 9 44.123
8- 2- 4- 10 -105.316 8- 2- 3- 12 -70.107
8- 2- 3- 14 170.697 9- 3- 12- 11 169.792
9- 3- 14- 13 -179.468 9- 3- 14- 16 -56.483
9- 3- 14- 18 67.060 10- 4- 1- 11 171.145
10- 4- 1- 13 -71.405 11- 1- 13- 14 54.601
11- 12- 3- 14 52.103 11- 1- 13- 15 -68.315
11- 1- 13- 17 167.217 12- 3- 14- 13 -67.529
12- 11- 1- 13 -72.935 12- 3- 14- 16 55.456
12- 3- 14- 18 178.999 13- 17- 19- 18 52.086
13- 14- 18- 19 20.717 14- 18- 19- 17 -45.062
14- 13- 17- 19 -38.207 15- 13- 14- 16 12.190
15- 13- 14- 18 -108.429 15- 13- 17- 19 81.415
16- 14- 13- 17 131.523 16- 14- 18- 19 -100.127
17- 13- 14- 18 10.904

MP2/6-311G*

Geometry information
Bond Lengths

I J R I J R I J R I J R
1) 1- 4 1.5209 1- 7 1.0939 1- 11 1.4335 1- 13 1.5256
5) 2- 3 1.5241 2- 4 1.5425 2- 5 1.0914 2- 8 1.0925
9) 3- 9 1.0944 3- 12 1.4334 3- 14 1.5262 4- 6 1.0930
13) 4- 10 1.0922 11- 12 1.4876 13- 14 1.5523 13- 15 1.0945
17) 13- 17 1.4181 14- 16 1.0942 14- 18 1.4221 17- 19 1.4356
21) 18- 19 1.4564
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.042 1- 4- 10 110.188 1- 11- 12 109.770
4) 1- 13- 14 107.499 1- 13- 15 112.343 1- 13- 17 111.333
7) 2- 3- 9 113.046 2- 3- 12 109.764 2- 3- 14 111.508
10) 2- 4- 6 111.028 2- 4- 10 111.861 3- 2- 4 107.034
13) 3- 2- 5 109.596 3- 2- 8 109.196 3- 14- 16 111.611
16) 3- 14- 18 109.672 4- 1- 7 112.448 4- 1- 11 110.947
19) 4- 1- 13 112.582 4- 2- 3 107.034 4- 2- 5 111.825
22) 4- 2- 8 110.976 5- 2- 3 109.596 5- 2- 4 111.825
25) 5- 2- 8 108.184 6- 4- 10 108.250 7- 1- 4 112.448
28) 7- 1- 11 102.922 7- 1- 13 112.317 8- 2- 3 109.196
31) 8- 2- 4 110.976 8- 2- 5 108.184 9- 3- 12 102.945
34) 9- 3- 14 111.383 10- 4- 6 108.250 11- 1- 4 110.947
37) 11- 1- 7 102.922 11- 1- 13 104.930 12- 3- 9 102.945
40) 12- 3- 14 107.722 13- 1- 4 112.582 13- 1- 7 112.317
43) 13- 1- 11 104.930 13- 14- 16 111.781 13- 14- 18 104.364
46) 13- 17- 19 100.846 14- 3- 9 111.383 14- 3- 12 107.722
49) 14- 13- 15 111.385 14- 13- 17 103.131 14- 18- 19 103.206
52) 15- 13- 14 111.385 15- 13- 17 110.736 16- 14- 18 111.316
55) 17- 13- 14 103.131 17- 13- 15 110.736 18- 14- 16 111.316
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 15.215 1- 11- 12- 3 18.947
1- 13- 14- 3 12.580 1- 4- 2- 5 -104.822
1- 4- 2- 8 134.277 1- 13- 14- 16 -110.431
1- 13- 14- 18 129.143 1- 13- 17- 19 -153.223
2- 4- 1- 7 178.711 2- 3- 12- 11 -71.046
2- 4- 1- 11 -66.629 2- 3- 14- 13 53.177
2- 4- 1- 13 50.628 2- 3- 14- 16 176.292
2- 3- 14- 18 -59.868 3- 2- 4- 6 -102.072
3- 2- 4- 10 136.881 3- 14- 13- 15 136.052
3- 14- 13- 17 -105.145 3- 14- 18- 19 135.034
4- 2- 3- 9 163.600 4- 1- 11- 12 47.725
4- 2- 3- 12 49.298 4- 1- 13- 14 -67.150
4- 2- 3- 14 -69.994 4- 1- 13- 15 169.966
4- 1- 13- 17 45.113 5- 2- 4- 6 137.890
5- 2- 3- 9 -74.947 5- 2- 4- 10 16.844
5- 2- 3- 12 170.752 5- 2- 3- 14 51.460
6- 4- 1- 7 -61.474 6- 4- 2- 8 16.990
6- 4- 1- 11 53.186 6- 4- 1- 13 170.443
7- 1- 4- 10 56.023 7- 1- 11- 12 168.210
7- 1- 13- 14 164.698 7- 1- 13- 15 41.815
7- 1- 13- 17 -83.039 8- 2- 3- 9 43.393
8- 2- 4- 10 -104.056 8- 2- 3- 12 -70.908
8- 2- 3- 14 169.800 9- 3- 12- 11 168.329
9- 3- 14- 13 -179.511 9- 3- 14- 16 -56.395
9- 3- 14- 18 67.444 10- 4- 1- 11 170.682
10- 4- 1- 13 -72.061 11- 1- 13- 14 53.622
11- 12- 3- 14 50.542 11- 1- 13- 15 -69.262
11- 1- 13- 17 165.884 12- 3- 14- 13 -67.320
12- 11- 1- 13 -74.120 12- 3- 14- 16 55.795
12- 3- 14- 18 179.635 13- 17- 19- 18 52.005
13- 14- 18- 19 19.782 14- 18- 19- 17 -44.527
14- 13- 17- 19 -38.226 15- 13- 14- 16 13.041

15- 13- 14- 18 -107.386 15- 13- 17- 19 81.028
16- 14- 13- 17 131.844 16- 14- 18- 19 -100.954
17- 13- 14- 18 11.417

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5293 1- 7 1.0945 1- 11 1.4331 1- 13 1.5369
5) 2- 3 1.5301 2- 4 1.5522 2- 5 1.0931 2- 8 1.0935
9) 3- 9 1.0945 3- 12 1.4335 3- 14 1.5377 4- 6 1.0940
13) 4- 10 1.0932 11- 12 1.4938 13- 14 1.5623 13- 15 1.0949
17) 13- 17 1.4236 14- 16 1.0950 14- 18 1.4242 17- 19 1.4477
21) 18- 19 1.4530
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.960 1- 4- 10 109.603 1- 11- 12 110.807
4) 1- 13- 14 108.050 1- 13- 15 111.145 1- 13- 17 110.986
7) 2- 3- 9 112.325 2- 3- 12 110.685 2- 3- 14 112.363
10) 2- 4- 6 111.120 2- 4- 10 111.664 3- 2- 4 108.250
13) 3- 2- 5 109.321 3- 2- 8 108.442 3- 14- 16 111.117
16) 3- 14- 18 110.755 4- 1- 7 112.244 4- 1- 11 110.790
19) 4- 1- 13 112.691 4- 2- 3 108.250 4- 2- 5 111.632
22) 4- 2- 8 111.089 5- 2- 3 109.321 5- 2- 4 111.632
25) 5- 2- 8 108.049 6- 4- 10 108.095 7- 1- 4 112.244
28) 7- 1- 11 102.793 7- 1- 13 111.589 8- 2- 3 108.442
31) 8- 2- 4 111.089 8- 2- 5 108.049 9- 3- 12 102.822
34) 9- 3- 14 111.521 10- 4- 6 108.095 11- 1- 4 110.790
37) 11- 1- 7 102.793 11- 1- 13 106.110 12- 3- 9 102.822
40) 12- 3- 14 106.555 13- 1- 4 112.691 13- 1- 7 111.589
43) 13- 1- 11 106.110 13- 14- 16 111.276 13- 14- 18 104.162
46) 13- 17- 19 102.393 14- 3- 9 111.521 14- 3- 12 106.555
49) 14- 13- 15 111.251 14- 13- 17 103.845 14- 18- 19 102.846
52) 15- 13- 14 111.251 15- 13- 17 111.296 16- 14- 18 111.313
55) 17- 13- 14 103.845 17- 13- 15 111.296 18- 14- 16 111.313
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 3.253 1- 11- 12- 3 3.591
1- 13- 14- 3 2.568 1- 4- 2- 5 -117.115
1- 4- 2- 8 122.211 1- 13- 14- 16 -119.620
1- 13- 14- 18 120.345 1- 13- 17- 19 -146.666
2- 4- 1- 7 -174.463 2- 3- 12- 11 -61.806
2- 4- 1- 11 -60.185 2- 3- 14- 13 58.995
2- 4- 1- 13 58.531 2- 3- 14- 16 -178.719
2- 3- 14- 18 -54.454 3- 2- 4- 6 -115.183
3- 2- 4- 10 124.041 3- 14- 13- 15 124.832
3- 14- 13- 17 -115.354 3- 14- 18- 19 142.684
4- 2- 3- 9 170.572 4- 1- 11- 12 57.641
4- 2- 3- 12 56.274 4- 1- 13- 14 -61.912
4- 2- 3- 14 -62.717 4- 1- 13- 15 175.759
4- 1- 13- 17 51.327 5- 2- 4- 6 124.450
5- 2- 3- 9 -67.629 5- 2- 4- 10 3.674
5- 2- 3- 12 178.073 5- 2- 3- 14 59.081
6- 4- 1- 7 -54.039 6- 4- 2- 8 3.776
6- 4- 1- 11 60.239 6- 4- 1- 13 178.955
7- 1- 4- 10 63.479 7- 1- 11- 12 177.736
7- 1- 13- 14 170.735 7- 1- 13- 15 48.406
7- 1- 13- 17 -76.026 8- 2- 3- 9 49.952
8- 2- 4- 10 -117.000 8- 2- 3- 12 -64.347

8- 2- 3- 14 176.662 9- 3- 12- 11 178.038
9- 3- 14- 13 -173.864 9- 3- 14- 16 -51.578
9- 3- 14- 18 72.687 10- 4- 1- 11 177.757
10- 4- 1- 13 -63.527 11- 1- 13- 14 59.503
11- 12- 3- 14 60.641 11- 1- 13- 15 -62.827
11- 1- 13- 17 172.742 12- 3- 14- 13 -62.389
12- 11- 1- 13 -64.985 12- 3- 14- 16 59.897
12- 3- 14- 18 -175.838 13- 17- 19- 18 48.730
13- 14- 18- 19 26.848 14- 18- 19- 17 -47.114
14- 13- 17- 19 -30.796 15- 13- 14- 16 2.644
15- 13- 14- 18 -117.391 15- 13- 17- 19 88.987
16- 14- 13- 17 122.458 16- 14- 18- 19 -93.162
17- 13- 14- 18 2.423

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5284 1- 7 1.0939 1- 11 1.4392 1- 13 1.5376
5) 2- 3 1.5285 2- 4 1.5506 2- 5 1.0930 2- 8 1.0934
9) 3- 9 1.0939 3- 12 1.4392 3- 14 1.5376 4- 6 1.0934
13) 4- 10 1.0930 11- 12 1.4953 13- 14 1.5614 13- 15 1.0937
17) 13- 17 1.4295 14- 16 1.0937 14- 18 1.4295 17- 19 1.4509
21) 18- 19 1.4510
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.205 1- 4- 10 109.336 1- 11- 12 110.784
4) 1- 13- 14 108.093 1- 13- 15 111.219 1- 13- 17 110.903
7) 2- 3- 9 112.394 2- 3- 12 110.706 2- 3- 14 112.808
10) 2- 4- 6 111.203 2- 4- 10 111.783 3- 2- 4 108.413
13) 3- 2- 5 109.338 3- 2- 8 108.229 3- 14- 16 111.213
16) 3- 14- 18 110.873 4- 1- 7 112.388 4- 1- 11 110.738
19) 4- 1- 13 112.824 4- 2- 3 108.413 4- 2- 5 111.784
22) 4- 2- 8 111.200 5- 2- 3 109.338 5- 2- 4 111.784
25) 5- 2- 8 107.806 6- 4- 10 107.807 7- 1- 4 112.388
28) 7- 1- 11 102.701 7- 1- 13 111.577 8- 2- 3 108.229
31) 8- 2- 4 111.200 8- 2- 5 107.806 9- 3- 12 102.704
34) 9- 3- 14 111.566 10- 4- 6 107.807 11- 1- 4 110.738
37) 11- 1- 7 102.701 11- 1- 13 105.947 12- 3- 9 102.704
40) 12- 3- 14 106.001 13- 1- 4 112.824 13- 1- 7 111.577
43) 13- 1- 11 105.947 13- 14- 16 111.345 13- 14- 18 104.024
46) 13- 17- 19 102.586 14- 3- 9 111.566 14- 3- 12 106.001
49) 14- 13- 15 111.337 14- 13- 17 104.004 14- 18- 19 102.622
52) 15- 13- 14 111.337 15- 13- 17 111.029 16- 14- 18 111.030
55) 17- 13- 14 104.004 17- 13- 15 111.029 18- 14- 16 111.030
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 0.226 1- 11- 12- 3 0.313
1- 13- 14- 3 0.190 1- 4- 2- 5 -120.363
1- 4- 2- 8 119.092 1- 13- 14- 16 -122.253
1- 13- 14- 18 118.095 1- 13- 17- 19 -144.934
2- 4- 1- 7 -172.614 2- 3- 12- 11 -59.865
2- 4- 1- 11 -58.395 2- 3- 14- 13 60.013
2- 4- 1- 13 60.165 2- 3- 14- 16 -177.464
2- 3- 14- 18 -53.409 3- 2- 4- 6 -118.625
3- 2- 4- 10 120.827 3- 14- 13- 15 122.628
3- 14- 13- 17 -117.737 3- 14- 18- 19 144.670
4- 2- 3- 9 172.354 4- 1- 11- 12 59.473
4- 2- 3- 12 58.147 4- 1- 13- 14 -60.226

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4- 2- 3- 14 -60.450 4- 1- 13- 15 177.263
4- 1- 13- 17 53.183 5- 2- 4- 6 120.786
5- 2- 3- 9 -65.551 5- 2- 4- 10 0.238
5- 2- 3- 12 -179.757 5- 2- 3- 14 61.646
6- 4- 1- 7 -51.888 6- 4- 2- 8 0.241
6- 4- 1- 11 62.332 6- 4- 1- 13 -179.108
7- 1- 4- 10 65.278 7- 1- 11- 12 179.659
7- 1- 13- 14 172.126 7- 1- 13- 15 49.615
7- 1- 13- 17 -74.465 8- 2- 3- 9 51.629
8- 2- 4- 10 -120.308 8- 2- 3- 12 -62.578
8- 2- 3- 14 178.825 9- 3- 12- 11 179.955
9- 3- 14- 13 -172.353 9- 3- 14- 16 -49.830
9- 3- 14- 18 74.225 10- 4- 1- 11 179.498
10- 4- 1- 13 -61.942 11- 1- 13- 14 61.093
11- 12- 3- 14 62.786 11- 1- 13- 15 -61.418
11- 1- 13- 17 174.503 12- 3- 14- 13 -61.293
12- 11- 1- 13 -63.182 12- 3- 14- 16 61.230
12- 3- 14- 18 -174.716 13- 17- 19- 18 48.019
13- 14- 18- 19 28.695 14- 18- 19- 17 -47.908
14- 13- 17- 19 -28.965 15- 13- 14- 16 0.186
15- 13- 14- 18 -119.467 15- 13- 17- 19 90.879
16- 14- 13- 17 119.821 16- 14- 18- 19 -91.171
17- 13- 14- 18 0.169
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Optimised structures for primary ozonide (15b) *endo-endo* at all levels reported.

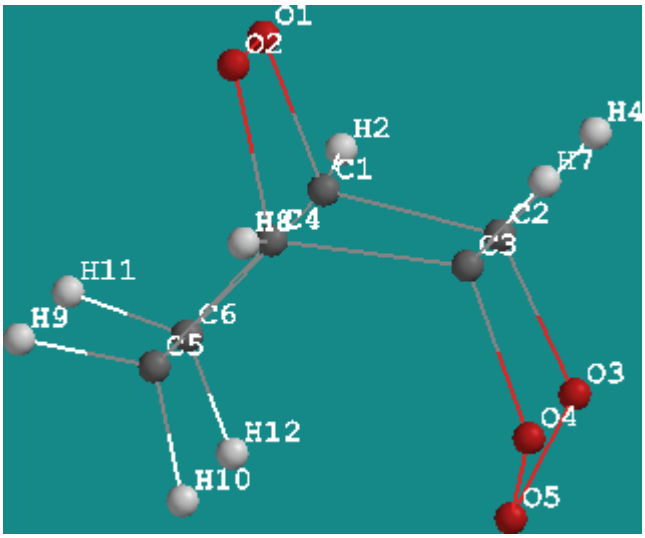

Figure S4: Optimised geometry for *endo-endo* primary ozonide **15b**

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5230 1- 7 1.0807 1- 11 1.4161 1- 13 1.5281
5) 2- 3 1.5230 2- 4 1.5454 2- 5 1.0818 2- 8 1.0830
9) 3- 9 1.0807 3- 12 1.4161 3- 14 1.5281 4- 6 1.0830
13) 4- 10 1.0818 11- 12 1.4180 13- 14 1.5404 13- 15 1.0793
17) 13- 17 1.4055 14- 16 1.0793 14- 18 1.4055 17- 19 1.3848
21) 18- 19 1.3848
```

Bond Angles

I	J	K	Theta	I	J	K	Theta	I	J	K	Theta
1)	1-	4-	6 107.998	1-	4-	10	110.080	1-	11-	12	112.119
4)	1-	13-	14 107.992	1-	13-	15	110.591	1-	13-	17	114.750
7)	2-	3-	9 112.099	2-	3-	12	109.646	2-	3-	14	113.527
10)	2-	4-	6 111.018	2-	4-	10	111.862	3-	2-	4	107.955
13)	3-	2-	5 110.080	3-	2-	8	107.998	3-	14-	16	110.591
16)	3-	14-	18 114.750	4-	1-	7	112.099	4-	1-	11	109.646
19)	4-	1-	13 113.527	4-	2-	3	107.955	4-	2-	5	111.862
22)	4-	2-	8 111.018	5-	2-	3	110.080	5-	2-	4	111.862
25)	5-	2-	8 107.865	6-	4-	10	107.865	7-	1-	4	112.099
28)	7-	1-	11 104.020	7-	1-	13	111.235	8-	2-	3	107.998
31)	8-	2-	4 111.018	8-	2-	5	107.865	9-	3-	12	104.020
34)	9-	3-	14 111.235	10-	4-	6	107.865	11-	1-	4	109.646
37)	11-	1-	7 104.020	11-	1-	13	105.660	12-	3-	9	104.020
40)	12-	3-	14 105.660	13-	1-	4	113.527	13-	1-	7	111.235
43)	13-	1-	11 105.660	13-	14-	16	113.250	13-	14-	18	103.172
46)	13-	17-	19 104.478	14-	3-	9	111.235	14-	3-	12	105.660
49)	14-	13-	15 113.250	14-	13-	17	103.172	14-	18-	19	104.478
52)	15-	13-	14 113.250	15-	13-	17	107.004	16-	14-	18	107.004
55)	17-	13-	14 103.172	17-	13-	15	107.004	18-	14-	16	107.004

Dihedrals

I	J	K	L	Theta	I	J	K	L	Theta
1-	4-	2-	3	-0.000	1-	11-	12-	3	-0.000
1-	13-	14-	3	-0.000	1-	4-	2-	5	-121.257
1-	4-	2-	8	118.194	1-	13-	14-	16	-122.819
1-	13-	14-	18	121.876	1-	13-	17-	19	-90.803
2-	4-	1-	7	-172.590	2-	3-	12-	11	-60.104
2-	4-	1-	11	-57.591	2-	3-	14-	13	60.336
2-	4-	1-	13	60.315	2-	3-	14-	16	-175.236
2-	3-	14-	18	-54.092	3-	2-	4-	6	-118.194
3-	2-	4-	10	121.257	3-	14-	13-	15	122.819
3-	14-	13-	17	-121.876	3-	14-	18-	19	90.803
4-	2-	3-	9	172.590	4-	1-	11-	12	60.104
4-	2-	3-	12	57.591	4-	1-	13-	14	-60.336
4-	2-	3-	14	-60.315	4-	1-	13-	15	175.236
4-	1-	13-	17	54.092	5-	2-	4-	6	120.548
5-	2-	3-	9	-65.052	5-	2-	4-	10	-0.000
5-	2-	3-	12	179.950	5-	2-	3-	14	62.043
6-	4-	1-	7	-52.477	6-	4-	2-	8	-0.000
6-	4-	1-	11	62.521	6-	4-	1-	13	-179.572
7-	1-	4-	10	65.052	7-	1-	11-	12	-179.838
7-	1-	13-	14	172.118	7-	1-	13-	15	47.690
7-	1-	13-	17	-73.454	8-	2-	3-	9	52.477
8-	2-	4-	10	-120.548	8-	2-	3-	12	-62.521
8-	2-	3-	14	179.572	9-	3-	12-	11	179.838
9-	3-	14-	13	-172.118	9-	3-	14-	16	-47.690
9-	3-	14-	18	73.454	10-	4-	1-	11	-179.950
10-	4-	1-	13	-62.043	11-	1-	13-	14	59.855
11-	12-	3-	14	62.599	11-	1-	13-	15	-64.573
11-	1-	13-	17	174.283	12-	3-	14-	13	-59.855
12-	11-	1-	13	-62.599	12-	3-	14-	16	64.573
12-	3-	14-	18	-174.283	13-	17-	19-	18	-44.626
13-	14-	18-	19	-26.404	14-	18-	19-	17	44.626
14-	13-	17-	19	26.404	15-	13-	14-	16	-0.000
15-	13-	14-	18	-115.305	15-	13-	17-	19	146.108
16-	14-	13-	17	115.305	16-	14-	18-	19	-146.108
17-	13-	14-	18	-0.000					

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5221 1- 7 1.0802 1- 11 1.4216 1- 13 1.5280
5) 2- 3 1.5221 2- 4 1.5447 2- 5 1.0816 2- 8 1.0826
9) 3- 9 1.0802 3- 12 1.4216 3- 14 1.5280 4- 6 1.0826
13) 4- 10 1.0816 11- 12 1.4184 13- 14 1.5393 13- 15 1.0787
17) 13- 17 1.4105 14- 16 1.0787 14- 18 1.4105 17- 19 1.3851
21) 18- 19 1.3851
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.993 1- 4- 10 110.003 1- 11- 12 112.086
4) 1- 13- 14 108.074 1- 13- 15 110.720 1- 13- 17 114.663
7) 2- 3- 9 112.229 2- 3- 12 109.535 2- 3- 14 113.725
10) 2- 4- 6 111.081 2- 4- 10 111.924 3- 2- 4 108.041
13) 3- 2- 5 110.003 3- 2- 8 107.993 3- 14- 16 110.720
16) 3- 14- 18 114.663 4- 1- 7 112.229 4- 1- 11 109.535
19) 4- 1- 13 113.725 4- 2- 3 108.041 4- 2- 5 111.924
22) 4- 2- 8 111.081 5- 2- 3 110.003 5- 2- 4 111.924
25) 5- 2- 8 107.732 6- 4- 10 107.732 7- 1- 4 112.229
28) 7- 1- 11 103.935 7- 1- 13 111.272 8- 2- 3 107.993
31) 8- 2- 4 111.081 8- 2- 5 107.732 9- 3- 12 103.935
34) 9- 3- 14 111.272 10- 4- 6 107.732 11- 1- 4 109.535
37) 11- 1- 7 103.935 11- 1- 13 105.438 12- 3- 9 103.935
40) 12- 3- 14 105.438 13- 1- 4 113.725 13- 1- 7 111.272
43) 13- 1- 11 105.438 13- 14- 16 113.310 13- 14- 18 103.175
46) 13- 17- 19 104.515 14- 3- 9 111.272 14- 3- 12 105.438
49) 14- 13- 15 113.310 14- 13- 17 103.175 14- 18- 19 104.515
52) 15- 13- 14 113.310 15- 13- 17 106.808 16- 14- 18 106.808
55) 17- 13- 14 103.175 17- 13- 15 106.808 18- 14- 16 106.808
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 14- 3 -0.000 1- 4- 2- 5 -121.258
1- 4- 2- 8 118.277 1- 13- 14- 16 -123.082
1- 13- 14- 18 121.816 1- 13- 17- 19 -90.950
2- 4- 1- 7 -172.547 2- 3- 12- 11 -60.092
2- 4- 1- 11 -57.646 2- 3- 14- 13 60.048
2- 4- 1- 13 60.029 2- 3- 14- 16 -175.309
2- 3- 14- 18 -54.387 3- 2- 4- 6 -118.277
3- 2- 4- 10 121.258 3- 14- 13- 15 123.082
3- 14- 13- 17 -121.816 3- 14- 18- 19 90.950
4- 2- 3- 9 172.547 4- 1- 11- 12 60.092
4- 2- 3- 12 57.646 4- 1- 13- 14 -60.048
4- 2- 3- 14 -60.029 4- 1- 13- 15 175.309
4- 1- 13- 17 54.387 5- 2- 4- 6 120.465
5- 2- 3- 9 -65.011 5- 2- 4- 10 -0.000
5- 2- 3- 12 -179.912 5- 2- 3- 14 62.413
6- 4- 1- 7 -52.313 6- 4- 2- 8 -0.000
6- 4- 1- 11 62.588 6- 4- 1- 13 -179.737
7- 1- 4- 10 65.011 7- 1- 11- 12 -179.801
7- 1- 13- 14 172.034 7- 1- 13- 15 47.391
7- 1- 13- 17 -73.531 8- 2- 3- 9 52.313
8- 2- 4- 10 -120.465 8- 2- 3- 12 -62.588
8- 2- 3- 14 179.737 9- 3- 12- 11 179.801
9- 3- 14- 13 -172.034 9- 3- 14- 16 -47.391
9- 3- 14- 18 73.531 10- 4- 1- 11 179.912
10- 4- 1- 13 -62.413 11- 1- 13- 14 59.972
11- 12- 3- 14 62.652 11- 1- 13- 15 -64.672
11- 1- 13- 17 174.407 12- 3- 14- 13 -59.972
12- 11- 1- 13 -62.652 12- 3- 14- 16 64.672
12- 3- 14- 18 -174.407 13- 17- 19- 18 -44.490

13- 14- 18- 19 -26.315 14- 18- 19- 17 44.490
14- 13- 17- 19 26.315 15- 13- 14- 16 -0.000
15- 13- 14- 18 -115.102 15- 13- 17- 19 146.000
16- 14- 13- 17 115.102 16- 14- 18- 19 -146.000
17- 13- 14- 18 -0.000

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5203 1- 7 1.0957 1- 11 1.4388 1- 13 1.5269
5) 2- 3 1.5203 2- 4 1.5423 2- 5 1.0931 2- 8 1.0937
9) 3- 9 1.0957 3- 12 1.4388 3- 14 1.5269 4- 6 1.0937
13) 4- 10 1.0931 11- 12 1.5132 13- 14 1.5507 13- 15 1.0939
17) 13- 17 1.4286 14- 16 1.0939 14- 18 1.4286 17- 19 1.4656
21) 18- 19 1.4656
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.749 1- 4- 10 109.611 1- 11- 12 109.955
4) 1- 13- 14 108.019 1- 13- 15 110.876 1- 13- 17 114.442
7) 2- 3- 9 112.134 2- 3- 12 110.609 2- 3- 14 113.520
10) 2- 4- 6 111.259 2- 4- 10 111.901 3- 2- 4 108.267
13) 3- 2- 5 109.611 3- 2- 8 107.749 3- 14- 16 110.876
16) 3- 14- 18 114.442 4- 1- 7 112.134 4- 1- 11 110.609
19) 4- 1- 13 113.520 4- 2- 3 108.267 4- 2- 5 111.901
22) 4- 2- 8 111.259 5- 2- 3 109.611 5- 2- 4 111.901
25) 5- 2- 8 107.967 6- 4- 10 107.967 7- 1- 4 112.134
28) 7- 1- 11 102.516 7- 1- 13 110.935 8- 2- 3 107.749
31) 8- 2- 4 111.259 8- 2- 5 107.967 9- 3- 12 102.516
34) 9- 3- 14 110.935 10- 4- 6 107.967 11- 1- 4 110.609
37) 11- 1- 7 102.516 11- 1- 13 106.415 12- 3- 9 102.516
40) 12- 3- 14 106.415 13- 1- 4 113.520 13- 1- 7 110.935
43) 13- 1- 11 106.415 13- 14- 16 112.846 13- 14- 18 104.548
46) 13- 17- 19 102.099 14- 3- 9 110.935 14- 3- 12 106.415
49) 14- 13- 15 112.846 14- 13- 17 104.548 14- 18- 19 102.099
52) 15- 13- 14 112.846 15- 13- 17 106.055 16- 14- 18 106.055
55) 17- 13- 14 104.548 17- 13- 15 106.055 18- 14- 16 106.055
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 14- 3 -0.000 1- 4- 2- 5 -120.906
1- 4- 2- 8 118.221 1- 13- 14- 16 -122.933
1- 13- 14- 18 122.272 1- 13- 17- 19 -88.809
2- 4- 1- 7 -173.222 2- 3- 12- 11 -60.475
2- 4- 1- 11 -59.463 2- 3- 14- 13 59.931
2- 4- 1- 13 60.071 2- 3- 14- 16 -175.943
2- 3- 14- 18 -56.044 3- 2- 4- 6 -118.221
3- 2- 4- 10 120.906 3- 14- 13- 15 122.933
3- 14- 13- 17 -122.272 3- 14- 18- 19 88.809
4- 2- 3- 9 173.222 4- 1- 11- 12 60.475
4- 2- 3- 12 59.463 4- 1- 13- 14 -59.931
4- 2- 3- 14 -60.071 4- 1- 13- 15 175.943
4- 1- 13- 17 56.044 5- 2- 4- 6 120.873
5- 2- 3- 9 -64.461 5- 2- 4- 10 -0.000
5- 2- 3- 12 -178.221 5- 2- 3- 14 62.245
6- 4- 1- 7 -52.788 6- 4- 2- 8 -0.000
6- 4- 1- 11 60.972 6- 4- 1- 13 -179.494
7- 1- 4- 10 64.461 7- 1- 11- 12 -179.802
7- 1- 13- 14 172.736 7- 1- 13- 15 48.610

7- 1- 13- 17 -71.289 8- 2- 3- 9 52.788
8- 2- 4- 10 -120.873 8- 2- 3- 12 -60.972
8- 2- 3- 14 179.494 9- 3- 12- 11 179.802
9- 3- 14- 13 -172.736 9- 3- 14- 16 -48.610
9- 3- 14- 18 71.289 10- 4- 1- 11 178.221
10- 4- 1- 13 -62.245 11- 1- 13- 14 61.968
11- 12- 3- 14 63.254 11- 1- 13- 15 -62.158
11- 1- 13- 17 177.943 12- 3- 14- 13 -61.968
12- 11- 1- 13 -63.254 12- 3- 14- 16 62.158
12- 3- 14- 18 -177.943 13- 17- 19- 18 -48.125
13- 14- 18- 19 -29.159 14- 18- 19- 17 48.125
14- 13- 17- 19 29.159 15- 13- 14- 16 -0.000
15- 13- 14- 18 -114.795 15- 13- 17- 19 148.636
16- 14- 13- 17 114.795 16- 14- 18- 19 -148.636
17- 13- 14- 18 -0.000

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5217 1- 7 1.0947 1- 11 1.4318 1- 13 1.5278
5) 2- 3 1.5217 2- 4 1.5442 2- 5 1.0919 2- 8 1.0929
9) 3- 9 1.0947 3- 12 1.4318 3- 14 1.5278 4- 6 1.0929
13) 4- 10 1.0919 11- 12 1.4941 13- 14 1.5528 13- 15 1.0924
17) 13- 17 1.4205 14- 16 1.0924 14- 18 1.4205 17- 19 1.4457
21) 18- 19 1.4457
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.654 1- 4- 10 109.881 1- 11- 12 110.332
4) 1- 13- 14 107.845 1- 13- 15 111.045 1- 13- 17 114.616
7) 2- 3- 9 112.162 2- 3- 12 110.539 2- 3- 14 113.312
10) 2- 4- 6 111.135 2- 4- 10 112.016 3- 2- 4 108.089
13) 3- 2- 5 109.881 3- 2- 8 107.654 3- 14- 16 111.045
16) 3- 14- 18 114.616 4- 1- 7 112.162 4- 1- 11 110.539
19) 4- 1- 13 113.312 4- 2- 3 108.089 4- 2- 5 112.016
22) 4- 2- 8 111.135 5- 2- 3 109.881 5- 2- 4 112.016
25) 5- 2- 8 107.977 6- 4- 10 107.977 7- 1- 4 112.162
28) 7- 1- 11 102.562 7- 1- 13 110.902 8- 2- 3 107.654
31) 8- 2- 4 111.135 8- 2- 5 107.977 9- 3- 12 102.562
34) 9- 3- 14 110.902 10- 4- 6 107.977 11- 1- 4 110.539
37) 11- 1- 7 102.562 11- 1- 13 106.690 12- 3- 9 102.562
40) 12- 3- 14 106.690 13- 1- 4 113.312 13- 1- 7 110.902
43) 13- 1- 11 106.690 13- 14- 16 112.796 13- 14- 18 104.172
46) 13- 17- 19 102.419 14- 3- 9 110.902 14- 3- 12 106.690
49) 14- 13- 15 112.796 14- 13- 17 104.172 14- 18- 19 102.419
52) 15- 13- 14 112.796 15- 13- 17 106.286 16- 14- 18 106.286
55) 17- 13- 14 104.172 17- 13- 15 106.286 18- 14- 16 106.286
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 14- 3 -0.000 1- 4- 2- 5 -121.196
1- 4- 2- 8 117.925 1- 13- 14- 16 -122.991
1- 13- 14- 18 122.183 1- 13- 17- 19 -88.867
2- 4- 1- 7 -172.945 2- 3- 12- 11 -60.499
2- 4- 1- 11 -59.155 2- 3- 14- 13 60.402
2- 4- 1- 13 60.542 2- 3- 14- 16 -175.542
2- 3- 14- 18 -55.091 3- 2- 4- 6 -117.925

3- 2- 4- 10 121.196 3- 14- 13- 15 122.991
3- 14- 13- 17 -122.183 3- 14- 18- 19 88.867
4- 2- 3- 9 172.945 4- 1- 11- 12 60.499
4- 2- 3- 12 59.155 4- 1- 13- 14 -60.402
4- 2- 3- 14 -60.542 4- 1- 13- 15 175.542
4- 1- 13- 17 55.091 5- 2- 4- 6 120.879
5- 2- 3- 9 -64.543 5- 2- 4- 10 -0.000
5- 2- 3- 12 -178.334 5- 2- 3- 14 61.970
6- 4- 1- 7 -52.812 6- 4- 2- 8 -0.000
6- 4- 1- 11 60.978 6- 4- 1- 13 -179.325
7- 1- 4- 10 64.543 7- 1- 11- 12 -179.752
7- 1- 13- 14 172.422 7- 1- 13- 15 48.366
7- 1- 13- 17 -72.084 8- 2- 3- 9 52.812
8- 2- 4- 10 -120.879 8- 2- 3- 12 -60.978
8- 2- 3- 14 179.325 9- 3- 12- 11 179.752
9- 3- 14- 13 -172.422 9- 3- 14- 16 -48.366
9- 3- 14- 18 72.084 10- 4- 1- 11 178.334
10- 4- 1- 13 -61.970 11- 1- 13- 14 61.471
11- 12- 3- 14 63.110 11- 1- 13- 15 -62.584
11- 1- 13- 17 176.965 12- 3- 14- 13 -61.471
12- 11- 1- 13 -63.110 12- 3- 14- 16 62.584
12- 3- 14- 18 -176.965 13- 17- 19- 18 -47.851
13- 14- 18- 19 -28.737 14- 18- 19- 17 47.851
14- 13- 17- 19 28.737 15- 13- 14- 16 -0.000
15- 13- 14- 18 -114.826 15- 13- 17- 19 148.083
16- 14- 13- 17 114.826 16- 14- 18- 19 -148.083
17- 13- 14- 18 -0.000

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5296 1- 7 1.0948 1- 11 1.4352 1- 13 1.5398
5) 2- 3 1.5296 2- 4 1.5509 2- 5 1.0934 2- 8 1.0940
9) 3- 9 1.0948 3- 12 1.4352 3- 14 1.5398 4- 6 1.0940
13) 4- 10 1.0934 11- 12 1.4966 13- 14 1.5600 13- 15 1.0928
17) 13- 17 1.4253 14- 16 1.0928 14- 18 1.4253 17- 19 1.4508
21) 18- 19 1.4508
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.047 1- 4- 10 109.679 1- 11- 12 110.557
4) 1- 13- 14 107.861 1- 13- 15 110.463 1- 13- 17 115.367
7) 2- 3- 9 112.140 2- 3- 12 110.456 2- 3- 14 113.490
10) 2- 4- 6 111.245 2- 4- 10 111.735 3- 2- 4 108.163
13) 3- 2- 5 109.679 3- 2- 8 108.047 3- 14- 16 110.463
16) 3- 14- 18 115.367 4- 1- 7 112.140 4- 1- 11 110.456
19) 4- 1- 13 113.490 4- 2- 3 108.163 4- 2- 5 111.735
22) 4- 2- 8 111.245 5- 2- 3 109.679 5- 2- 4 111.735
25) 5- 2- 8 107.903 6- 4- 10 107.903 7- 1- 4 112.140
28) 7- 1- 11 102.868 7- 1- 13 110.911 8- 2- 3 108.047
31) 8- 2- 4 111.245 8- 2- 5 107.903 9- 3- 12 102.868
34) 9- 3- 14 110.911 10- 4- 6 107.903 11- 1- 4 110.456
37) 11- 1- 7 102.868 11- 1- 13 106.289 12- 3- 9 102.868
40) 12- 3- 14 106.289 13- 1- 4 113.490 13- 1- 7 110.911
43) 13- 1- 11 106.289 13- 14- 16 112.689 13- 14- 18 104.254
46) 13- 17- 19 103.064 14- 3- 9 110.911 14- 3- 12 106.289
49) 14- 13- 15 112.689 14- 13- 17 104.254 14- 18- 19 103.064
52) 15- 13- 14 112.689 15- 13- 17 106.176 16- 14- 18 106.176
55) 17- 13- 14 104.254 17- 13- 15 106.176 18- 14- 16 106.176

Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 14- 3 -0.000 1- 4- 2- 5 -120.819
1- 4- 2- 8 118.513 1- 13- 14- 16 -122.196
1- 13- 14- 18 123.111 1- 13- 17- 19 -90.281
2- 4- 1- 7 -172.986 2- 3- 12- 11 -60.316
2- 4- 1- 11 -58.882 2- 3- 14- 13 60.188
2- 4- 1- 13 60.361 2- 3- 14- 16 -176.253
2- 3- 14- 18 -55.856 3- 2- 4- 6 -118.513
3- 2- 4- 10 120.819 3- 14- 13- 15 122.196
3- 14- 13- 17 -123.111 3- 14- 18- 19 90.281
4- 2- 3- 9 172.986 4- 1- 11- 12 60.316
4- 2- 3- 12 58.882 4- 1- 13- 14 -60.188
4- 2- 3- 14 -60.361 4- 1- 13- 15 176.253
4- 1- 13- 17 55.856 5- 2- 4- 6 120.668
5- 2- 3- 9 -64.925 5- 2- 4- 10 -0.000
5- 2- 3- 12 -179.028 5- 2- 3- 14 61.729
6- 4- 1- 7 -52.456 6- 4- 2- 8 -0.000
6- 4- 1- 11 61.647 6- 4- 1- 13 -179.110
7- 1- 4- 10 64.925 7- 1- 11- 12 -179.829
7- 1- 13- 14 172.514 7- 1- 13- 15 48.956
7- 1- 13- 17 -71.441 8- 2- 3- 9 52.456
8- 2- 4- 10 -120.668 8- 2- 3- 12 -61.647
8- 2- 3- 14 179.110 9- 3- 12- 11 179.829
9- 3- 14- 13 -172.514 9- 3- 14- 16 -48.956
9- 3- 14- 18 71.441 10- 4- 1- 11 179.028
10- 4- 1- 13 -61.729 11- 1- 13- 14 61.412
11- 12- 3- 14 63.202 11- 1- 13- 15 -62.146
11- 1- 13- 17 177.457 12- 3- 14- 13 -61.412
12- 11- 1- 13 -63.202 12- 3- 14- 16 62.146
12- 3- 14- 18 -177.457 13- 17- 19- 18 -46.185
13- 14- 18- 19 -27.796 14- 18- 19- 17 46.185
14- 13- 17- 19 27.796 15- 13- 14- 16 -0.000
15- 13- 14- 18 -114.692 15- 13- 17- 19 147.010
16- 14- 13- 17 114.692 16- 14- 18- 19 -147.010
17- 13- 14- 18 -0.000

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5284 1- 7 1.0941 1- 11 1.4414 1- 13 1.5396
5) 2- 3 1.5284 2- 4 1.5500 2- 5 1.0932 2- 8 1.0937
9) 3- 9 1.0941 3- 12 1.4414 3- 14 1.5396 4- 6 1.0937
13) 4- 10 1.0932 11- 12 1.4976 13- 14 1.5589 13- 15 1.0921
17) 13- 17 1.4308 14- 16 1.0921 14- 18 1.4308 17- 19 1.4515
21) 18- 19 1.4515
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.072 1- 4- 10 109.595 1- 11- 12 110.511
4) 1- 13- 14 107.947 1- 13- 15 110.628 1- 13- 17 115.284
7) 2- 3- 9 112.272 2- 3- 12 110.345 2- 3- 14 113.677
10) 2- 4- 6 111.319 2- 4- 10 111.812 3- 2- 4 108.258
13) 3- 2- 5 109.595 3- 2- 8 108.072 3- 14- 16 110.628
16) 3- 14- 18 115.284 4- 1- 7 112.272 4- 1- 11 110.345
19) 4- 1- 13 113.677 4- 2- 3 108.258 4- 2- 5 111.812
22) 4- 2- 8 111.319 5- 2- 3 109.595 5- 2- 4 111.812
25) 5- 2- 8 107.713 6- 4- 10 107.713 7- 1- 4 112.272

28) 7- 1- 11 102.788 7- 1- 13 110.946 8- 2- 3 108.072
31) 8- 2- 4 111.319 8- 2- 5 107.713 9- 3- 12 102.788
34) 9- 3- 14 110.946 10- 4- 6 107.713 11- 1- 4 110.345
37) 11- 1- 7 102.788 11- 1- 13 106.075 12- 3- 9 102.788
40) 12- 3- 14 106.075 13- 1- 4 113.677 13- 1- 7 110.946
43) 13- 1- 11 106.075 13- 14- 16 112.737 13- 14- 18 104.256
46) 13- 17- 19 103.150 14- 3- 9 110.946 14- 3- 12 106.075
49) 14- 13- 15 112.737 14- 13- 17 104.256 14- 18- 19 103.150
52) 15- 13- 14 112.737 15- 13- 17 105.945 16- 14- 18 105.945
55) 17- 13- 14 104.256 17- 13- 15 105.945 18- 14- 16 105.945
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 14- 3 -0.000 1- 4- 2- 5 -120.825
1- 4- 2- 8 118.646 1- 13- 14- 16 -122.497
1- 13- 14- 18 123.059 1- 13- 17- 19 -90.453
2- 4- 1- 7 -172.961 2- 3- 12- 11 -60.299
2- 4- 1- 11 -58.947 2- 3- 14- 13 59.893
2- 4- 1- 13 60.069 2- 3- 14- 16 -176.325
2- 3- 14- 18 -56.164 3- 2- 4- 6 -118.646
3- 2- 4- 10 120.825 3- 14- 13- 15 122.497
3- 14- 13- 17 -123.059 3- 14- 18- 19 90.453
4- 2- 3- 9 172.961 4- 1- 11- 12 60.299
4- 2- 3- 12 58.947 4- 1- 13- 14 -59.893
4- 2- 3- 14 -60.069 4- 1- 13- 15 176.325
4- 1- 13- 17 56.164 5- 2- 4- 6 120.529
5- 2- 3- 9 -64.847 5- 2- 4- 10 -0.000
5- 2- 3- 12 -178.861 5- 2- 3- 14 62.123
6- 4- 1- 7 -52.274 6- 4- 2- 8 -0.000
6- 4- 1- 11 61.740 6- 4- 1- 13 -179.244
7- 1- 4- 10 64.847 7- 1- 11- 12 -179.790
7- 1- 13- 14 172.448 7- 1- 13- 15 48.666
7- 1- 13- 17 -71.495 8- 2- 3- 9 52.274
8- 2- 4- 10 -120.529 8- 2- 3- 12 -61.740
8- 2- 3- 14 179.244 9- 3- 12- 11 179.790
9- 3- 14- 13 -172.448 9- 3- 14- 16 -48.666
9- 3- 14- 18 71.495 10- 4- 1- 11 178.861
10- 4- 1- 13 -62.123 11- 1- 13- 14 61.535
11- 12- 3- 14 63.245 11- 1- 13- 15 -62.247
11- 1- 13- 17 177.592 12- 3- 14- 13 -61.535
12- 11- 1- 13 -63.245 12- 3- 14- 16 62.247
12- 3- 14- 18 -177.592 13- 17- 19- 18 -45.989
13- 14- 18- 19 -27.686 14- 18- 19- 17 45.989
14- 13- 17- 19 27.686 15- 13- 14- 16 -0.000
15- 13- 14- 18 -114.444 15- 13- 17- 19 146.852
16- 14- 13- 17 114.444 16- 14- 18- 19 -146.852
17- 13- 14- 18 -0.000

Optimised structures for primary ozonide (15c) *exo-endo* at all levels reported.

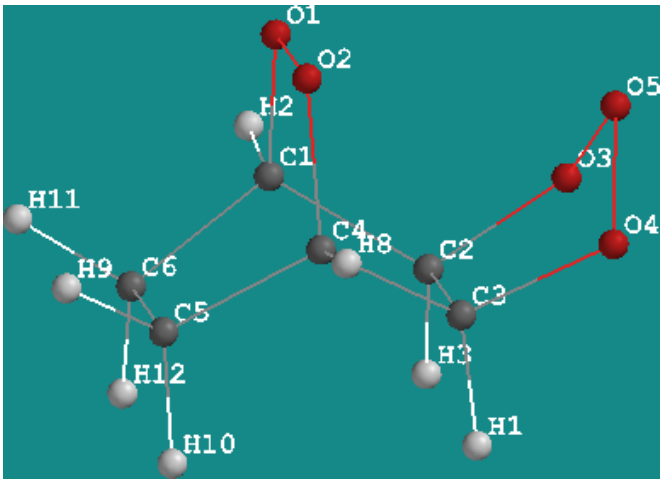

Figure S5: Optimised geometry for *exo-endo* primary ozonide **15c**

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5279 1- 7 1.0807 1- 11 1.4080 1- 13 1.5240
5) 2- 3 1.5279 2- 4 1.5508 2- 5 1.0854 2- 8 1.0820
9) 3- 9 1.0807 3- 12 1.4080 3- 15 1.5240 4- 6 1.0820
13) 4- 10 1.0854 11- 12 1.4141 13- 14 1.0812 13- 15 1.5424
17) 13- 17 1.4015 15- 16 1.0812 15- 18 1.4015 17- 19 1.3842
21) 18- 19 1.3842
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.592 1- 4- 10 110.429 1- 11- 12 112.285
4) 1- 13- 14 110.920 1- 13- 15 107.956 1- 13- 17 114.639
7) 2- 3- 9 112.777 2- 3- 12 109.197 2- 3- 15 109.491
10) 2- 4- 6 110.869 2- 4- 10 111.769 3- 2- 4 107.744
13) 3- 2- 5 110.429 3- 2- 8 108.592 3- 15- 16 110.920
16) 3- 15- 18 114.639 4- 1- 7 112.777 4- 1- 11 109.197
19) 4- 1- 13 109.491 4- 2- 3 107.744 4- 2- 5 111.769
22) 4- 2- 8 110.869 5- 2- 3 110.429 5- 2- 4 111.769
25) 5- 2- 8 107.410 6- 4- 10 107.410 7- 1- 4 112.777
28) 7- 1- 11 103.964 7- 1- 13 111.164 8- 2- 3 108.592
31) 8- 2- 4 110.869 8- 2- 5 107.410 9- 3- 12 103.964
34) 9- 3- 15 111.164 10- 4- 6 107.410 11- 1- 4 109.197
37) 11- 1- 7 103.964 11- 1- 13 110.107 12- 3- 9 103.964
40) 12- 3- 15 110.107 13- 1- 4 109.491 13- 1- 7 111.164
43) 13- 1- 11 110.107 13- 15- 16 113.585 13- 15- 18 103.039
46) 13- 17- 19 104.606 14- 13- 15 113.585 14- 13- 17 106.598
49) 15- 3- 9 111.164 15- 3- 12 110.107 15- 13- 14 113.585
52) 15- 13- 17 103.039 15- 18- 19 104.606 16- 15- 18 106.598
55) 17- 13- 14 106.598 17- 13- 15 103.039 18- 15- 16 106.598
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.494
1- 4- 2- 8 118.701 1- 13- 15- 16 123.438
1- 13- 15- 18 -121.661 1- 13- 17- 19 90.360
2- 4- 1- 7 -172.836 2- 3- 12- 11 -60.564
2- 4- 1- 11 -57.791 2- 3- 15- 13 62.965
2- 4- 1- 13 62.831 2- 3- 15- 16 -62.076
2- 3- 15- 18 177.141 3- 2- 4- 6 -118.701
3- 2- 4- 10 121.494 3- 15- 13- 14 -123.438
```

3- 15- 13- 17 121.661 3- 15- 18- 19 -90.360
4- 2- 3- 9 172.836 4- 1- 11- 12 60.564
4- 2- 3- 12 57.791 4- 1- 13- 14 62.076
4- 1- 13- 15 -62.965 4- 2- 3- 15 -62.831
4- 1- 13- 17 -177.141 5- 2- 4- 6 119.805
5- 2- 3- 9 -64.839 5- 2- 4- 10 -0.000
5- 2- 3- 12 -179.885 5- 2- 3- 15 59.493
6- 4- 1- 7 -52.687 6- 4- 2- 8 -0.000
6- 4- 1- 11 62.359 6- 4- 1- 13 -177.019
7- 1- 4- 10 64.839 7- 1- 11- 12 -178.838
7- 1- 13- 14 -63.193 7- 1- 13- 15 171.766
7- 1- 13- 17 57.589 8- 2- 3- 9 52.687
8- 2- 4- 10 -119.805 8- 2- 3- 12 -62.359
8- 2- 3- 15 177.019 9- 3- 12- 11 178.838
9- 3- 15- 13 -171.766 9- 3- 15- 16 63.193
9- 3- 15- 18 -57.589 10- 4- 1- 11 179.885
10- 4- 1- 13 -59.493 11- 1- 13- 14 -177.857
11- 1- 13- 15 57.102 11- 12- 3- 15 59.680
11- 1- 13- 17 -57.074 12- 3- 15- 13 -57.102
12- 11- 1- 13 -59.680 12- 3- 15- 16 177.857
12- 3- 15- 18 57.074 13- 17- 19- 18 44.955
13- 15- 18- 19 26.663 14- 13- 15- 16 -0.000
14- 13- 15- 18 114.901 14- 13- 17- 19 -146.503
15- 18- 19- 17 -44.955 15- 13- 17- 19 -26.663
16- 15- 13- 17 -114.901 16- 15- 18- 19 146.503
17- 13- 15- 18 -0.000

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5260 1- 7 1.0803 1- 11 1.4166 1- 13 1.5224
5) 2- 3 1.5260 2- 4 1.5493 2- 5 1.0842 2- 8 1.0818
9) 3- 9 1.0803 3- 12 1.4166 3- 15 1.5224 4- 6 1.0818
13) 4- 10 1.0842 11- 12 1.4152 13- 14 1.0801 13- 15 1.5411
17) 13- 17 1.4103 15- 16 1.0801 15- 18 1.4103 17- 19 1.3846
21) 18- 19 1.3846
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.585 1- 4- 10 110.140 1- 11- 12 112.181
4) 1- 13- 14 111.016 1- 13- 15 108.055 1- 13- 17 114.613
7) 2- 3- 9 112.910 2- 3- 12 109.282 2- 3- 15 109.503
10) 2- 4- 6 111.023 2- 4- 10 111.831 3- 2- 4 107.848
13) 3- 2- 5 110.140 3- 2- 8 108.585 3- 15- 16 111.016
16) 3- 15- 18 114.613 4- 1- 7 112.910 4- 1- 11 109.282
19) 4- 1- 13 109.503 4- 2- 3 107.848 4- 2- 5 111.831
22) 4- 2- 8 111.023 5- 2- 3 110.140 5- 2- 4 111.831
25) 5- 2- 8 107.379 6- 4- 10 107.379 7- 1- 4 112.910
28) 7- 1- 11 103.819 7- 1- 13 111.253 8- 2- 3 108.585
31) 8- 2- 4 111.023 8- 2- 5 107.379 9- 3- 12 103.819
34) 9- 3- 15 111.253 10- 4- 6 107.379 11- 1- 4 109.282
37) 11- 1- 7 103.819 11- 1- 13 109.919 12- 3- 9 103.819
40) 12- 3- 15 109.919 13- 1- 4 109.503 13- 1- 7 111.253
43) 13- 1- 11 109.919 13- 15- 16 113.664 13- 15- 18 103.041
46) 13- 17- 19 104.662 14- 13- 15 113.664 14- 13- 17 106.340
49) 15- 3- 9 111.253 15- 3- 12 109.919 15- 13- 14 113.664
52) 15- 13- 17 103.041 15- 18- 19 104.662 16- 15- 18 106.340
55) 17- 13- 14 106.340 17- 13- 15 103.041 18- 15- 16 106.340
Dihedrals
I J K L Theta I J K L Theta

1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.242
1- 4- 2- 8 118.846 1- 13- 15- 16 123.688
1- 13- 15- 18 -121.679 1- 13- 17- 19 90.632
2- 4- 1- 7 -172.799 2- 3- 12- 11 -60.443
2- 4- 1- 11 -57.803 2- 3- 15- 13 62.778
2- 4- 1- 13 62.648 2- 3- 15- 16 -62.496
2- 3- 15- 18 177.007 3- 2- 4- 6 -118.846
3- 2- 4- 10 121.242 3- 15- 13- 14 -123.688
3- 15- 13- 17 121.679 3- 15- 18- 19 -90.632
4- 2- 3- 9 172.799 4- 1- 11- 12 60.443
4- 2- 3- 12 57.803 4- 1- 13- 14 62.496
4- 1- 13- 15 -62.778 4- 2- 3- 15 -62.648
4- 1- 13- 17 -177.007 5- 2- 4- 6 119.912
5- 2- 3- 9 -64.911 5- 2- 4- 10 -0.000
5- 2- 3- 12 -179.907 5- 2- 3- 15 59.642
6- 4- 1- 7 -52.409 6- 4- 2- 8 -0.000
6- 4- 1- 11 62.588 6- 4- 1- 13 -176.962
7- 1- 4- 10 64.911 7- 1- 11- 12 -178.843
7- 1- 13- 14 -63.016 7- 1- 13- 15 171.711
7- 1- 13- 17 57.481 8- 2- 3- 9 52.409
8- 2- 4- 10 -119.912 8- 2- 3- 12 -62.588
8- 2- 3- 15 176.962 9- 3- 12- 11 178.843
9- 3- 15- 13 -171.711 9- 3- 15- 16 63.016
9- 3- 15- 18 -57.481 10- 4- 1- 11 179.907
10- 4- 1- 13 -59.642 11- 1- 13- 14 -177.442
11- 1- 13- 15 57.284 11- 12- 3- 15 59.753
11- 1- 13- 17 -56.945 12- 3- 15- 13 -57.284
12- 11- 1- 13 -59.753 12- 3- 15- 16 177.442
12- 3- 15- 18 56.945 13- 17- 19- 18 44.718
13- 15- 18- 19 26.500 14- 13- 15- 16 -0.000
14- 13- 15- 18 114.632 14- 13- 17- 19 -146.318
15- 18- 19- 17 -44.718 15- 13- 17- 19 -26.500
16- 15- 13- 17 -114.632 16- 15- 18- 19 146.318
17- 13- 15- 18 -0.000

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5267 1- 7 1.0957 1- 11 1.4297 1- 13 1.5242
5) 2- 3 1.5267 2- 4 1.5480 2- 5 1.0963 2- 8 1.0928
9) 3- 9 1.0957 3- 12 1.4297 3- 15 1.5242 4- 6 1.0928
13) 4- 10 1.0963 11- 12 1.5077 13- 14 1.0962 13- 15 1.5521
17) 13- 17 1.4240 15- 16 1.0962 15- 18 1.4240 17- 19 1.4647
21) 18- 19 1.4647
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.129 1- 4- 10 110.286 1- 11- 12 110.132
4) 1- 13- 14 111.222 1- 13- 15 107.954 1- 13- 17 114.429
7) 2- 3- 9 112.832 2- 3- 12 109.991 2- 3- 15 110.051
10) 2- 4- 6 111.038 2- 4- 10 111.900 3- 2- 4 108.007
13) 3- 2- 5 110.286 3- 2- 8 108.129 3- 15- 16 111.222
16) 3- 15- 18 114.429 4- 1- 7 112.832 4- 1- 11 109.991
19) 4- 1- 13 110.051 4- 2- 3 108.007 4- 2- 5 111.900
22) 4- 2- 8 111.038 5- 2- 3 110.286 5- 2- 4 111.900
25) 5- 2- 8 107.428 6- 4- 10 107.428 7- 1- 4 112.832
28) 7- 1- 11 102.334 7- 1- 13 110.771 8- 2- 3 108.129
31) 8- 2- 4 111.038 8- 2- 5 107.428 9- 3- 12 102.334
34) 9- 3- 15 110.771 10- 4- 6 107.428 11- 1- 4 109.991
37) 11- 1- 7 102.334 11- 1- 13 110.644 12- 3- 9 102.334

40) 12- 3- 15 110.644 13- 1- 4 110.051 13- 1- 7 110.771
43) 13- 1- 11 110.644 13- 15- 16 113.111 13- 15- 18 104.419
46) 13- 17- 19 101.990 14- 13- 15 113.111 14- 13- 17 105.629
49) 15- 3- 9 110.771 15- 3- 12 110.644 15- 13- 14 113.111
52) 15- 13- 17 104.419 15- 18- 19 101.990 16- 15- 18 105.629
55) 17- 13- 14 105.629 17- 13- 15 104.419 18- 15- 16 105.629
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.572
1- 4- 2- 8 118.396 1- 13- 15- 16 123.505
1- 13- 15- 18 -122.153 1- 13- 17- 19 88.190
2- 4- 1- 7 -173.342 2- 3- 12- 11 -61.072
2- 4- 1- 11 -59.777 2- 3- 15- 13 62.342
2- 4- 1- 13 62.375 2- 3- 15- 16 -62.301
2- 3- 15- 18 178.107 3- 2- 4- 6 -118.396
3- 2- 4- 10 121.572 3- 15- 13- 14 -123.505
3- 15- 13- 17 122.153 3- 15- 18- 19 -88.190
4- 2- 3- 9 173.342 4- 1- 11- 12 61.072
4- 2- 3- 12 59.777 4- 1- 13- 14 62.301
4- 1- 13- 15 -62.342 4- 2- 3- 15 -62.375
4- 1- 13- 17 -178.107 5- 2- 4- 6 120.031
5- 2- 3- 9 -64.092 5- 2- 4- 10 -0.000
5- 2- 3- 12 -177.657 5- 2- 3- 15 60.192
6- 4- 1- 7 -53.102 6- 4- 2- 8 -0.000
6- 4- 1- 11 60.463 6- 4- 1- 13 -177.385
7- 1- 4- 10 64.092 7- 1- 11- 12 -178.782
7- 1- 13- 14 -63.165 7- 1- 13- 15 172.192
7- 1- 13- 17 56.427 8- 2- 3- 9 53.102
8- 2- 4- 10 -120.031 8- 2- 3- 12 -60.463
8- 2- 3- 15 177.385 9- 3- 12- 11 178.782
9- 3- 15- 13 -172.192 9- 3- 15- 16 63.165
9- 3- 15- 18 -56.427 10- 4- 1- 11 177.657
10- 4- 1- 13 -60.192 11- 1- 13- 14 -175.935
11- 1- 13- 15 59.422 11- 12- 3- 15 60.727
11- 1- 13- 17 -56.343 12- 3- 15- 13 -59.422
12- 11- 1- 13 -60.727 12- 3- 15- 16 175.935
12- 3- 15- 18 56.343 13- 17- 19- 18 48.827
13- 15- 18- 19 29.608 14- 13- 15- 16 -0.000
14- 13- 15- 18 114.342 14- 13- 17- 19 -149.131
15- 18- 19- 17 -48.827 15- 13- 17- 19 -29.608
16- 15- 13- 17 -114.342 16- 15- 18- 19 149.131
17- 13- 15- 18 -0.000

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5277 1- 7 1.0948 1- 11 1.4229 1- 13 1.5248
5) 2- 3 1.5277 2- 4 1.5502 2- 5 1.0953 2- 8 1.0921
9) 3- 9 1.0948 3- 12 1.4229 3- 15 1.5248 4- 6 1.0921
13) 4- 10 1.0953 11- 12 1.4882 13- 14 1.0947 13- 15 1.5541
17) 13- 17 1.4164 15- 16 1.0947 15- 18 1.4164 17- 19 1.4445
21) 18- 19 1.4445
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.183 1- 4- 10 110.401 1- 11- 12 110.525
4) 1- 13- 14 111.298 1- 13- 15 107.793 1- 13- 17 114.777
7) 2- 3- 9 112.952 2- 3- 12 110.056 2- 3- 15 109.563

10) 2- 4- 6 110.920 2- 4- 10 111.963 3- 2- 4 107.833
13) 3- 2- 5 110.401 3- 2- 8 108.183 3- 15- 16 111.298
16) 3- 15- 18 114.777 4- 1- 7 112.952 4- 1- 11 110.056
19) 4- 1- 13 109.563 4- 2- 3 107.833 4- 2- 5 111.963
22) 4- 2- 8 110.920 5- 2- 3 110.401 5- 2- 4 111.963
25) 5- 2- 8 107.490 6- 4- 10 107.490 7- 1- 4 112.952
28) 7- 1- 11 102.411 7- 1- 13 110.715 8- 2- 3 108.183
31) 8- 2- 4 110.920 8- 2- 5 107.490 9- 3- 12 102.411
34) 9- 3- 15 110.715 10- 4- 6 107.490 11- 1- 4 110.056
37) 11- 1- 7 102.411 11- 1- 13 110.988 12- 3- 9 102.411
40) 12- 3- 15 110.988 13- 1- 4 109.563 13- 1- 7 110.715
43) 13- 1- 11 110.988 13- 15- 16 113.145 13- 15- 18 104.034
46) 13- 17- 19 102.415 14- 13- 15 113.145 14- 13- 17 105.706
49) 15- 3- 9 110.715 15- 3- 12 110.988 15- 13- 14 113.145
52) 15- 13- 17 104.034 15- 18- 19 102.415 16- 15- 18 105.706
55) 17- 13- 14 105.706 17- 13- 15 104.034 18- 15- 16 105.706
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.640
1- 4- 2- 8 118.288 1- 13- 15- 16 123.507
1- 13- 15- 18 -122.270 1- 13- 17- 19 88.431
2- 4- 1- 7 -173.137 2- 3- 12- 11 -61.001
2- 4- 1- 11 -59.367 2- 3- 15- 13 62.910
2- 4- 1- 13 62.935 2- 3- 15- 16 -61.713
2- 3- 15- 18 178.291 3- 2- 4- 6 -118.288
3- 2- 4- 10 121.640 3- 15- 13- 14 -123.507
3- 15- 13- 17 122.270 3- 15- 18- 19 -88.431
4- 2- 3- 9 173.137 4- 1- 11- 12 61.001
4- 2- 3- 12 59.367 4- 1- 13- 14 61.713
4- 1- 13- 15 -62.910 4- 2- 3- 15 -62.935
4- 1- 13- 17 -178.291 5- 2- 4- 6 120.072
5- 2- 3- 9 -64.259 5- 2- 4- 10 -0.000
5- 2- 3- 12 -178.029 5- 2- 3- 15 59.668
6- 4- 1- 7 -53.106 6- 4- 2- 8 -0.000
6- 4- 1- 11 60.664 6- 4- 1- 13 -177.034
7- 1- 4- 10 64.259 7- 1- 11- 12 -178.641
7- 1- 13- 14 -63.515 7- 1- 13- 15 171.862
7- 1- 13- 17 56.481 8- 2- 3- 9 53.106
8- 2- 4- 10 -120.072 8- 2- 3- 12 -60.664
8- 2- 3- 15 177.034 9- 3- 12- 11 178.641
9- 3- 15- 13 -171.862 9- 3- 15- 16 63.515
9- 3- 15- 18 -56.481 10- 4- 1- 11 178.029
10- 4- 1- 13 -59.668 11- 1- 13- 14 -176.542
11- 1- 13- 15 58.834 11- 12- 3- 15 60.455
11- 1- 13- 17 -56.546 12- 3- 15- 13 -58.834
12- 11- 1- 13 -60.455 12- 3- 15- 16 176.542
12- 3- 15- 18 56.546 13- 17- 19- 18 48.393
13- 15- 18- 19 29.104 14- 13- 15- 16 -0.000
14- 13- 15- 18 114.223 14- 13- 17- 19 -148.521
15- 18- 19- 17 -48.393 15- 13- 17- 19 -29.104
16- 15- 13- 17 -114.223 16- 15- 18- 19 148.521
17- 13- 15- 18 -0.000

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5367 1- 7 1.0947 1- 11 1.4262 1- 13 1.5364
5) 2- 3 1.5367 2- 4 1.5569 2- 5 1.0966 2- 8 1.0933
9) 3- 9 1.0947 3- 12 1.4262 3- 15 1.5364 4- 6 1.0933

13) 4- 10 1.0966 11- 12 1.4913 13- 14 1.0949 13- 15 1.5620
17) 13- 17 1.4204 15- 16 1.0949 15- 18 1.4204 17- 19 1.4495
21) 18- 19 1.4495
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.403 1- 4- 10 110.393 1- 11- 12 110.728
4) 1- 13- 14 110.828 1- 13- 15 107.791 1- 13- 17 115.246
7) 2- 3- 9 112.677 2- 3- 12 109.860 2- 3- 15 109.692
10) 2- 4- 6 111.001 2- 4- 10 111.764 3- 2- 4 107.887
13) 3- 2- 5 110.393 3- 2- 8 108.403 3- 15- 16 110.828
16) 3- 15- 18 115.246 4- 1- 7 112.677 4- 1- 11 109.860
19) 4- 1- 13 109.692 4- 2- 3 107.887 4- 2- 5 111.764
22) 4- 2- 8 111.001 5- 2- 3 110.393 5- 2- 4 111.764
25) 5- 2- 8 107.357 6- 4- 10 107.357 7- 1- 4 112.677
28) 7- 1- 11 102.853 7- 1- 13 110.791 8- 2- 3 108.403
31) 8- 2- 4 111.001 8- 2- 5 107.357 9- 3- 12 102.853
34) 9- 3- 15 110.791 10- 4- 6 107.357 11- 1- 4 109.860
37) 11- 1- 7 102.853 11- 1- 13 110.811 12- 3- 9 102.853
40) 12- 3- 15 110.811 13- 1- 4 109.692 13- 1- 7 110.791
43) 13- 1- 11 110.811 13- 15- 16 113.007 13- 15- 18 104.095
46) 13- 17- 19 102.977 14- 13- 15 113.007 14- 13- 17 105.826
49) 15- 3- 9 110.791 15- 3- 12 110.811 15- 13- 14 113.007
52) 15- 13- 17 104.095 15- 18- 19 102.977 16- 15- 18 105.826
55) 17- 13- 14 105.826 17- 13- 15 104.095 18- 15- 16 105.826
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.542
1- 4- 2- 8 118.635 1- 13- 15- 16 122.816
1- 13- 15- 18 -122.847 1- 13- 17- 19 89.522
2- 4- 1- 7 -173.235 2- 3- 12- 11 -60.931
2- 4- 1- 11 -59.202 2- 3- 15- 13 62.777
2- 4- 1- 13 62.837 2- 3- 15- 16 -61.365
2- 3- 15- 18 178.504 3- 2- 4- 6 -118.635
3- 2- 4- 10 121.542 3- 15- 13- 14 -122.816
3- 15- 13- 17 122.847 3- 15- 18- 19 -89.522
4- 2- 3- 9 173.235 4- 1- 11- 12 60.931
4- 2- 3- 12 59.202 4- 1- 13- 14 61.365
4- 1- 13- 15 -62.777 4- 2- 3- 15 -62.837
4- 1- 13- 17 -178.504 5- 2- 4- 6 119.823
5- 2- 3- 9 -64.377 5- 2- 4- 10 -0.000
5- 2- 3- 12 -178.410 5- 2- 3- 15 59.551
6- 4- 1- 7 -52.953 6- 4- 2- 8 -0.000
6- 4- 1- 11 61.080 6- 4- 1- 13 -176.881
7- 1- 4- 10 64.377 7- 1- 11- 12 -178.879
7- 1- 13- 14 -63.658 7- 1- 13- 15 172.201
7- 1- 13- 17 56.474 8- 2- 3- 9 52.953
8- 2- 4- 10 -119.823 8- 2- 3- 12 -61.080
8- 2- 3- 15 176.881 9- 3- 12- 11 178.879
9- 3- 15- 13 -172.201 9- 3- 15- 16 63.658
9- 3- 15- 18 -56.474 10- 4- 1- 11 178.410
10- 4- 1- 13 -59.551 11- 1- 13- 14 -177.166
11- 1- 13- 15 58.693 11- 12- 3- 15 60.440
11- 1- 13- 17 -57.034 12- 3- 15- 13 -58.693
12- 11- 1- 13 -60.440 12- 3- 15- 16 177.166
12- 3- 15- 18 57.034 13- 17- 19- 18 46.979
13- 15- 18- 19 28.298 14- 13- 15- 16 -0.000
14- 13- 15- 18 114.337 14- 13- 17- 19 -147.641
15- 18- 19- 17 -46.979 15- 13- 17- 19 -28.298
16- 15- 13- 17 -114.337 16- 15- 18- 19 147.641
17- 13- 15- 18 -0.000

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5339 1- 7 1.0942 1- 11 1.4367 1- 13 1.5338
5) 2- 3 1.5339 2- 4 1.5550 2- 5 1.0951 2- 8 1.0930
9) 3- 9 1.0942 3- 12 1.4367 3- 15 1.5338 4- 6 1.0930
13) 4- 10 1.0951 11- 12 1.4930 13- 14 1.0933 13- 15 1.5598
17) 13- 17 1.4305 15- 16 1.0933 15- 18 1.4305 17- 19 1.4504
21) 18- 19 1.4504
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.466 1- 4- 10 109.994 1- 11- 12 110.589
4) 1- 13- 14 110.945 1- 13- 15 107.916 1- 13- 17 115.213
7) 2- 3- 9 112.793 2- 3- 12 110.004 2- 3- 15 109.724
10) 2- 4- 6 111.230 2- 4- 10 111.805 3- 2- 4 108.010
13) 3- 2- 5 109.994 3- 2- 8 108.466 3- 15- 16 110.945
16) 3- 15- 18 115.213 4- 1- 7 112.793 4- 1- 11 110.004
19) 4- 1- 13 109.724 4- 2- 3 108.010 4- 2- 5 111.805
22) 4- 2- 8 111.230 5- 2- 3 109.994 5- 2- 4 111.805
25) 5- 2- 8 107.294 6- 4- 10 107.294 7- 1- 4 112.793
28) 7- 1- 11 102.689 7- 1- 13 110.919 8- 2- 3 108.466
31) 8- 2- 4 111.230 8- 2- 5 107.294 9- 3- 12 102.689
34) 9- 3- 15 110.919 10- 4- 6 107.294 11- 1- 4 110.004
37) 11- 1- 7 102.689 11- 1- 13 110.539 12- 3- 9 102.689
40) 12- 3- 15 110.539 13- 1- 4 109.724 13- 1- 7 110.919
43) 13- 1- 11 110.539 13- 15- 16 113.072 13- 15- 18 104.114
46) 13- 17- 19 103.070 14- 13- 15 113.072 14- 13- 17 105.524
49) 15- 3- 9 110.919 15- 3- 12 110.539 15- 13- 14 113.072
52) 15- 13- 17 104.114 15- 18- 19 103.070 16- 15- 18 105.524
55) 17- 13- 14 105.524 17- 13- 15 104.114 18- 15- 16 105.524
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.151
1- 4- 2- 8 118.921 1- 13- 15- 16 123.097
1- 13- 15- 18 -122.882 1- 13- 17- 19 89.875
2- 4- 1- 7 -173.199 2- 3- 12- 11 -60.776
2- 4- 1- 11 -59.212 2- 3- 15- 13 62.542
2- 4- 1- 13 62.601 2- 3- 15- 16 -61.842
2- 3- 15- 18 178.359 3- 2- 4- 6 -118.921
3- 2- 4- 10 121.151 3- 15- 13- 14 -123.097
3- 15- 13- 17 122.882 3- 15- 18- 19 -89.875
4- 2- 3- 9 173.199 4- 1- 11- 12 60.776
4- 2- 3- 12 59.212 4- 1- 13- 14 61.842
4- 1- 13- 15 -62.542 4- 2- 3- 15 -62.601
4- 1- 13- 17 -178.359 5- 2- 4- 6 119.928
5- 2- 3- 9 -64.530 5- 2- 4- 10 -0.000
5- 2- 3- 12 -178.517 5- 2- 3- 15 59.669
6- 4- 1- 7 -52.535 6- 4- 2- 8 -0.000
6- 4- 1- 11 61.452 6- 4- 1- 13 -176.735
7- 1- 4- 10 64.530 7- 1- 11- 12 -178.922
7- 1- 13- 14 -63.442 7- 1- 13- 15 172.174
7- 1- 13- 17 56.358 8- 2- 3- 9 52.535
8- 2- 4- 10 -119.928 8- 2- 3- 12 -61.452
8- 2- 3- 15 176.735 9- 3- 12- 11 178.922
9- 3- 15- 13 -172.174 9- 3- 15- 16 63.442
9- 3- 15- 18 -56.358 10- 4- 1- 11 178.517
10- 4- 1- 13 -59.669 11- 1- 13- 14 -176.665

```
11- 1- 13- 15 58.950 11- 12- 3- 15 60.551
11- 1- 13- 17 -56.866 12- 3- 15- 13 -58.950
12- 11- 1- 13 -60.551 12- 3- 15- 16 176.665
12- 3- 15- 18 56.866 13- 17- 19- 18 46.656
13- 15- 18- 19 28.093 14- 13- 15- 16 -0.000
14- 13- 15- 18 114.020 14- 13- 17- 19 -147.383
15- 18- 19- 17 -46.656 15- 13- 17- 19 -28.093
16- 15- 13- 17 -114.020 16- 15- 18- 19 147.383
17- 13- 15- 18 -0.000
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Optimised structures for primary ozonide (15d) *exo-exo* at all levels reported.

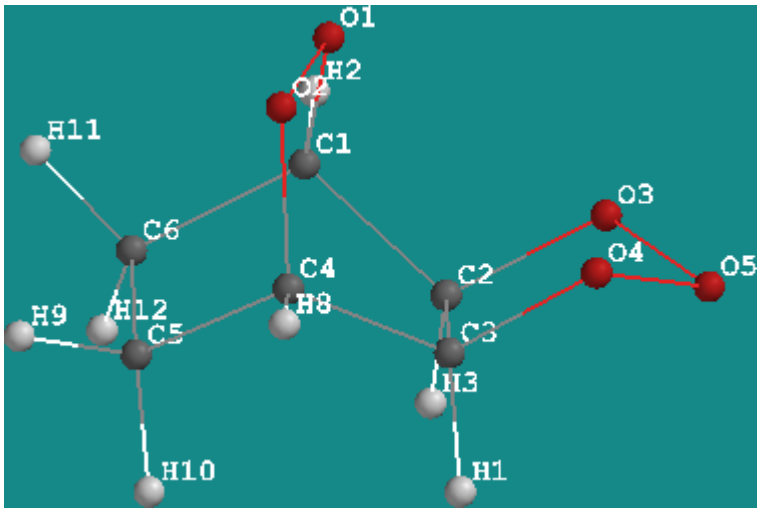

Figure S6: Optimised geometry for *exo-exo* primary ozonide **15d**

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5285 1- 7 1.0807 1- 11 1.4061 1- 13 1.5217
5) 2- 3 1.5288 2- 4 1.5506 2- 5 1.0852 2- 8 1.0819
9) 3- 9 1.0807 3- 12 1.4060 3- 15 1.5216 4- 6 1.0820
13) 4- 10 1.0851 11- 12 1.4135 13- 14 1.0835 13- 15 1.5423
17) 13- 17 1.4013 15- 16 1.0835 15- 18 1.4009 17- 19 1.3834
21) 18- 19 1.3828
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.425 1- 4- 10 110.401 1- 11- 12 112.416
4) 1- 13- 14 111.435 1- 13- 15 108.004 1- 13- 17 111.182
7) 2- 3- 9 112.659 2- 3- 12 109.193 2- 3- 15 109.149
10) 2- 4- 6 110.837 2- 4- 10 111.769 3- 2- 4 107.751
13) 3- 2- 5 110.413 3- 2- 8 108.585 3- 15- 16 111.280
16) 3- 15- 18 111.351 4- 1- 7 112.625 4- 1- 11 109.375
19) 4- 1- 13 109.333 4- 2- 3 107.751 4- 2- 5 111.764
22) 4- 2- 8 110.849 5- 2- 3 110.413 5- 2- 4 111.764
25) 5- 2- 8 107.449 6- 4- 10 107.475 7- 1- 4 112.625
```

28) 7- 1- 11 104.005 7- 1- 13 111.633 8- 2- 3 108.585
31) 8- 2- 4 110.849 8- 2- 5 107.449 9- 3- 12 104.021
34) 9- 3- 15 111.629 10- 4- 6 107.475 11- 1- 4 109.375
37) 11- 1- 7 104.005 11- 1- 13 109.724 12- 3- 9 104.021
40) 12- 3- 15 110.066 13- 1- 4 109.333 13- 1- 7 111.633
43) 13- 1- 11 109.724 13- 15- 16 112.469 13- 15- 18 102.886
46) 13- 17- 19 103.707 14- 13- 15 112.522 14- 13- 17 110.438
49) 15- 3- 9 111.629 15- 3- 12 110.066 15- 13- 14 112.522
52) 15- 13- 17 102.951 15- 18- 19 103.514 16- 15- 18 110.415
55) 17- 13- 14 110.438 17- 13- 15 102.951 18- 15- 16 110.415
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 1.385 1- 11- 12- 3 2.006
1- 13- 15- 3 1.049 1- 4- 2- 5 -120.091
1- 4- 2- 8 120.071 1- 13- 15- 16 124.337
1- 13- 15- 18 -116.857 1- 13- 17- 19 142.713
2- 4- 1- 7 -173.388 2- 3- 12- 11 -61.539
2- 4- 1- 11 -58.270 2- 3- 15- 13 62.355
2- 4- 1- 13 61.897 2- 3- 15- 16 -61.650
2- 3- 15- 18 174.695 3- 2- 4- 6 -117.189
3- 2- 4- 10 122.946 3- 15- 13- 14 -122.369
3- 15- 13- 17 118.733 3- 15- 18- 19 -144.264
4- 2- 3- 9 171.766 4- 1- 11- 12 59.054
4- 2- 3- 12 56.722 4- 1- 13- 14 60.579
4- 1- 13- 15 -63.496 4- 2- 3- 15 -63.639
4- 1- 13- 17 -175.747 5- 2- 4- 6 121.336
5- 2- 3- 9 -65.921 5- 2- 4- 10 1.470
5- 2- 3- 12 179.035 5- 2- 3- 15 58.674
6- 4- 1- 7 -53.284 6- 4- 2- 8 1.497
6- 4- 1- 11 61.834 6- 4- 1- 13 -177.999
7- 1- 4- 10 64.207 7- 1- 11- 12 179.585
7- 1- 13- 14 -64.712 7- 1- 13- 15 171.213
7- 1- 13- 17 58.961 8- 2- 3- 9 51.639
8- 2- 4- 10 -118.368 8- 2- 3- 12 -63.404
8- 2- 3- 15 176.234 9- 3- 12- 11 177.972
9- 3- 15- 13 -172.449 9- 3- 15- 16 63.546
9- 3- 15- 18 -60.109 10- 4- 1- 11 179.325
10- 4- 1- 13 -60.509 11- 1- 13- 14 -179.468
11- 1- 13- 15 56.457 11- 12- 3- 15 58.258
11- 1- 13- 17 -55.795 12- 3- 15- 13 -57.469
12- 11- 1- 13 -60.873 12- 3- 15- 16 178.526
12- 3- 15- 18 54.871 13- 17- 19- 18 -47.146
13- 15- 18- 19 -28.639 14- 13- 15- 16 0.919
14- 13- 15- 18 119.725 14- 13- 17- 19 -93.048
15- 18- 19- 17 47.704 15- 13- 17- 19 27.292
16- 15- 13- 17 -117.979 16- 15- 18- 19 91.592
17- 13- 15- 18 0.827

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5268 1- 7 1.0803 1- 11 1.4147 1- 13 1.5204
5) 2- 3 1.5267 2- 4 1.5491 2- 5 1.0840 2- 8 1.0816
9) 3- 9 1.0803 3- 12 1.4147 3- 15 1.5204 4- 6 1.0816
13) 4- 10 1.0840 11- 12 1.4145 13- 14 1.0817 13- 15 1.5410
17) 13- 17 1.4107 15- 16 1.0817 15- 18 1.4108 17- 19 1.3834
21) 18- 19 1.3835
Bond Angles
I J K Theta I J K Theta I J K Theta

1) 1- 4- 6 108.477 1- 4- 10 110.117 1- 11- 12 112.336
4) 1- 13- 14 111.461 1- 13- 15 108.195 1- 13- 17 111.239
7) 2- 3- 9 112.773 2- 3- 12 109.393 2- 3- 15 109.301
10) 2- 4- 6 110.995 2- 4- 10 111.840 3- 2- 4 107.957
13) 3- 2- 5 110.113 3- 2- 8 108.448 3- 15- 16 111.490
16) 3- 15- 18 111.208 4- 1- 7 112.780 4- 1- 11 109.355
19) 4- 1- 13 109.267 4- 2- 3 107.957 4- 2- 5 111.840
22) 4- 2- 8 110.995 5- 2- 3 110.113 5- 2- 4 111.840
25) 5- 2- 8 107.445 6- 4- 10 107.441 7- 1- 4 112.780
28) 7- 1- 11 103.884 7- 1- 13 111.705 8- 2- 3 108.448
31) 8- 2- 4 110.995 8- 2- 5 107.445 9- 3- 12 103.881
34) 9- 3- 15 111.708 10- 4- 6 107.441 11- 1- 4 109.355
37) 11- 1- 7 103.884 11- 1- 13 109.699 12- 3- 9 103.881
40) 12- 3- 15 109.631 13- 1- 4 109.267 13- 1- 7 111.705
43) 13- 1- 11 109.699 13- 15- 16 112.690 13- 15- 18 102.922
46) 13- 17- 19 103.599 14- 13- 15 112.680 14- 13- 17 110.058
49) 15- 3- 9 111.708 15- 3- 12 109.631 15- 13- 14 112.680
52) 15- 13- 17 102.907 15- 18- 19 103.638 16- 15- 18 110.062
55) 17- 13- 14 110.058 17- 13- 15 102.907 18- 15- 16 110.062
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.273 1- 11- 12- 3 -0.400
1- 13- 15- 3 -0.212 1- 4- 2- 5 -121.561
1- 4- 2- 8 118.456 1- 13- 15- 16 123.505
1- 13- 15- 18 -117.980 1- 13- 17- 19 143.648
2- 4- 1- 7 -172.396 2- 3- 12- 11 -59.914
2- 4- 1- 11 -57.348 2- 3- 15- 13 62.830
2- 4- 1- 13 62.735 2- 3- 15- 16 -61.607
2- 3- 15- 18 175.149 3- 2- 4- 6 -119.021
3- 2- 4- 10 121.000 3- 15- 13- 14 -123.906
3- 15- 13- 17 117.597 3- 15- 18- 19 -143.330
4- 2- 3- 9 172.714 4- 1- 11- 12 60.412
4- 2- 3- 12 57.651 4- 1- 13- 14 61.828
4- 1- 13- 15 -62.597 4- 2- 3- 15 -62.393
4- 1- 13- 17 -174.931 5- 2- 4- 6 119.692
5- 2- 3- 9 -64.932 5- 2- 4- 10 -0.287
5- 2- 3- 12 -179.995 5- 2- 3- 15 59.961
6- 4- 1- 7 -52.054 6- 4- 2- 8 -0.292
6- 4- 1- 11 62.994 6- 4- 1- 13 -176.923
7- 1- 4- 10 65.265 7- 1- 11- 12 -178.952
7- 1- 13- 14 -63.666 7- 1- 13- 15 171.909
7- 1- 13- 17 59.575 8- 2- 3- 9 52.373
8- 2- 4- 10 -120.271 8- 2- 3- 12 -62.690
8- 2- 3- 15 177.266 9- 3- 12- 11 179.443
9- 3- 15- 13 -171.660 9- 3- 15- 16 63.904
9- 3- 15- 18 -59.341 10- 4- 1- 11 -179.687
10- 4- 1- 13 -59.604 11- 1- 13- 14 -178.301
11- 1- 13- 15 57.274 11- 12- 3- 15 59.927
11- 1- 13- 17 -55.060 12- 3- 15- 13 -57.068
12- 11- 1- 13 -59.405 12- 3- 15- 16 178.496
12- 3- 15- 18 55.251 13- 17- 19- 18 -47.379
13- 15- 18- 19 -27.727 14- 13- 15- 16 -0.189
14- 13- 15- 18 118.326 14- 13- 17- 19 -92.312
15- 18- 19- 17 47.263 15- 13- 17- 19 28.006
16- 15- 13- 17 -118.686 16- 15- 18- 19 92.612
17- 13- 15- 18 -0.171

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R

1) 1- 4 1.5269 1- 7 1.0956 1- 11 1.4312 1- 13 1.5223
5) 2- 3 1.5308 2- 4 1.5456 2- 5 1.0968 2- 8 1.0929
9) 3- 9 1.0952 3- 12 1.4301 3- 15 1.5215 4- 6 1.0928
13) 4- 10 1.0951 11- 12 1.5024 13- 14 1.0988 13- 15 1.5512
17) 13- 17 1.4245 15- 16 1.0979 15- 18 1.4201 17- 19 1.4743
21) 18- 19 1.4563

Bond Angles

I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.486 1- 4- 10 110.498 1- 11- 12 109.565
4) 1- 13- 14 112.505 1- 13- 15 107.104 1- 13- 17 109.433
7) 2- 3- 9 113.265 2- 3- 12 108.851 2- 3- 15 108.339
10) 2- 4- 6 110.867 2- 4- 10 111.839 3- 2- 4 106.967
13) 3- 2- 5 110.353 3- 2- 8 109.178 3- 15- 16 111.124
16) 3- 15- 18 110.984 4- 1- 7 112.838 4- 1- 11 110.388
19) 4- 1- 13 110.164 4- 2- 3 106.967 4- 2- 5 111.903
22) 4- 2- 8 111.004 5- 2- 3 110.353 5- 2- 4 111.903
25) 5- 2- 8 107.432 6- 4- 10 107.733 7- 1- 4 112.838
28) 7- 1- 11 102.877 7- 1- 13 111.864 8- 2- 3 109.178
31) 8- 2- 4 111.004 8- 2- 5 107.432 9- 3- 12 103.061
34) 9- 3- 15 111.719 10- 4- 6 107.733 11- 1- 4 110.388
37) 11- 1- 7 102.877 11- 1- 13 108.415 12- 3- 9 103.061
40) 12- 3- 15 111.547 13- 1- 4 110.164 13- 1- 7 111.864
43) 13- 1- 11 108.415 13- 15- 16 111.368 13- 15- 18 103.820
46) 13- 17- 19 102.413 14- 13- 15 111.832 14- 13- 17 110.924
49) 15- 3- 9 111.719 15- 3- 12 111.547 15- 13- 14 111.832
52) 15- 13- 17 104.679 15- 18- 19 100.339 16- 15- 18 110.707
55) 17- 13- 14 110.924 17- 13- 15 104.679 18- 15- 16 110.707

Dihedrals

I J K L Theta I J K L Theta
1- 4- 2- 3 14.903 1- 11- 12- 3 19.205
1- 13- 15- 3 11.557 1- 4- 2- 5 -106.066
1- 4- 2- 8 133.918 1- 13- 15- 16 134.239
1- 13- 15- 18 -106.601 1- 13- 17- 19 136.691
2- 4- 1- 7 178.435 2- 3- 12- 11 -71.967
2- 4- 1- 11 -67.078 2- 3- 15- 13 55.454
2- 4- 1- 13 52.624 2- 3- 15- 16 -67.376
2- 3- 15- 18 168.971 3- 2- 4- 6 -102.814
3- 2- 4- 10 136.926 3- 15- 13- 14 -112.134
3- 15- 13- 17 127.690 3- 15- 18- 19 -153.944
4- 2- 3- 9 164.311 4- 1- 11- 12 48.209
4- 2- 3- 12 50.312 4- 1- 13- 14 55.109
4- 1- 13- 15 -68.167 4- 2- 3- 15 -71.156
4- 1- 13- 17 178.896 5- 2- 4- 6 136.216
5- 2- 3- 9 -73.740 5- 2- 4- 10 15.956
5- 2- 3- 12 172.261 5- 2- 3- 15 50.793
6- 4- 1- 7 -61.707 6- 4- 2- 8 16.200
6- 4- 1- 11 52.780 6- 4- 1- 13 172.482
7- 1- 4- 10 55.596 7- 1- 11- 12 168.854
7- 1- 13- 14 -71.251 7- 1- 13- 15 165.473
7- 1- 13- 17 52.536 8- 2- 3- 9 44.121
8- 2- 4- 10 -104.060 8- 2- 3- 12 -69.878
8- 2- 3- 15 168.654 9- 3- 12- 11 167.525
9- 3- 15- 13 -179.098 9- 3- 15- 16 58.071
9- 3- 15- 18 -65.582 10- 4- 1- 11 170.083
10- 4- 1- 13 -70.215 11- 1- 13- 14 176.000
11- 1- 13- 15 52.725 11- 12- 3- 15 47.523
11- 1- 13- 17 -60.213 12- 3- 15- 13 -64.338
12- 11- 1- 13 -72.543 12- 3- 15- 16 172.831
12- 3- 15- 18 49.179 13- 17- 19- 18 -46.240
13- 15- 18- 19 -37.446 14- 13- 15- 16 10.549
14- 13- 15- 18 129.709 14- 13- 17- 19 -98.597
15- 18- 19- 17 52.337 15- 13- 17- 19 22.183

16- 15- 13- 17 -109.627 16- 15- 18- 19 82.165
17- 13- 15- 18 9.533

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5276 1- 7 1.0945 1- 11 1.4248 1- 13 1.5226
5) 2- 3 1.5329 2- 4 1.5472 2- 5 1.0959 2- 8 1.0922
9) 3- 9 1.0941 3- 12 1.4238 3- 15 1.5213 4- 6 1.0920
13) 4- 10 1.0941 11- 12 1.4816 13- 14 1.0973 13- 15 1.5541
17) 13- 17 1.4173 15- 16 1.0968 15- 18 1.4125 17- 19 1.4546
21) 18- 19 1.4352
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.486 1- 4- 10 110.666 1- 11- 12 109.690
4) 1- 13- 14 112.853 1- 13- 15 106.764 1- 13- 17 109.654
7) 2- 3- 9 113.533 2- 3- 12 108.727 2- 3- 15 107.572
10) 2- 4- 6 110.657 2- 4- 10 111.948 3- 2- 4 106.516
13) 3- 2- 5 110.515 3- 2- 8 109.420 3- 15- 16 111.127
16) 3- 15- 18 111.812 4- 1- 7 112.970 4- 1- 11 110.424
19) 4- 1- 13 109.876 4- 2- 3 106.516 4- 2- 5 111.910
22) 4- 2- 8 110.958 5- 2- 3 110.515 5- 2- 4 111.910
25) 5- 2- 8 107.528 6- 4- 10 107.862 7- 1- 4 112.970
28) 7- 1- 11 103.065 7- 1- 13 111.893 8- 2- 3 109.420
31) 8- 2- 4 110.958 8- 2- 5 107.528 9- 3- 12 103.237
34) 9- 3- 15 111.759 10- 4- 6 107.862 11- 1- 4 110.424
37) 11- 1- 7 103.065 11- 1- 13 108.342 12- 3- 9 103.237
40) 12- 3- 15 112.024 13- 1- 4 109.876 13- 1- 7 111.893
43) 13- 1- 11 108.342 13- 15- 16 111.372 13- 15- 18 103.442
46) 13- 17- 19 102.777 14- 13- 15 112.071 14- 13- 17 110.818
49) 15- 3- 9 111.759 15- 3- 12 112.024 15- 13- 14 112.071
52) 15- 13- 17 104.260 15- 18- 19 100.695 16- 15- 18 110.376
55) 17- 13- 14 110.818 17- 13- 15 104.260 18- 15- 16 110.376
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 16.738 1- 11- 12- 3 21.811
1- 13- 15- 3 12.505 1- 4- 2- 5 -104.143
1- 4- 2- 8 135.747 1- 13- 15- 16 135.102
1- 13- 15- 18 -106.347 1- 13- 17- 19 135.515
2- 4- 1- 7 177.596 2- 3- 12- 11 -73.312
2- 4- 1- 11 -67.580 2- 3- 15- 13 55.469
2- 4- 1- 13 51.872 2- 3- 15- 16 -67.276
2- 3- 15- 18 168.897 3- 2- 4- 6 -100.740
3- 2- 4- 10 138.906 3- 15- 13- 14 -111.538
3- 15- 13- 17 128.545 3- 15- 18- 19 -153.643
4- 2- 3- 9 162.936 4- 1- 11- 12 46.417
4- 2- 3- 12 48.645 4- 1- 13- 14 54.504
4- 1- 13- 15 -69.056 4- 2- 3- 15 -72.868
4- 1- 13- 17 178.564 5- 2- 4- 6 138.378
5- 2- 3- 9 -75.294 5- 2- 4- 10 18.025
5- 2- 3- 12 170.416 5- 2- 3- 15 48.903
6- 4- 1- 7 -62.906 6- 4- 2- 8 18.268
6- 4- 1- 11 51.919 6- 4- 1- 13 171.370
7- 1- 4- 10 54.644 7- 1- 11- 12 167.342
7- 1- 13- 14 -71.831 7- 1- 13- 15 164.609
7- 1- 13- 17 52.229 8- 2- 3- 9 42.928
8- 2- 4- 10 -102.085 8- 2- 3- 12 -71.363
8- 2- 3- 15 167.124 9- 3- 12- 11 165.834

9- 3- 15- 13 -179.266 9- 3- 15- 16 57.988
9- 3- 15- 18 -65.838 10- 4- 1- 11 169.469
10- 4- 1- 13 -71.080 11- 1- 13- 14 175.220
11- 1- 13- 15 51.660 11- 12- 3- 15 45.439
11- 1- 13- 17 -60.720 12- 3- 15- 13 -63.963
12- 11- 1- 13 -73.958 12- 3- 15- 16 173.292
12- 3- 15- 18 49.465 13- 17- 19- 18 -45.776
13- 15- 18- 19 -37.131 14- 13- 15- 16 11.058
14- 13- 15- 18 129.609 14- 13- 17- 19 -99.245
15- 18- 19- 17 52.075 15- 13- 17- 19 21.513
16- 15- 13- 17 -108.859 16- 15- 18- 19 82.109
17- 13- 15- 18 9.692

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5377 1- 7 1.0947 1- 11 1.4241 1- 13 1.5337
5) 2- 3 1.5378 2- 4 1.5556 2- 5 1.0961 2- 8 1.0930
9) 3- 9 1.0947 3- 12 1.4240 3- 15 1.5334 4- 6 1.0930
13) 4- 10 1.0962 11- 12 1.4921 13- 14 1.0979 13- 15 1.5622
17) 13- 17 1.4190 15- 16 1.0978 15- 18 1.4190 17- 19 1.4489
21) 18- 19 1.4495
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.221 1- 4- 10 110.261 1- 11- 12 110.910
4) 1- 13- 14 111.261 1- 13- 15 108.024 1- 13- 17 110.911
7) 2- 3- 9 112.412 2- 3- 12 109.978 2- 3- 15 109.250
10) 2- 4- 6 110.926 2- 4- 10 111.879 3- 2- 4 108.068
13) 3- 2- 5 110.320 3- 2- 8 108.199 3- 15- 16 111.285
16) 3- 15- 18 110.889 4- 1- 7 112.495 4- 1- 11 109.936
19) 4- 1- 13 109.203 4- 2- 3 108.068 4- 2- 5 111.837
22) 4- 2- 8 110.935 5- 2- 3 110.320 5- 2- 4 111.837
25) 5- 2- 8 107.431 6- 4- 10 107.453 7- 1- 4 112.495
28) 7- 1- 11 102.914 7- 1- 13 111.520 8- 2- 3 108.199
31) 8- 2- 4 110.935 8- 2- 5 107.431 9- 3- 12 102.907
34) 9- 3- 15 111.563 10- 4- 6 107.453 11- 1- 4 109.936
37) 11- 1- 7 102.914 11- 1- 13 110.650 12- 3- 9 102.907
40) 12- 3- 15 110.604 13- 1- 4 109.203 13- 1- 7 111.520
43) 13- 1- 11 110.650 13- 15- 16 111.386 13- 15- 18 104.108
46) 13- 17- 19 102.297 14- 13- 15 111.324 14- 13- 17 111.008
49) 15- 3- 9 111.563 15- 3- 12 110.604 15- 13- 14 111.324
52) 15- 13- 17 104.055 15- 18- 19 102.318 16- 15- 18 110.977
55) 17- 13- 14 111.008 17- 13- 15 104.055 18- 15- 16 110.977
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.290 1- 11- 12- 3 -0.415
1- 13- 15- 3 -0.245 1- 4- 2- 5 -121.908
1- 4- 2- 8 118.170 1- 13- 15- 16 122.203
1- 13- 15- 18 -118.137 1- 13- 17- 19 145.060
2- 4- 1- 7 -172.698 2- 3- 12- 11 -60.274
2- 4- 1- 11 -58.649 2- 3- 15- 13 62.865
2- 4- 1- 13 62.923 2- 3- 15- 16 -59.646
2- 3- 15- 18 176.305 3- 2- 4- 6 -118.761
3- 2- 4- 10 121.267 3- 15- 13- 14 -122.683
3- 15- 13- 17 117.683 3- 15- 18- 19 -144.637
4- 2- 3- 9 172.977 4- 1- 11- 12 60.796

4- 2- 3- 12 58.959 4- 1- 13- 14 59.905
4- 1- 13- 15 -62.571 4- 2- 3- 15 -62.612
4- 1- 13- 17 -176.007 5- 2- 4- 6 119.622
5- 2- 3- 9 -64.473 5- 2- 4- 10 -0.350
5- 2- 3- 12 -178.491 5- 2- 3- 15 59.938
6- 4- 1- 7 -52.515 6- 4- 2- 8 -0.301
6- 4- 1- 11 61.534 6- 4- 1- 13 -176.894
7- 1- 4- 10 64.749 7- 1- 11- 12 -179.156
7- 1- 13- 14 -65.044 7- 1- 13- 15 172.480
7- 1- 13- 17 59.044 8- 2- 3- 9 52.786
8- 2- 4- 10 -120.273 8- 2- 3- 12 -61.232
8- 2- 3- 15 177.196 9- 3- 12- 11 179.759
9- 3- 15- 13 -172.228 9- 3- 15- 16 65.261
9- 3- 15- 18 -58.788 10- 4- 1- 11 178.798
10- 4- 1- 13 -59.630 11- 1- 13- 14 -178.957
11- 1- 13- 15 58.567 11- 12- 3- 15 60.486
11- 1- 13- 17 -54.869 12- 3- 15- 13 -58.327
12- 11- 1- 13 -59.907 12- 3- 15- 16 179.162
12- 3- 15- 18 55.113 13- 17- 19- 18 -48.372
13- 15- 18- 19 -28.798 14- 13- 15- 16 -0.234
14- 13- 15- 18 119.425 14- 13- 17- 19 -90.707
15- 18- 19- 17 48.224 15- 13- 17- 19 29.141
16- 15- 13- 17 -119.868 16- 15- 18- 19 91.138
17- 13- 15- 18 -0.208

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5353 1- 7 1.0941 1- 11 1.4343 1- 13 1.5319
5) 2- 3 1.5354 2- 4 1.5541 2- 5 1.0945 2- 8 1.0927
9) 3- 9 1.0941 3- 12 1.4343 3- 15 1.5319 4- 6 1.0927
13) 4- 10 1.0945 11- 12 1.4926 13- 14 1.0950 13- 15 1.5607
17) 13- 17 1.4302 15- 16 1.0950 15- 18 1.4302 17- 19 1.4498
21) 18- 19 1.4498
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.232 1- 4- 10 109.951 1- 11- 12 110.821
4) 1- 13- 14 111.434 1- 13- 15 108.092 1- 13- 17 110.829
7) 2- 3- 9 112.578 2- 3- 12 110.100 2- 3- 15 109.263
10) 2- 4- 6 111.174 2- 4- 10 111.789 3- 2- 4 108.180
13) 3- 2- 5 109.949 3- 2- 8 108.233 3- 15- 16 111.434
16) 3- 15- 18 110.828 4- 1- 7 112.578 4- 1- 11 110.098
19) 4- 1- 13 109.265 4- 2- 3 108.180 4- 2- 5 111.793
22) 4- 2- 8 111.173 5- 2- 3 109.949 5- 2- 4 111.793
25) 5- 2- 8 107.459 6- 4- 10 107.460 7- 1- 4 112.578
28) 7- 1- 11 102.783 7- 1- 13 111.647 8- 2- 3 108.233
31) 8- 2- 4 111.173 8- 2- 5 107.459 9- 3- 12 102.784
34) 9- 3- 15 111.646 10- 4- 6 107.460 11- 1- 4 110.098
37) 11- 1- 7 102.783 11- 1- 13 110.328 12- 3- 9 102.784
40) 12- 3- 15 110.329 13- 1- 4 109.265 13- 1- 7 111.647
43) 13- 1- 11 110.328 13- 15- 16 111.553 13- 15- 18 104.069
46) 13- 17- 19 102.341 14- 13- 15 111.552 14- 13- 17 110.608
49) 15- 3- 9 111.646 15- 3- 12 110.329 15- 13- 14 111.552
52) 15- 13- 17 104.070 15- 18- 19 102.340 16- 15- 18 110.608
55) 17- 13- 14 110.608 17- 13- 15 104.070 18- 15- 16 110.608
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 0.007 1- 11- 12- 3 0.004

1- 13- 15- 3 0.003 1- 4- 2- 5 -121.194
1- 4- 2- 8 118.715 1- 13- 15- 16 122.848
1- 13- 15- 18 -117.869 1- 13- 17- 19 144.810
2- 4- 1- 7 -172.807 2- 3- 12- 11 -60.360
2- 4- 1- 11 -58.771 2- 3- 15- 13 62.491
2- 4- 1- 13 62.544 2- 3- 15- 16 -60.426
2- 3- 15- 18 175.938 3- 2- 4- 6 -118.701
3- 2- 4- 10 121.208 3- 15- 13- 14 -122.841
3- 15- 13- 17 117.876 3- 15- 18- 19 -144.814
4- 2- 3- 9 172.803 4- 1- 11- 12 60.357
4- 2- 3- 12 58.764 4- 1- 13- 14 60.421
4- 1- 13- 15 -62.495 4- 2- 3- 15 -62.552
4- 1- 13- 17 -175.943 5- 2- 4- 6 120.098
5- 2- 3- 9 -64.861 5- 2- 4- 10 0.008
5- 2- 3- 12 -178.900 5- 2- 3- 15 59.784
6- 4- 1- 7 -52.247 6- 4- 2- 8 0.007
6- 4- 1- 11 61.789 6- 4- 1- 13 -176.896
7- 1- 4- 10 64.859 7- 1- 11- 12 -179.494
7- 1- 13- 14 -64.769 7- 1- 13- 15 172.314
7- 1- 13- 17 58.866 8- 2- 3- 9 52.243
8- 2- 4- 10 -120.083 8- 2- 3- 12 -61.796
8- 2- 3- 15 176.888 9- 3- 12- 11 179.489
9- 3- 15- 13 -172.321 9- 3- 15- 16 64.762
9- 3- 15- 18 -58.874 10- 4- 1- 11 178.895
10- 4- 1- 13 -59.790 11- 1- 13- 14 -178.403
11- 1- 13- 15 58.681 11- 12- 3- 15 60.317
11- 1- 13- 17 -54.767 12- 3- 15- 13 -58.687
12- 11- 1- 13 -60.322 12- 3- 15- 16 178.396
12- 3- 15- 18 54.761 13- 17- 19- 18 -48.153
13- 15- 18- 19 -28.846 14- 13- 15- 16 0.004
14- 13- 15- 18 119.287 14- 13- 17- 19 -91.082
15- 18- 19- 17 48.155 15- 13- 17- 19 28.841
16- 15- 13- 17 -119.279 16- 15- 18- 19 91.078
17- 13- 15- 18 0.004

Optimised structures for ozonide 19a.at all levels reported.

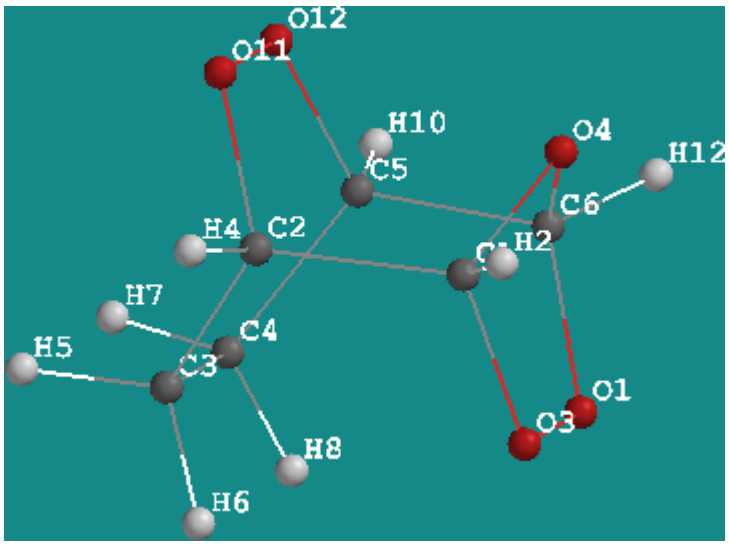

Figure S7: Optimised geometry for ozonide **19a**.

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5585 1- 10 1.0774 1- 17 1.4076 1- 18 1.3775
5) 2- 4 1.5421 2- 6 1.5262 2- 7 1.0807 2- 11 1.0830
9) 3- 4 1.5262 3- 5 1.5585 3- 8 1.0820 3- 16 1.4064
13) 4- 9 1.0830 4- 12 1.0807 5- 13 1.0774 5- 18 1.3775
17) 5- 19 1.4076 6- 14 1.0820 6- 15 1.4064 15- 16 1.4139
21) 17- 19 1.4120
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 108.225 1- 6- 15 109.900 1- 17- 19 104.867
4) 2- 4- 9 110.170 2- 4- 12 111.840 2- 6- 14 110.095
7) 2- 6- 15 109.949 3- 4- 9 107.055 3- 4- 12 110.337
10) 3- 5- 13 112.404 3- 5- 18 111.037 3- 5- 19 112.054
13) 4- 2- 6 109.489 4- 2- 7 111.840 4- 2- 11 110.170
16) 4- 3- 5 115.250 4- 3- 8 110.095 4- 3- 16 109.949
19) 5- 3- 4 115.250 5- 3- 8 108.225 5- 3- 16 109.900
22) 6- 1- 10 112.404 6- 1- 17 112.054 6- 1- 18 111.037
25) 6- 2- 4 109.489 6- 2- 7 110.337 6- 2- 11 107.055
28) 6- 15- 16 114.052 7- 2- 4 111.840 7- 2- 6 110.337
31) 7- 2- 11 107.825 8- 3- 4 110.095 8- 3- 5 108.225
34) 8- 3- 16 102.667 9- 4- 12 107.825 10- 1- 6 112.404
37) 10- 1- 17 107.676 10- 1- 18 109.614 11- 2- 4 110.170
40) 11- 2- 6 107.055 11- 2- 7 107.825 12- 4- 9 107.825
43) 13- 5- 18 109.614 13- 5- 19 107.676 14- 6- 15 102.667
46) 15- 6- 14 102.667 16- 3- 4 109.949 16- 3- 5 109.900
49) 16- 3- 8 102.667 17- 1- 6 112.054 17- 1- 10 107.676
52) 17- 1- 18 103.647 18- 1- 6 111.037 18- 1- 10 109.614
55) 18- 1- 17 103.647 18- 5- 13 109.614 18- 5- 19 103.647
58) 19- 5- 13 107.676 19- 5- 18 103.647
Dihedrals
I J K L Theta I J K L Theta
1- 18- 5- 3 76.135 1- 6- 2- 4 -70.901
1- 17- 19- 5 -0.000 1- 6- 2- 7 52.606
1- 6- 2- 11 169.683 1- 18- 5- 13 -159.075
1- 6- 15- 16 71.293 1- 18- 5- 19 -44.353
```

2- 4- 3- 5 70.901 2- 4- 3- 8 -166.364
2- 6- 1- 10 -134.445 2- 4- 3- 16 -53.957
2- 6- 15- 16 -56.587 2- 6- 1- 17 -13.022
2- 6- 1- 18 102.354 3- 4- 2- 6 -0.000
3- 16- 15- 6 -0.000 3- 4- 2- 7 -122.617
3- 4- 2- 11 117.479 3- 5- 19- 17 -92.581
4- 3- 5- 13 134.445 4- 2- 6- 14 166.364
4- 2- 6- 15 53.957 4- 3- 16- 15 56.587
4- 3- 5- 18 -102.354 4- 3- 5- 19 13.022
5- 18- 1- 6 -76.135 5- 3- 4- 9 -169.683
5- 18- 1- 10 159.075 5- 3- 4- 12 -52.606
5- 3- 16- 15 -71.293 5- 18- 1- 17 44.353
6- 2- 4- 9 -117.479 6- 2- 4- 12 122.617
6- 1- 17- 19 92.581 7- 2- 4- 9 119.904
7- 2- 4- 12 -0.000 7- 2- 6- 14 -70.129
7- 2- 6- 15 177.464 8- 3- 4- 9 -46.948
8- 3- 4- 12 70.129 8- 3- 5- 13 10.719
8- 3- 16- 15 173.730 8- 3- 5- 18 133.919
8- 3- 5- 19 -110.705 9- 4- 2- 11 -0.000
9- 4- 3- 16 65.459 10- 1- 6- 14 -10.719
10- 1- 6- 15 100.671 10- 1- 17- 19 -143.315
11- 2- 4- 12 -119.904 11- 2- 6- 14 46.948
11- 2- 6- 15 -65.459 12- 4- 3- 16 -177.464
13- 5- 3- 16 -100.671 13- 5- 19- 17 143.315
14- 6- 15- 16 -173.730 14- 6- 1- 17 110.705
14- 6- 1- 18 -133.919 15- 6- 1- 17 -137.905
15- 6- 1- 18 -22.529 16- 3- 5- 18 22.529
16- 3- 5- 19 137.905 17- 19- 5- 18 27.216
18- 1- 17- 19 -27.216

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5572 1- 10 1.0773 1- 17 1.4104 1- 18 1.3800
5) 2- 4 1.5411 2- 6 1.5251 2- 7 1.0805 2- 11 1.0825
9) 3- 4 1.5251 3- 5 1.5572 3- 8 1.0814 3- 16 1.4123
13) 4- 9 1.0825 4- 12 1.0805 5- 13 1.0773 5- 18 1.3800
17) 5- 19 1.4104 6- 14 1.0814 6- 15 1.4123 15- 16 1.4148
21) 17- 19 1.4123
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 108.196 1- 6- 15 109.679 1- 17- 19 104.903
4) 2- 4- 9 110.247 2- 4- 12 111.932 2- 6- 14 110.194
7) 2- 6- 15 109.903 3- 4- 9 107.028 3- 4- 12 110.212
10) 3- 5- 13 112.439 3- 5- 18 111.164 3- 5- 19 112.158
13) 4- 2- 6 109.590 4- 2- 7 111.932 4- 2- 11 110.247
16) 4- 3- 5 115.474 4- 3- 8 110.194 4- 3- 16 109.903
19) 5- 3- 4 115.474 5- 3- 8 108.196 5- 3- 16 109.679
22) 6- 1- 10 112.439 6- 1- 17 112.158 6- 1- 18 111.164
25) 6- 2- 4 109.590 6- 2- 7 110.212 6- 2- 11 107.028
28) 6- 15- 16 114.001 7- 2- 4 111.932 7- 2- 6 110.212
31) 7- 2- 11 107.700 8- 3- 4 110.194 8- 3- 5 108.196
34) 8- 3- 16 102.608 9- 4- 12 107.700 10- 1- 6 112.439
37) 10- 1- 17 107.551 10- 1- 18 109.603 11- 2- 4 110.247
40) 11- 2- 6 107.028 11- 2- 7 107.700 12- 4- 9 107.700
43) 13- 5- 18 109.603 13- 5- 19 107.551 14- 6- 15 102.608
46) 15- 6- 14 102.608 16- 3- 4 109.903 16- 3- 5 109.679
49) 16- 3- 8 102.608 17- 1- 6 112.158 17- 1- 10 107.551

52) 17- 1- 18 103.493 18- 1- 6 111.164 18- 1- 10 109.603
55) 18- 1- 17 103.493 18- 5- 13 109.603 18- 5- 19 103.493
58) 19- 5- 13 107.551 19- 5- 18 103.493
Dihedrals
I J K L Theta I J K L Theta
1- 18- 5- 3 75.982 1- 6- 2- 4 -70.711
1- 17- 19- 5 -0.000 1- 6- 2- 7 52.896
1- 6- 2- 11 169.741 1- 18- 5- 13 -159.102
1- 6- 15- 16 71.444 1- 18- 5- 19 -44.604
2- 4- 3- 5 70.711 2- 4- 3- 8 -166.349
2- 6- 1- 10 -134.561 2- 4- 3- 16 -53.984
2- 6- 15- 16 -56.528 2- 6- 1- 17 -13.197
2- 6- 1- 18 102.132 3- 4- 2- 6 -0.000
3- 16- 15- 6 -0.000 3- 4- 2- 7 -122.590
3- 4- 2- 11 117.552 3- 5- 19- 17 -92.546
4- 3- 5- 13 134.561 4- 2- 6- 14 166.349
4- 2- 6- 15 53.984 4- 3- 16- 15 56.528
4- 3- 5- 18 -102.132 4- 3- 5- 19 13.197
5- 18- 1- 6 -75.982 5- 3- 4- 9 -169.741
5- 18- 1- 10 159.102 5- 3- 4- 12 -52.896
5- 3- 16- 15 -71.444 5- 18- 1- 17 44.604
6- 2- 4- 9 -117.552 6- 2- 4- 12 122.590
6- 1- 17- 19 92.546 7- 2- 4- 9 119.857
7- 2- 4- 12 -0.000 7- 2- 6- 14 -70.045
7- 2- 6- 15 177.590 8- 3- 4- 9 -46.801
8- 3- 4- 12 70.045 8- 3- 5- 13 10.568
8- 3- 16- 15 173.732 8- 3- 5- 18 133.875
8- 3- 5- 19 -110.796 9- 4- 2- 11 -0.000
9- 4- 3- 16 65.565 10- 1- 6- 14 -10.568
10- 1- 6- 15 100.629 10- 1- 17- 19 -143.324
11- 2- 4- 12 -119.857 11- 2- 6- 14 46.801
11- 2- 6- 15 -65.565 12- 4- 3- 16 -177.590
13- 5- 3- 16 -100.629 13- 5- 19- 17 143.324
14- 6- 15- 16 -173.732 14- 6- 1- 17 110.796
14- 6- 1- 18 -133.875 15- 6- 1- 17 -138.008
15- 6- 1- 18 -22.678 16- 3- 5- 18 22.678
16- 3- 5- 19 138.008 17- 19- 5- 18 27.362
18- 1- 17- 19 -27.362

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 2 1.0933 2- 7 1.5580 2- 14 1.4035 2- 19 1.4340
5) 3- 5 1.5379 3- 7 1.5241 3- 8 1.0934 3- 11 1.0919
9) 4- 5 1.5241 4- 6 1.5580 4- 12 1.0974 4- 17 1.4266
13) 5- 9 1.0919 5- 13 1.0934 6- 14 1.4035 6- 15 1.0933
17) 6- 18 1.4340 7- 10 1.0974 7- 16 1.4266 16- 17 1.5100
21) 18- 19 1.5011
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 2- 7 112.745 1- 2- 14 108.300 1- 2- 19 106.526
4) 2- 7- 10 107.892 2- 7- 16 110.489 3- 5- 9 111.825
7) 3- 5- 13 110.413 3- 7- 10 109.977 3- 7- 16 111.181
10) 4- 5- 9 109.795 4- 5- 13 106.864 4- 6- 14 111.688
13) 4- 6- 15 112.745 4- 6- 18 112.141 5- 3- 7 109.793
16) 5- 3- 8 110.413 5- 3- 11 111.825 5- 4- 6 115.244
19) 5- 4- 12 109.977 5- 4- 17 111.181 6- 4- 5 115.244
22) 6- 4- 12 107.892 6- 4- 17 110.489 6- 18- 19 103.182
25) 7- 2- 14 111.688 7- 2- 19 112.141 7- 3- 5 109.793
28) 7- 3- 8 106.864 7- 3- 11 109.795 7- 16- 17 111.811

31) 8- 3- 5 110.413 8- 3- 7 106.864 8- 3- 11 108.013
34) 9- 5- 13 108.013 10- 7- 16 101.071 11- 3- 5 111.825
37) 11- 3- 7 109.795 11- 3- 8 108.013 12- 4- 5 109.977
40) 12- 4- 6 107.892 12- 4- 17 101.071 13- 5- 9 108.013
43) 14- 2- 7 111.688 14- 2- 19 104.996 14- 6- 15 108.300
46) 14- 6- 18 104.996 15- 6- 14 108.300 15- 6- 18 106.526
49) 16- 7- 10 101.071 17- 4- 5 111.181 17- 4- 6 110.489
52) 17- 4- 12 101.071 18- 6- 14 104.996 18- 6- 15 106.526
55) 19- 2- 7 112.141 19- 2- 14 104.996
Dihedrals
I J K L Theta I J K L Theta
1- 2- 7- 3 135.238 1- 2- 14- 6 -159.914
1- 2- 7- 10 11.931 1- 2- 7- 16 -97.705
1- 2- 19- 18 143.211 2- 14- 6- 4 -75.351
2- 7- 3- 5 70.965 2- 19- 18- 6 -0.000
2- 7- 3- 8 -169.271 2- 7- 3- 11 -52.364
2- 14- 6- 15 159.914 2- 7- 16- 17 -72.383
2- 14- 6- 18 46.414 3- 5- 4- 6 -70.965
3- 5- 4- 12 166.840 3- 7- 2- 14 -102.545
3- 5- 4- 17 55.742 3- 7- 16- 17 56.892
3- 7- 2- 19 15.001 4- 5- 3- 7 -0.000
4- 17- 16- 7 -0.000 4- 5- 3- 8 -117.575
4- 5- 3- 11 122.129 4- 6- 18- 19 93.001
5- 3- 7- 10 -166.840 5- 4- 6- 14 102.545
5- 4- 6- 15 -135.238 5- 3- 7- 16 -55.742
5- 4- 17- 16 -56.892 5- 4- 6- 18 -15.001
6- 14- 2- 7 75.351 6- 4- 5- 9 52.364
6- 4- 5- 13 169.271 6- 4- 17- 16 72.383
6- 14- 2- 19 -46.414 7- 3- 5- 9 -122.129
7- 3- 5- 13 117.575 7- 2- 19- 18 -93.001
8- 3- 5- 9 120.297 8- 3- 7- 10 -47.076
8- 3- 5- 13 -0.000 8- 3- 7- 16 64.023
9- 5- 3- 11 -0.000 9- 5- 4- 12 -69.831
9- 5- 4- 17 179.071 10- 7- 3- 11 69.831
10- 7- 2- 14 134.148 10- 7- 16- 17 173.581
10- 7- 2- 19 -108.305 11- 3- 5- 13 -120.297
11- 3- 7- 16 -179.071 12- 4- 5- 13 47.076
12- 4- 6- 14 -134.148 12- 4- 6- 15 -11.931
12- 4- 17- 16 -173.581 12- 4- 6- 18 108.305
13- 5- 4- 17 -64.023 14- 2- 7- 16 24.513
14- 6- 4- 17 -24.513 14- 2- 19- 18 28.468
14- 6- 18- 19 -28.468 15- 6- 4- 17 97.705
15- 6- 18- 19 -143.211 16- 7- 2- 19 142.059
17- 4- 6- 18 -142.059

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 2 1.0921 2- 7 1.5605 2- 14 1.3971 2- 19 1.4259
5) 3- 5 1.5399 3- 7 1.5253 3- 8 1.0928 3- 11 1.0908
9) 4- 5 1.5253 4- 6 1.5605 4- 12 1.0960 4- 17 1.4202
13) 5- 9 1.0908 5- 13 1.0928 6- 14 1.3971 6- 15 1.0921
17) 6- 18 1.4259 7- 10 1.0960 7- 16 1.4202 16- 17 1.4909
21) 18- 19 1.4809
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 2- 7 112.690 1- 2- 14 108.405 1- 2- 19 106.419
4) 2- 7- 10 107.890 2- 7- 16 110.835 3- 5- 9 111.888
7) 3- 5- 13 110.321 3- 7- 10 110.007 3- 7- 16 111.029
10) 4- 5- 9 110.068 4- 5- 13 106.838 4- 6- 14 111.661

13) 4- 6- 15 112.690 4- 6- 18 112.233 5- 3- 7 109.524
16) 5- 3- 8 110.321 5- 3- 11 111.888 5- 4- 6 115.004
19) 5- 4- 12 110.007 5- 4- 17 111.029 6- 4- 5 115.004
22) 6- 4- 12 107.890 6- 4- 17 110.835 6- 18- 19 103.372
25) 7- 2- 14 111.661 7- 2- 19 112.233 7- 3- 5 109.524
28) 7- 3- 8 106.838 7- 3- 11 110.068 7- 16- 17 112.097
31) 8- 3- 5 110.321 8- 3- 7 106.838 8- 3- 11 108.067
34) 9- 5- 13 108.067 10- 7- 16 101.128 11- 3- 5 111.888
37) 11- 3- 7 110.068 11- 3- 8 108.067 12- 4- 5 110.007
40) 12- 4- 6 107.890 12- 4- 17 101.128 13- 5- 9 108.067
43) 14- 2- 7 111.661 14- 2- 19 104.989 14- 6- 15 108.405
46) 14- 6- 18 104.989 15- 6- 14 108.405 15- 6- 18 106.419
49) 16- 7- 10 101.128 17- 4- 5 111.029 17- 4- 6 110.835
52) 17- 4- 12 101.128 18- 6- 14 104.989 18- 6- 15 106.419
55) 19- 2- 7 112.233 19- 2- 14 104.989
Dihedrals
I J K L Theta I J K L Theta
1- 2- 7- 3 134.583 1- 2- 14- 6 -159.671
1- 2- 7- 10 11.404 1- 2- 7- 16 -98.464
1- 2- 19- 18 143.321 2- 14- 6- 4 -75.608
2- 7- 3- 5 71.183 2- 19- 18- 6 -0.000
2- 7- 3- 8 -169.327 2- 7- 3- 11 -52.229
2- 14- 6- 15 159.671 2- 7- 16- 17 -71.968
2- 14- 6- 18 46.250 3- 5- 4- 6 -71.183
3- 5- 4- 12 166.774 3- 7- 2- 14 -103.122
3- 5- 4- 17 55.672 3- 7- 16- 17 57.144
3- 7- 2- 19 14.458 4- 5- 3- 7 -0.000
4- 17- 16- 7 -0.000 4- 5- 3- 8 -117.326
4- 5- 3- 11 122.331 4- 6- 18- 19 92.975
5- 3- 7- 10 -166.774 5- 4- 6- 14 103.122
5- 4- 6- 15 -134.583 5- 3- 7- 16 -55.672
5- 4- 17- 16 -57.144 5- 4- 6- 18 -14.458
6- 14- 2- 7 75.608 6- 4- 5- 9 52.229
6- 4- 5- 13 169.327 6- 4- 17- 16 71.968
6- 14- 2- 19 -46.250 7- 3- 5- 9 -122.331
7- 3- 5- 13 117.326 7- 2- 19- 18 -92.975
8- 3- 5- 9 120.343 8- 3- 7- 10 -47.284
8- 3- 5- 13 -0.000 8- 3- 7- 16 63.819
9- 5- 3- 11 -0.000 9- 5- 4- 12 -69.814
9- 5- 4- 17 179.083 10- 7- 3- 11 69.814
10- 7- 2- 14 133.699 10- 7- 16- 17 173.837
10- 7- 2- 19 -108.721 11- 3- 5- 13 -120.343
11- 3- 7- 16 -179.083 12- 4- 5- 13 47.284
12- 4- 6- 14 -133.699 12- 4- 6- 15 -11.404
12- 4- 17- 16 -173.837 12- 4- 6- 18 108.721
13- 5- 4- 17 -63.819 14- 2- 7- 16 23.831
14- 6- 4- 17 -23.831 14- 2- 19- 18 28.508
14- 6- 18- 19 -28.508 15- 6- 4- 17 98.464
15- 6- 18- 19 -143.321 16- 7- 2- 19 141.411
17- 4- 6- 18 -141.411

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 2 1.0926 2- 7 1.5734 2- 14 1.4019 2- 19 1.4312
5) 3- 5 1.5477 3- 7 1.5336 3- 8 1.0940 3- 11 1.0923
9) 4- 5 1.5336 4- 6 1.5734 4- 12 1.0964 4- 17 1.4229
13) 5- 9 1.0923 5- 13 1.0940 6- 14 1.4019 6- 15 1.0926

17) 6- 18 1.4312 7- 10 1.0964 7- 16 1.4229 16- 17 1.4960
21) 18- 19 1.4851
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 2- 7 112.493 1- 2- 14 108.642 1- 2- 19 106.930
4) 2- 7- 10 107.954 2- 7- 16 110.527 3- 5- 9 111.710
7) 3- 5- 13 110.327 3- 7- 10 110.055 3- 7- 16 110.840
10) 4- 5- 9 109.927 4- 5- 13 107.156 4- 6- 14 111.325
13) 4- 6- 15 112.493 4- 6- 18 112.441 5- 3- 7 109.716
16) 5- 3- 8 110.327 5- 3- 11 111.710 5- 4- 6 115.014
19) 5- 4- 12 110.055 5- 4- 17 110.840 6- 4- 5 115.014
22) 6- 4- 12 107.954 6- 4- 17 110.527 6- 18- 19 103.631
25) 7- 2- 14 111.325 7- 2- 19 112.441 7- 3- 5 109.716
28) 7- 3- 8 107.156 7- 3- 11 109.927 7- 16- 17 112.445
31) 8- 3- 5 110.327 8- 3- 7 107.156 8- 3- 11 107.886
34) 9- 5- 13 107.886 10- 7- 16 101.568 11- 3- 5 111.710
37) 11- 3- 7 109.927 11- 3- 8 107.886 12- 4- 5 110.055
40) 12- 4- 6 107.954 12- 4- 17 101.568 13- 5- 9 107.886
43) 14- 2- 7 111.325 14- 2- 19 104.591 14- 6- 15 108.642
46) 14- 6- 18 104.591 15- 6- 14 108.642 15- 6- 18 106.930
49) 16- 7- 10 101.568 17- 4- 5 110.840 17- 4- 6 110.527
52) 17- 4- 12 101.568 18- 6- 14 104.591 18- 6- 15 106.930
55) 19- 2- 7 112.441 19- 2- 14 104.591
Dihedrals
I J K L Theta I J K L Theta
1- 2- 7- 3 135.222 1- 2- 14- 6 -159.789
1- 2- 7- 10 11.925 1- 2- 7- 16 -98.343
1- 2- 19- 18 143.222 2- 14- 6- 4 -75.800
2- 7- 3- 5 71.051 2- 19- 18- 6 -0.000
2- 7- 3- 8 -169.159 2- 7- 3- 11 -52.171
2- 14- 6- 15 159.789 2- 7- 16- 17 -71.946
2- 14- 6- 18 45.873 3- 5- 4- 6 -71.051
3- 5- 4- 12 166.778 3- 7- 2- 14 -102.566
3- 5- 4- 17 55.223 3- 7- 16- 17 56.784
3- 7- 2- 19 14.424 4- 5- 3- 7 -0.000
4- 17- 16- 7 -0.000 4- 5- 3- 8 -117.833
4- 5- 3- 11 122.166 4- 6- 18- 19 92.834
5- 3- 7- 10 -166.778 5- 4- 6- 14 102.566
5- 4- 6- 15 -135.222 5- 3- 7- 16 -55.223
5- 4- 17- 16 -56.784 5- 4- 6- 18 -14.424
6- 14- 2- 7 75.800 6- 4- 5- 9 52.171
6- 4- 5- 13 169.159 6- 4- 17- 16 71.946
6- 14- 2- 19 -45.873 7- 3- 5- 9 -122.166
7- 3- 5- 13 117.833 7- 2- 19- 18 -92.834
8- 3- 5- 9 120.001 8- 3- 7- 10 -46.988
8- 3- 5- 13 -0.000 8- 3- 7- 16 64.566
9- 5- 3- 11 -0.000 9- 5- 4- 12 -70.000
9- 5- 4- 17 178.446 10- 7- 3- 11 70.000
10- 7- 2- 14 134.137 10- 7- 16- 17 173.685
10- 7- 2- 19 -108.873 11- 3- 5- 13 -120.001
11- 3- 7- 16 -178.446 12- 4- 5- 13 46.988
12- 4- 6- 14 -134.137 12- 4- 6- 15 -11.925
12- 4- 17- 16 -173.685 12- 4- 6- 18 108.873
13- 5- 4- 17 -64.566 14- 2- 7- 16 23.869
14- 6- 4- 17 -23.869 14- 2- 19- 18 28.102
14- 6- 18- 19 -28.102 15- 6- 4- 17 98.343
15- 6- 18- 19 -143.222 16- 7- 2- 19 140.859
17- 4- 6- 18 -140.859

DFT/6-31G* (DICHLOROMETHANE)

Geometry information

Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5708 1- 10 1.0923 1- 17 1.4347 1- 18 1.4050
5) 2- 4 1.5466 2- 6 1.5326 2- 7 1.0919 2- 11 1.0935
9) 3- 4 1.5326 3- 5 1.5708 3- 8 1.0956 3- 16 1.4298
13) 4- 9 1.0935 4- 12 1.0919 5- 13 1.0923 5- 18 1.4050
17) 5- 19 1.4347 6- 14 1.0956 6- 15 1.4298 15- 16 1.4975
21) 17- 19 1.4859
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 107.894 1- 6- 15 110.284 1- 17- 19 103.653
4) 2- 4- 9 110.439 2- 4- 12 111.842 2- 6- 14 110.115
7) 2- 6- 15 110.740 3- 4- 9 107.080 3- 4- 12 109.830
10) 3- 5- 13 112.481 3- 5- 18 111.481 3- 5- 19 112.621
13) 4- 2- 6 109.808 4- 2- 7 111.842 4- 2- 11 110.439
16) 4- 3- 5 115.366 4- 3- 8 110.115 4- 3- 16 110.740
19) 5- 3- 4 115.366 5- 3- 8 107.894 5- 3- 16 110.284
22) 6- 1- 10 112.481 6- 1- 17 112.621 6- 1- 18 111.481
25) 6- 2- 4 109.808 6- 2- 7 109.830 6- 2- 11 107.080
28) 6- 15- 16 112.358 7- 2- 4 111.842 7- 2- 6 109.830
31) 7- 2- 11 107.710 8- 3- 4 110.115 8- 3- 5 107.894
34) 8- 3- 16 101.508 9- 4- 12 107.710 10- 1- 6 112.481
37) 10- 1- 17 106.765 10- 1- 18 108.644 11- 2- 4 110.439
40) 11- 2- 6 107.080 11- 2- 7 107.710 12- 4- 9 107.710
43) 13- 5- 18 108.644 13- 5- 19 106.765 14- 6- 15 101.508
46) 15- 6- 14 101.508 16- 3- 4 110.740 16- 3- 5 110.284
49) 16- 3- 8 101.508 17- 1- 6 112.621 17- 1- 10 106.765
52) 17- 1- 18 104.405 18- 1- 6 111.481 18- 1- 10 108.644
55) 18- 1- 17 104.405 18- 5- 13 108.644 18- 5- 19 104.405
58) 19- 5- 13 106.765 19- 5- 18 104.405
Dihedrals
I J K L Theta I J K L Theta
1- 18- 5- 3 75.616 1- 6- 2- 4 -70.804
1- 17- 19- 5 -0.000 1- 6- 2- 7 52.580
1- 6- 2- 11 169.265 1- 18- 5- 13 -159.881
1- 6- 15- 16 72.127 1- 18- 5- 19 -46.243
2- 4- 3- 5 70.804 2- 4- 3- 8 -166.799
2- 6- 1- 10 -135.355 2- 4- 3- 16 -55.338
2- 6- 15- 16 -56.800 2- 6- 1- 17 -14.650
2- 6- 1- 18 102.325 3- 4- 2- 6 -0.000
3- 16- 15- 6 -0.000 3- 4- 2- 7 -122.196
3- 4- 2- 11 117.864 3- 5- 19- 17 -92.784
4- 3- 5- 13 135.355 4- 2- 6- 14 166.799
4- 2- 6- 15 55.338 4- 3- 16- 15 56.800
4- 3- 5- 18 -102.325 4- 3- 5- 19 14.650
5- 18- 1- 6 -75.616 5- 3- 4- 9 -169.265
5- 18- 1- 10 159.881 5- 3- 4- 12 -52.580
5- 3- 16- 15 -72.127 5- 18- 1- 17 46.243
6- 2- 4- 9 -117.864 6- 2- 4- 12 122.196
6- 1- 17- 19 92.784 7- 2- 4- 9 119.941
7- 2- 4- 12 -0.000 7- 2- 6- 14 -69.816
7- 2- 6- 15 178.722 8- 3- 4- 9 -46.868
8- 3- 4- 12 69.816 8- 3- 5- 13 11.780
8- 3- 16- 15 173.697 8- 3- 5- 18 134.100
8- 3- 5- 19 -108.925 9- 4- 2- 11 -0.000
9- 4- 3- 16 64.593 10- 1- 6- 14 -11.780
10- 1- 6- 15 98.270 10- 1- 17- 19 -143.288
11- 2- 4- 12 -119.941 11- 2- 6- 14 46.868
11- 2- 6- 15 -64.593 12- 4- 3- 16 -178.722
13- 5- 3- 16 -98.270 13- 5- 19- 17 143.288
14- 6- 15- 16 -173.697 14- 6- 1- 17 108.925
14- 6- 1- 18 -134.100 15- 6- 1- 17 -141.025

```
15- 6- 1- 18 -24.050 16- 3- 5- 18 24.050
16- 3- 5- 19 141.025 17- 19- 5- 18 28.322
18- 1- 17- 19 -28.322
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Optimised structures for ozonide 19b.at all levels reported.

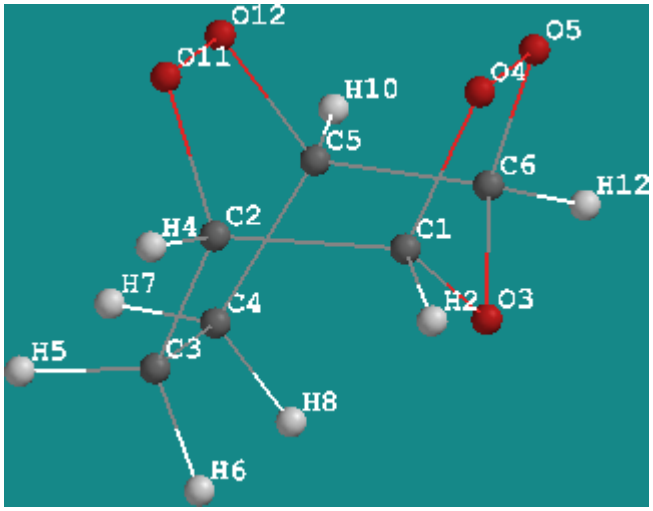

Figure S8: Optimised geometry for ozonide **19b**.

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5512 1- 10 1.0785 1- 17 1.3854 1- 18 1.3977
5) 2- 4 1.5492 2- 6 1.5270 2- 7 1.0833 2- 11 1.0827
9) 3- 4 1.5270 3- 5 1.5515 3- 8 1.0821 3- 16 1.4025
13) 4- 9 1.0829 4- 12 1.0835 5- 13 1.0786 5- 17 1.3853
17) 5- 19 1.3983 6- 14 1.0820 6- 15 1.4028 15- 16 1.4066
21) 18- 19 1.4111
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 108.240 1- 6- 15 112.747 1- 18- 19 105.000
4) 2- 4- 9 110.263 2- 4- 12 111.294 2- 6- 14 111.330
7) 2- 6- 15 110.010 3- 4- 9 107.907 3- 4- 12 110.249
10) 3- 5- 13 111.761 3- 5- 17 111.072 3- 5- 19 112.165
13) 4- 2- 6 109.450 4- 2- 7 111.280 4- 2- 11 110.266
16) 4- 3- 5 111.848 4- 3- 8 111.334 4- 3- 16 109.947
19) 5- 3- 4 111.848 5- 3- 8 108.250 5- 3- 16 112.777
22) 6- 1- 10 111.767 6- 1- 17 111.079 6- 1- 18 112.192
25) 6- 2- 4 109.450 6- 2- 7 110.222 6- 2- 11 107.917
28) 6- 15- 16 114.413 7- 2- 4 111.280 7- 2- 6 110.222
31) 7- 2- 11 107.635 8- 3- 4 111.334 8- 3- 5 108.250
34) 8- 3- 16 102.298 9- 4- 12 107.641 10- 1- 6 111.767
37) 10- 1- 17 109.297 10- 1- 18 108.376 11- 2- 4 110.266
40) 11- 2- 6 107.917 11- 2- 7 107.635 12- 4- 9 107.641
43) 13- 5- 17 109.287 13- 5- 19 108.402 14- 6- 15 102.284
46) 15- 6- 14 102.284 16- 3- 4 109.947 16- 3- 5 112.777
49) 16- 3- 8 102.298 17- 1- 6 111.079 17- 1- 10 109.297
52) 17- 1- 18 103.790 17- 5- 13 109.287 17- 5- 19 103.818
55) 18- 1- 6 112.192 18- 1- 10 108.376 18- 1- 17 103.790
```

58) 19- 5- 13 108.402 19- 5- 17 103.818
Dihedrals
I J K L Theta I J K L Theta
1- 17- 5- 3 -76.585 1- 6- 2- 4 -72.552
1- 18- 19- 5 -0.276 1- 6- 2- 7 50.148
1- 6- 2- 11 167.432 1- 17- 5- 13 159.652
1- 6- 15- 16 69.438 1- 17- 5- 19 44.154
2- 4- 3- 5 72.585 2- 4- 3- 8 -166.163
2- 6- 1- 10 -95.667 2- 4- 3- 16 -53.518
2- 6- 15- 16 -56.154 2- 6- 1- 17 26.694
2- 6- 1- 18 142.360 3- 4- 2- 6 -0.109
3- 16- 15- 6 -0.336 3- 4- 2- 7 -122.178
3- 4- 2- 11 118.457 3- 5- 19- 18 92.824
4- 3- 5- 13 95.872 4- 2- 6- 14 166.215
4- 2- 6- 15 53.554 4- 3- 16- 15 56.618
4- 3- 5- 17 -26.467 4- 3- 5- 19 -142.147
5- 17- 1- 6 76.414 5- 3- 4- 9 -167.429
5- 17- 1- 10 -159.803 5- 3- 4- 12 -50.128
5- 3- 16- 15 -68.958 5- 17- 1- 18 -44.344
6- 2- 4- 9 -118.641 6- 2- 4- 12 121.979
6- 1- 18- 19 -92.376 7- 2- 4- 9 119.291
7- 2- 4- 12 -0.090 7- 2- 6- 14 -71.084
7- 2- 6- 15 176.255 8- 3- 4- 9 -46.177
8- 3- 4- 12 71.124 8- 3- 5- 13 -27.147
8- 3- 16- 15 174.992 8- 3- 5- 17 -149.486
8- 3- 5- 19 94.834 9- 4- 2- 11 -0.074
9- 4- 3- 16 66.468 10- 1- 6- 14 27.336
10- 1- 6- 15 139.737 10- 1- 18- 19 143.737
11- 2- 4- 12 -119.455 11- 2- 6- 14 46.200
11- 2- 6- 15 -66.461 12- 4- 3- 16 -176.231
13- 5- 3- 16 -139.587 13- 5- 19- 18 -143.299
14- 6- 15- 16 -174.545 14- 6- 1- 17 149.698
14- 6- 1- 18 -94.636 15- 6- 1- 17 -97.901
15- 6- 1- 18 17.765 16- 3- 5- 17 98.074
16- 3- 5- 19 -17.606 17- 5- 19- 18 -27.176
17- 1- 18- 19 27.628

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5494 1- 10 1.0782 1- 17 1.3845 1- 18 1.4055
5) 2- 4 1.5482 2- 6 1.5257 2- 7 1.0827 2- 11 1.0823
9) 3- 4 1.5257 3- 5 1.5496 3- 8 1.0815 3- 16 1.4095
13) 4- 9 1.0825 4- 12 1.0828 5- 13 1.0782 5- 17 1.3844
17) 5- 19 1.4059 6- 14 1.0814 6- 15 1.4097 15- 16 1.4074
21) 18- 19 1.4118
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 108.228 1- 6- 15 112.633 1- 18- 19 104.954
4) 2- 4- 9 110.372 2- 4- 12 111.395 2- 6- 14 111.470
7) 2- 6- 15 110.030 3- 4- 9 107.876 3- 4- 12 110.017
10) 3- 5- 13 111.807 3- 5- 17 111.357 3- 5- 19 112.186
13) 4- 2- 6 109.535 4- 2- 7 111.382 4- 2- 11 110.376
16) 4- 3- 5 111.907 4- 3- 8 111.471 4- 3- 16 109.988
19) 5- 3- 4 111.907 5- 3- 8 108.228 5- 3- 16 112.644
22) 6- 1- 10 111.808 6- 1- 17 111.353 6- 1- 18 112.213
25) 6- 2- 4 109.535 6- 2- 7 109.999 6- 2- 11 107.896
28) 6- 15- 16 114.326 7- 2- 4 111.382 7- 2- 6 109.999

31) 7- 2- 11 107.575 8- 3- 4 111.471 8- 3- 5 108.228
34) 8- 3- 16 102.206 9- 4- 12 107.577 10- 1- 6 111.808
37) 10- 1- 17 109.309 10- 1- 18 108.237 11- 2- 4 110.376
40) 11- 2- 6 107.896 11- 2- 7 107.575 12- 4- 9 107.577
43) 13- 5- 17 109.302 13- 5- 19 108.257 14- 6- 15 102.192
46) 15- 6- 14 102.192 16- 3- 4 109.988 16- 3- 5 112.644
49) 16- 3- 8 102.206 17- 1- 6 111.353 17- 1- 10 109.309
52) 17- 1- 18 103.553 17- 5- 13 109.302 17- 5- 19 103.567
55) 18- 1- 6 112.213 18- 1- 10 108.237 18- 1- 17 103.553
58) 19- 5- 13 108.257 19- 5- 17 103.567
Dihedrals
I J K L Theta I J K L Theta
1- 17- 5- 3 -76.135 1- 6- 2- 4 -72.479
1- 18- 19- 5 -0.154 1- 6- 2- 7 50.259
1- 6- 2- 11 167.336 1- 17- 5- 13 159.839
1- 6- 15- 16 69.409 1- 17- 5- 19 44.626
2- 4- 3- 5 72.435 2- 4- 3- 8 -166.202
2- 6- 1- 10 -95.918 2- 4- 3- 16 -53.569
2- 6- 15- 16 -56.180 2- 6- 1- 17 26.686
2- 6- 1- 18 142.245 3- 4- 2- 6 -0.018
3- 16- 15- 6 -0.157 3- 4- 2- 7 -121.931
3- 4- 2- 11 118.641 3- 5- 19- 18 92.774
4- 3- 5- 13 96.033 4- 2- 6- 14 166.170
4- 2- 6- 15 53.531 4- 3- 16- 15 56.409
4- 3- 5- 17 -26.564 4- 3- 5- 19 -142.125
5- 17- 1- 6 76.050 5- 3- 4- 9 -167.402
5- 17- 1- 10 -159.919 5- 3- 4- 12 -50.324
5- 3- 16- 15 -69.176 5- 17- 1- 18 -44.733
6- 2- 4- 9 -118.644 6- 2- 4- 12 121.918
6- 1- 18- 19 -92.523 7- 2- 4- 9 119.443
7- 2- 4- 12 0.006 7- 2- 6- 14 -71.092
7- 2- 6- 15 176.269 8- 3- 4- 9 -46.039
8- 3- 4- 12 71.039 8- 3- 5- 13 -27.184
8- 3- 16- 15 174.910 8- 3- 5- 17 -149.780
8- 3- 5- 19 94.658 9- 4- 2- 11 0.015
9- 4- 3- 16 66.593 10- 1- 6- 14 27.286
10- 1- 6- 15 139.509 10- 1- 18- 19 143.624
11- 2- 4- 12 -119.422 11- 2- 6- 14 45.985
11- 2- 6- 15 -66.654 12- 4- 3- 16 -176.328
13- 5- 3- 16 -139.429 13- 5- 19- 18 -143.379
14- 6- 15- 16 -174.691 14- 6- 1- 17 149.890
14- 6- 1- 18 -94.551 15- 6- 1- 17 -97.887
15- 6- 1- 18 17.672 16- 3- 5- 17 97.974
16- 3- 5- 19 -17.587 17- 5- 19- 18 -27.424
17- 1- 18- 19 27.677

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 2 1.0974 2- 5 1.5251 2- 14 1.4226 2- 17 1.5518
5) 3- 4 1.5251 3- 5 1.5467 3- 6 1.0934 3- 9 1.0945
9) 4- 7 1.0974 4- 13 1.4227 4- 15 1.5516 5- 8 1.0945
13) 5- 10 1.0934 11- 12 1.4992 11- 15 1.4221 12- 17 1.4230
17) 13- 14 1.4951 15- 16 1.0945 15- 19 1.4127 17- 18 1.0945
21) 17- 19 1.4126
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 2- 5 111.410 1- 2- 14 100.587 1- 2- 17 107.822
4) 2- 5- 8 109.921 2- 5- 10 107.729 2- 17- 18 112.022
7) 2- 17- 19 111.598 3- 4- 7 111.393 3- 4- 13 111.175

10) 3- 4- 15 111.962 3- 5- 8 111.304 3- 5- 10 110.436
13) 4- 3- 5 109.712 4- 3- 6 107.710 4- 3- 9 109.881
16) 4- 13- 14 112.302 4- 15- 16 112.042 4- 15- 19 111.638
19) 5- 2- 14 111.081 5- 2- 17 111.936 5- 3- 4 109.712
22) 5- 3- 6 110.445 5- 3- 9 111.292 6- 3- 4 107.710
25) 6- 3- 5 110.445 6- 3- 9 107.715 7- 4- 13 100.580
28) 7- 4- 15 107.770 8- 5- 10 107.728 9- 3- 4 109.881
31) 9- 3- 5 111.292 9- 3- 6 107.715 10- 5- 8 107.728
34) 11- 12- 17 103.412 11- 15- 16 107.274 11- 15- 19 105.157
37) 12- 11- 15 103.314 12- 17- 18 107.303 12- 17- 19 105.226
40) 13- 4- 7 100.580 13- 4- 15 113.371 14- 2- 5 111.081
43) 14- 2- 17 113.425 15- 4- 7 107.770 15- 4- 13 113.371
46) 15- 11- 12 103.314 16- 15- 19 108.032 17- 2- 5 111.936
49) 17- 2- 14 113.425 18- 17- 19 108.016 19- 15- 16 108.032
52) 19- 17- 18 108.016
Dihedrals
I J K L Theta I J K L Theta
1- 2- 5- 3 -166.385 1- 2- 5- 8 70.955
1- 2- 5- 10 -46.166 1- 2- 17- 12 93.577
1- 2- 14- 13 175.232 1- 2- 17- 18 -27.273
1- 2- 17- 19 -148.533 2- 5- 3- 4 -0.361
2- 14- 13- 4 -0.681 2- 5- 3- 6 118.221
2- 5- 3- 9 -122.187 2- 17- 12- 11 93.393
2- 17- 19- 15 -76.027 3- 4- 15- 11 143.996
3- 4- 13- 14 -56.290 3- 5- 2- 14 -55.122
3- 4- 15- 16 -95.167 3- 5- 2- 17 72.797
3- 4- 15- 19 26.158 4- 3- 5- 8 121.474
4- 3- 5- 10 -118.916 4- 15- 11- 12 -92.536
4- 15- 19- 17 75.644 5- 3- 4- 7 166.704
5- 2- 17- 12 -143.546 5- 2- 14- 13 57.194
5- 3- 4- 13 55.406 5- 3- 4- 15 -72.538
5- 2- 17- 18 95.604 5- 2- 17- 19 -25.657
6- 3- 4- 7 46.444 6- 3- 5- 8 -119.943
6- 3- 5- 10 -0.334 6- 3- 4- 13 -64.854
6- 3- 4- 15 167.202 7- 4- 3- 9 -70.630
7- 4- 15- 11 -93.167 7- 4- 13- 14 -174.343
7- 4- 15- 16 27.669 7- 4- 15- 19 148.994
8- 5- 3- 9 -0.352 8- 5- 2- 14 -177.782
8- 5- 2- 17 -49.862 9- 3- 5- 10 119.258
9- 3- 4- 13 178.072 9- 3- 4- 15 50.128
10- 5- 2- 14 65.097 10- 5- 2- 17 -166.984
11- 15- 4- 13 17.230 11- 15- 19- 17 -46.420
11- 12- 17- 18 -143.079 11- 12- 17- 19 -28.211
12- 17- 2- 14 -16.887 12- 17- 19- 15 46.041
12- 11- 15- 16 143.922 12- 11- 15- 19 29.081
13- 4- 15- 16 138.066 13- 14- 2- 17 -69.914
13- 4- 15- 19 -100.608 14- 13- 4- 15 70.889
14- 2- 17- 18 -137.736 14- 2- 17- 19 101.003
15- 11- 12- 17 -0.522 15- 19- 17- 18 160.413
16- 15- 19- 17 -160.733

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 2 1.0961 2- 5 1.5262 2- 14 1.4164 2- 17 1.5539
5) 3- 4 1.5262 3- 5 1.5489 3- 6 1.0927 3- 9 1.0935
9) 4- 7 1.0962 4- 13 1.4164 4- 15 1.5539 5- 8 1.0935
13) 5- 10 1.0927 11- 12 1.4792 11- 15 1.4151 12- 17 1.4151
17) 13- 14 1.4765 15- 16 1.0933 15- 19 1.4056 17- 18 1.0934
21) 17- 19 1.4057

Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 2- 5 111.522 1- 2- 14 100.635 1- 2- 17 107.636
4) 2- 5- 8 110.101 2- 5- 10 107.721 2- 17- 18 111.959
7) 2- 17- 19 111.700 3- 4- 7 111.517 3- 4- 13 111.012
10) 3- 4- 15 111.721 3- 5- 8 111.351 3- 5- 10 110.406
13) 4- 3- 5 109.373 4- 3- 6 107.718 4- 3- 9 110.094
16) 4- 13- 14 112.514 4- 15- 16 111.968 4- 15- 19 111.706
19) 5- 2- 14 111.011 5- 2- 17 111.711 5- 3- 4 109.373
22) 5- 3- 6 110.407 5- 3- 9 111.349 6- 3- 4 107.718
25) 6- 3- 5 110.407 6- 3- 9 107.823 7- 4- 13 100.639
28) 7- 4- 15 107.633 8- 5- 10 107.825 9- 3- 4 110.094
31) 9- 3- 5 111.349 9- 3- 6 107.823 10- 5- 8 107.825
34) 11- 12- 17 103.524 11- 15- 16 107.127 11- 15- 19 105.161
37) 12- 11- 15 103.513 12- 17- 18 107.126 12- 17- 19 105.163
40) 13- 4- 7 100.639 13- 4- 15 113.768 14- 2- 5 111.011
43) 14- 2- 17 113.774 15- 4- 7 107.633 15- 4- 13 113.768
46) 15- 11- 12 103.513 16- 15- 19 108.158 17- 2- 5 111.711
49) 17- 2- 14 113.774 18- 17- 19 108.159 19- 15- 16 108.158
52) 19- 17- 18 108.159
Dihedrals
I J K L Theta I J K L Theta
1- 2- 5- 3 -166.586 1- 2- 5- 8 70.763
1- 2- 5- 10 -46.569 1- 2- 17- 12 93.239
1- 2- 14- 13 175.267 1- 2- 17- 18 -27.373
1- 2- 17- 19 -148.847 2- 5- 3- 4 -0.050
2- 14- 13- 4 -0.065 2- 5- 3- 6 118.311
2- 5- 3- 9 -121.950 2- 17- 12- 11 92.975
2- 17- 19- 15 -75.950 3- 4- 15- 11 144.043
3- 4- 13- 14 -57.021 3- 5- 2- 14 -55.241
3- 4- 15- 16 -95.347 3- 5- 2- 17 72.912
3- 4- 15- 19 26.137 4- 3- 5- 8 121.852
4- 3- 5- 10 -118.406 4- 15- 11- 12 -92.930
4- 15- 19- 17 75.917 5- 3- 4- 7 166.640
5- 2- 17- 12 -144.014 5- 2- 14- 13 57.104
5- 3- 4- 13 55.293 5- 3- 4- 15 -72.859
5- 2- 17- 18 95.374 5- 2- 17- 19 -26.100
6- 3- 4- 7 46.615 6- 3- 5- 8 -119.787
6- 3- 5- 10 -0.045 6- 3- 4- 13 -64.731
6- 3- 4- 15 167.117 7- 4- 3- 9 -70.709
7- 4- 15- 11 -93.212 7- 4- 13- 14 -175.180
7- 4- 15- 16 27.398 7- 4- 15- 19 148.881
8- 5- 3- 9 -0.048 8- 5- 2- 14 -177.892
8- 5- 2- 17 -49.740 9- 3- 5- 10 119.694
9- 3- 4- 13 177.945 9- 3- 4- 15 49.793
10- 5- 2- 14 64.776 10- 5- 2- 17 -167.071
11- 15- 4- 13 17.376 11- 15- 19- 17 -46.218
11- 12- 17- 18 -143.665 11- 12- 17- 19 -28.743
12- 17- 2- 14 -17.350 12- 17- 19- 15 46.199
12- 11- 15- 16 143.708 12- 11- 15- 19 28.787
13- 4- 15- 16 137.986 13- 14- 2- 17 -69.925
13- 4- 15- 19 -100.530 14- 13- 4- 15 70.016
14- 2- 17- 18 -137.962 14- 2- 17- 19 100.564
15- 11- 12- 17 -0.026 15- 19- 17- 18 160.403
16- 15- 19- 17 -160.421

DFT/6-31G* (GAS)

Geometry information
Bond Lengths

I J R I J R I J R I J R
1) 1- 2 1.0962 2- 5 1.5347 2- 14 1.4194 2- 17 1.5679
5) 3- 4 1.5347 3- 5 1.5557 3- 6 1.0939 3- 9 1.0946
9) 4- 7 1.0960 4- 13 1.4194 4- 15 1.5677 5- 8 1.0946
13) 5- 10 1.0940 11- 12 1.4830 11- 15 1.4194 12- 17 1.4204
17) 13- 14 1.4823 15- 16 1.0936 15- 19 1.4113 17- 18 1.0936
21) 17- 19 1.4110
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 2- 5 111.334 1- 2- 14 101.258 1- 2- 17 107.955
4) 2- 5- 8 110.052 2- 5- 10 107.934 2- 17- 18 111.798
7) 2- 17- 19 111.476 3- 4- 7 111.263 3- 4- 13 110.865
10) 3- 4- 15 111.856 3- 5- 8 111.110 3- 5- 10 110.393
13) 4- 3- 5 109.656 4- 3- 6 107.856 4- 3- 9 110.089
16) 4- 13- 14 112.887 4- 15- 16 111.838 4- 15- 19 111.488
19) 5- 2- 14 110.740 5- 2- 17 111.803 5- 3- 4 109.656
22) 5- 3- 6 110.384 5- 3- 9 111.160 6- 3- 4 107.856
25) 6- 3- 5 110.384 6- 3- 9 107.621 7- 4- 13 101.261
28) 7- 4- 15 107.882 8- 5- 10 107.664 9- 3- 4 110.089
31) 9- 3- 5 111.160 9- 3- 6 107.621 10- 5- 8 107.664
34) 11- 12- 17 103.840 11- 15- 16 107.586 11- 15- 19 104.691
37) 12- 11- 15 103.785 12- 17- 18 107.625 12- 17- 19 104.760
40) 13- 4- 7 101.261 13- 4- 15 113.205 14- 2- 5 110.740
43) 14- 2- 17 113.257 15- 4- 7 107.882 15- 4- 13 113.205
46) 15- 11- 12 103.785 16- 15- 19 108.410 17- 2- 5 111.803
49) 17- 2- 14 113.257 18- 17- 19 108.373 19- 15- 16 108.410
52) 19- 17- 18 108.373
Dihedrals
I J K L Theta I J K L Theta
1- 2- 5- 3 -166.397 1- 2- 5- 8 71.116
1- 2- 5- 10 -46.120 1- 2- 17- 12 94.027
1- 2- 14- 13 175.151 1- 2- 17- 18 -27.182
1- 2- 17- 19 -148.658 2- 5- 3- 4 -0.334
2- 14- 13- 4 -0.642 2- 5- 3- 6 118.356
2- 5- 3- 9 -122.296 2- 17- 12- 11 93.231
2- 17- 19- 15 -76.199 3- 4- 15- 11 143.550
3- 4- 13- 14 -56.169 3- 5- 2- 14 -54.558
3- 4- 15- 16 -95.254 3- 5- 2- 17 72.760
3- 4- 15- 19 26.308 4- 3- 5- 8 121.523
4- 3- 5- 10 -119.101 4- 15- 11- 12 -92.479
4- 15- 19- 17 75.864 5- 3- 4- 7 166.746
5- 2- 17- 12 -143.185 5- 2- 14- 13 56.986
5- 3- 4- 13 54.872 5- 3- 4- 15 -72.516
5- 2- 17- 18 95.605 5- 2- 17- 19 -25.871
6- 3- 4- 7 46.505 6- 3- 5- 8 -119.788
6- 3- 5- 10 -0.412 6- 3- 4- 13 -65.369
6- 3- 4- 15 167.243 7- 4- 3- 9 -70.653
7- 4- 15- 11 -93.767 7- 4- 13- 14 -174.308
7- 4- 15- 16 27.430 7- 4- 15- 19 148.991
8- 5- 3- 9 -0.440 8- 5- 2- 14 -177.045
8- 5- 2- 17 -49.728 9- 3- 5- 10 118.936
9- 3- 4- 13 177.473 9- 3- 4- 15 50.084
10- 5- 2- 14 65.719 10- 5- 2- 17 -166.963
11- 15- 4- 13 17.430 11- 15- 19- 17 -45.994
11- 12- 17- 18 -143.202 11- 12- 17- 19 -28.006
12- 17- 2- 14 -17.235 12- 17- 19- 15 45.683
12- 11- 15- 16 143.923 12- 11- 15- 19 28.734
13- 4- 15- 16 138.626 13- 14- 2- 17 -69.529
13- 4- 15- 19 -99.813 14- 13- 4- 15 70.477
14- 2- 17- 18 -138.445 14- 2- 17- 19 100.079
15- 11- 12- 17 -0.444 15- 19- 17- 18 160.356
16- 15- 19- 17 -160.606

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5642 1- 10 1.0931 1- 17 1.4099 1- 18 1.4294
5) 2- 4 1.5540 2- 6 1.5327 2- 7 1.0938 2- 11 1.0934
9) 3- 4 1.5327 3- 5 1.5642 3- 8 1.0956 3- 16 1.4273
13) 4- 9 1.0934 4- 12 1.0938 5- 13 1.0931 5- 17 1.4099
17) 5- 19 1.4294 6- 14 1.0956 6- 15 1.4274 15- 16 1.4843
21) 18- 19 1.4844
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 107.879 1- 6- 15 113.081 1- 18- 19 103.746
4) 2- 4- 9 110.540 2- 4- 12 111.280 2- 6- 14 111.404
7) 2- 6- 15 110.879 3- 4- 9 107.866 3- 4- 12 109.802
10) 3- 5- 13 111.874 3- 5- 17 111.874 3- 5- 19 112.456
13) 4- 2- 6 109.737 4- 2- 7 111.281 4- 2- 11 110.538
16) 4- 3- 5 111.924 4- 3- 8 111.402 4- 3- 16 110.879
19) 5- 3- 4 111.924 5- 3- 8 107.878 5- 3- 16 113.086
22) 6- 1- 10 111.871 6- 1- 17 111.872 6- 1- 18 112.456
25) 6- 2- 4 109.737 6- 2- 7 109.801 6- 2- 11 107.865
28) 6- 15- 16 112.765 7- 2- 4 111.281 7- 2- 6 109.801
31) 7- 2- 11 107.535 8- 3- 4 111.402 8- 3- 5 107.878
34) 8- 3- 16 101.153 9- 4- 12 107.533 10- 1- 6 111.871
37) 10- 1- 17 108.417 10- 1- 18 107.450 11- 2- 4 110.538
40) 11- 2- 6 107.865 11- 2- 7 107.535 12- 4- 9 107.533
43) 13- 5- 17 108.416 13- 5- 19 107.450 14- 6- 15 101.153
46) 15- 6- 14 101.153 16- 3- 4 110.879 16- 3- 5 113.086
49) 16- 3- 8 101.153 17- 1- 6 111.872 17- 1- 10 108.417
52) 17- 1- 18 104.380 17- 5- 13 108.416 17- 5- 19 104.376
55) 18- 1- 6 112.456 18- 1- 10 107.450 18- 1- 17 104.380
58) 19- 5- 13 107.450 19- 5- 17 104.376
Dihedrals
I J K L Theta I J K L Theta
1- 17- 5- 3 -75.412 1- 6- 2- 4 -72.529
1- 18- 19- 5 0.026 1- 6- 2- 7 50.087
1- 6- 2- 11 166.990 1- 17- 5- 13 160.752
1- 6- 15- 16 70.153 1- 17- 5- 19 46.446
2- 4- 3- 5 72.529 2- 4- 3- 8 -166.596
2- 6- 1- 10 -95.682 2- 4- 3- 16 -54.765
2- 6- 15- 16 -56.500 2- 6- 1- 17 26.187
2- 6- 1- 18 143.284 3- 4- 2- 6 0.011
3- 16- 15- 6 0.018 3- 4- 2- 7 -121.723
3- 4- 2- 11 118.857 3- 5- 19- 18 92.872
4- 3- 5- 13 95.653 4- 2- 6- 14 166.592
4- 2- 6- 15 54.760 4- 3- 16- 15 56.477
4- 3- 5- 17 -26.217 4- 3- 5- 19 -143.311
5- 17- 1- 6 75.432 5- 3- 4- 9 -166.988
5- 17- 1- 10 -160.737 5- 3- 4- 12 -50.086
5- 3- 16- 15 -70.178 5- 17- 1- 18 -46.428
6- 2- 4- 9 -118.838 6- 2- 4- 12 121.745
6- 1- 18- 19 -92.914 7- 2- 4- 9 119.428
7- 2- 4- 12 0.011 7- 2- 6- 14 -70.793
7- 2- 6- 15 177.376 8- 3- 4- 9 -46.112
8- 3- 4- 12 70.790 8- 3- 5- 13 -27.244
8- 3- 16- 15 174.724 8- 3- 5- 17 -149.115
8- 3- 5- 19 93.792 9- 4- 2- 11 0.009
9- 4- 3- 16 65.718 10- 1- 6- 14 27.219
10- 1- 6- 15 138.222 10- 1- 18- 19 143.551

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11- 2- 4- 12 -119.409 11- 2- 6- 14 46.110
11- 2- 6- 15 -65.721 12- 4- 3- 16 -177.380
13- 5- 3- 16 -138.248 13- 5- 19- 18 -143.590
14- 6- 15- 16 -174.749 14- 6- 1- 17 149.089
14- 6- 1- 18 -93.814 15- 6- 1- 17 -99.909
15- 6- 1- 18 17.188 16- 3- 5- 17 99.881
16- 3- 5- 19 -17.212 17- 5- 19- 18 -28.602
17- 1- 18- 19 28.560
```

Optimised structures for the transition state for primary ozonide 14a.formation at all levels reported.

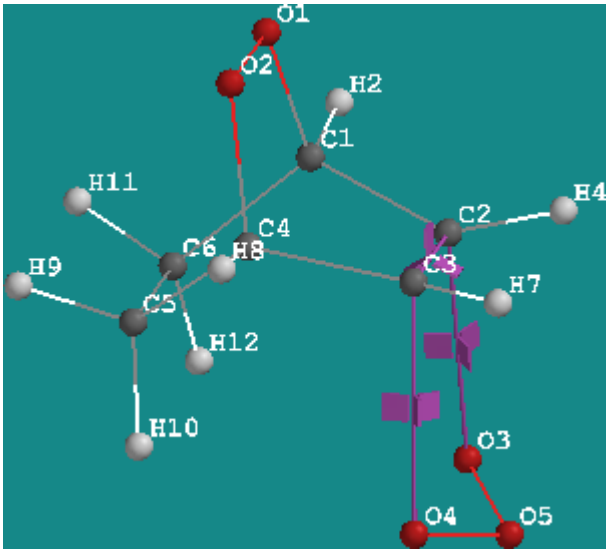

Figure S9: Optimised geometry for primary ozonide TS formation **14a**.

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5269 1- 7 1.0795 1- 11 1.4274 1- 13 1.5110
5) 2- 3 1.5269 2- 4 1.5463 2- 5 1.0804 2- 8 1.0831
9) 3- 9 1.0795 3- 12 1.4274 3- 14 1.5110 4- 6 1.0831
13) 4- 10 1.0804 11- 12 1.4122 13- 14 1.3622 13- 15 1.0716
17) 13- 17 2.2115 14- 16 1.0716 14- 18 2.2115 17- 19 1.2361
21) 18- 19 1.2361
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.838 1- 4- 10 110.505 1- 11- 12 111.532
4) 1- 13- 14 111.302 1- 13- 15 121.300 1- 13- 17 104.211
7) 2- 3- 9 112.739 2- 3- 12 107.663 2- 3- 14 112.477
10) 2- 4- 6 110.869 2- 4- 10 111.869 3- 2- 4 107.411
13) 3- 2- 5 110.504 3- 2- 8 107.840 3- 14- 16 121.300
16) 3- 14- 18 104.210 4- 1- 7 112.739 4- 1- 11 107.662
19) 4- 1- 13 112.479 4- 2- 3 107.411 4- 2- 5 111.869
22) 4- 2- 8 110.869 5- 2- 3 110.504 5- 2- 4 111.869
25) 5- 2- 8 108.281 6- 4- 10 108.281 7- 1- 4 112.739
28) 7- 1- 11 103.922 7- 1- 13 112.868 8- 2- 3 107.840
31) 8- 2- 4 110.869 8- 2- 5 108.281 9- 3- 12 103.922
34) 9- 3- 14 112.868 10- 4- 6 108.281 11- 1- 4 107.662
```

37) 11- 1- 7 103.922 11- 1- 13 106.450 12- 3- 9 103.922
40) 12- 3- 14 106.452 13- 1- 4 112.479 13- 1- 7 112.868
43) 13- 1- 11 106.450 13- 14- 16 123.649 13- 14- 18 99.145
46) 13- 17- 19 97.332 14- 3- 9 112.868 14- 3- 12 106.452
49) 14- 13- 15 123.649 14- 13- 17 99.142 14- 18- 19 97.331
52) 15- 13- 14 123.649 15- 13- 17 86.940 16- 14- 18 86.935
55) 17- 13- 14 99.142 17- 13- 15 86.940 18- 14- 16 86.935
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 0.008 1- 11- 12- 3 0.008
1- 13- 14- 3 0.005 1- 4- 2- 5 -121.419
1- 4- 2- 8 117.600 1- 13- 14- 16 -158.335
1- 13- 14- 18 109.252 1- 13- 17- 19 -143.964
2- 4- 1- 7 -173.803 2- 3- 12- 11 -62.409
2- 4- 1- 11 -59.771 2- 3- 14- 13 59.406
2- 4- 1- 13 57.190 2- 3- 14- 16 -141.668
2- 3- 14- 18 -46.538 3- 2- 4- 6 -117.581
3- 2- 4- 10 121.438 3- 14- 13- 15 158.343
3- 14- 13- 17 -109.241 3- 14- 18- 19 143.950
4- 2- 3- 9 173.792 4- 1- 11- 12 62.400
4- 2- 3- 12 59.761 4- 1- 13- 14 -59.412
4- 2- 3- 14 -57.201 4- 1- 13- 15 141.666
4- 1- 13- 17 46.530 5- 2- 4- 6 120.991
5- 2- 3- 9 -63.928 5- 2- 4- 10 0.010
5- 2- 3- 12 -177.960 5- 2- 3- 14 65.078
6- 4- 1- 7 -54.258 6- 4- 2- 8 0.010
6- 4- 1- 11 59.774 6- 4- 1- 13 176.735
7- 1- 4- 10 63.916 7- 1- 11- 12 -177.807
7- 1- 13- 14 171.648 7- 1- 13- 15 12.725
7- 1- 13- 17 -82.411 8- 2- 3- 9 54.246
8- 2- 4- 10 -120.970 8- 2- 3- 12 -59.785
8- 2- 3- 14 -176.747 9- 3- 12- 11 177.798
9- 3- 14- 13 -171.654 9- 3- 14- 16 -12.729
9- 3- 14- 18 82.402 10- 4- 1- 11 177.948
10- 4- 1- 13 -65.091 11- 1- 13- 14 58.269
11- 12- 3- 14 58.413 11- 1- 13- 15 -100.654
11- 1- 13- 17 164.210 12- 3- 14- 13 -58.274
12- 11- 1- 13 -58.424 12- 3- 14- 16 100.651
12- 3- 14- 18 -164.219 13- 17- 19- 18 60.865
13- 14- 18- 19 29.095 14- 18- 19- 17 -60.860
14- 13- 17- 19 -29.109 15- 13- 14- 16 0.003
15- 13- 14- 18 -92.410 15- 13- 17- 19 94.493
16- 14- 13- 17 92.419 16- 14- 18- 19 -94.507
17- 13- 14- 18 0.006

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5260 1- 7 1.0791 1- 11 1.4346 1- 13 1.5099
5) 2- 3 1.5260 2- 4 1.5455 2- 5 1.0802 2- 8 1.0829
9) 3- 9 1.0791 3- 12 1.4346 3- 14 1.5099 4- 6 1.0829
13) 4- 10 1.0802 11- 12 1.4131 13- 14 1.3624 13- 15 1.0714
17) 13- 17 2.2180 14- 16 1.0714 14- 18 2.2180 17- 19 1.2364
21) 18- 19 1.2364
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.916 1- 4- 10 110.368 1- 11- 12 111.469
4) 1- 13- 14 111.377 1- 13- 15 121.272 1- 13- 17 104.273

7) 2- 3- 9 112.820 2- 3- 12 107.540 2- 3- 14 112.622
10) 2- 4- 6 110.947 2- 4- 10 111.901 3- 2- 4 107.499
13) 3- 2- 5 110.368 3- 2- 8 107.916 3- 14- 16 121.272
16) 3- 14- 18 104.273 4- 1- 7 112.820 4- 1- 11 107.540
19) 4- 1- 13 112.622 4- 2- 3 107.499 4- 2- 5 111.901
22) 4- 2- 8 110.947 5- 2- 3 110.368 5- 2- 4 111.901
25) 5- 2- 8 108.145 6- 4- 10 108.145 7- 1- 4 112.820
28) 7- 1- 11 103.783 7- 1- 13 112.979 8- 2- 3 107.916
31) 8- 2- 4 110.947 8- 2- 5 108.145 9- 3- 12 103.783
34) 9- 3- 14 112.979 10- 4- 6 108.145 11- 1- 4 107.540
37) 11- 1- 7 103.783 11- 1- 13 106.320 12- 3- 9 103.783
40) 12- 3- 14 106.320 13- 1- 4 112.622 13- 1- 7 112.979
43) 13- 1- 11 106.320 13- 14- 16 123.657 13- 14- 18 99.122
46) 13- 17- 19 97.259 14- 3- 9 112.979 14- 3- 12 106.320
49) 14- 13- 15 123.657 14- 13- 17 99.122 14- 18- 19 97.259
52) 15- 13- 14 123.657 15- 13- 17 86.759 16- 14- 18 86.758
55) 17- 13- 14 99.122 17- 13- 15 86.759 18- 14- 16 86.758
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 0.000 1- 11- 12- 3 0.000
1- 13- 14- 3 0.000 1- 4- 2- 5 -121.336
1- 4- 2- 8 117.780 1- 13- 14- 16 -158.486
1- 13- 14- 18 109.330 1- 13- 17- 19 -144.093
2- 4- 1- 7 -173.694 2- 3- 12- 11 -62.409
2- 4- 1- 11 -59.861 2- 3- 14- 13 59.141
2- 4- 1- 13 56.946 2- 3- 14- 16 -141.784
2- 3- 14- 18 -46.837 3- 2- 4- 6 -117.779
3- 2- 4- 10 121.337 3- 14- 13- 15 158.486
3- 14- 13- 17 -109.329 3- 14- 18- 19 144.092
4- 2- 3- 9 173.693 4- 1- 11- 12 62.408
4- 2- 3- 12 59.860 4- 1- 13- 14 -59.141
4- 2- 3- 14 -56.947 4- 1- 13- 15 141.784
4- 1- 13- 17 46.836 5- 2- 4- 6 120.885
5- 2- 3- 9 -64.014 5- 2- 4- 10 0.001
5- 2- 3- 12 -177.848 5- 2- 3- 14 65.346
6- 4- 1- 7 -53.966 6- 4- 2- 8 0.001
6- 4- 1- 11 59.868 6- 4- 1- 13 176.674
7- 1- 4- 10 64.014 7- 1- 11- 12 -177.833
7- 1- 13- 14 171.581 7- 1- 13- 15 12.505
7- 1- 13- 17 -82.442 8- 2- 3- 9 53.965
8- 2- 4- 10 -120.883 8- 2- 3- 12 -59.868
8- 2- 3- 14 -176.675 9- 3- 12- 11 177.832
9- 3- 14- 13 -171.581 9- 3- 14- 16 -12.506
9- 3- 14- 18 82.442 10- 4- 1- 11 177.847
10- 4- 1- 13 -65.346 11- 1- 13- 14 58.389
11- 12- 3- 14 58.448 11- 1- 13- 15 -100.686
11- 1- 13- 17 164.366 12- 3- 14- 13 -58.390
12- 11- 1- 13 -58.448 12- 3- 14- 16 100.686
12- 3- 14- 18 -164.367 13- 17- 19- 18 61.029
13- 14- 18- 19 29.145 14- 18- 19- 17 -61.029
14- 13- 17- 19 -29.146 15- 13- 14- 16 0.000
15- 13- 14- 18 -92.184 15- 13- 17- 19 94.435
16- 14- 13- 17 92.184 16- 14- 18- 19 -94.436
17- 13- 14- 18 0.000

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5227 1- 7 1.0947 1- 11 1.4545 1- 13 1.5034
5) 2- 3 1.5225 2- 4 1.5430 2- 5 1.0925 2- 8 1.0936

9) 3- 9 1.0946 3- 12 1.4543 3- 14 1.5036 4- 6 1.0936
13) 4- 10 1.0925 11- 12 1.5045 13- 14 1.3969 13- 15 1.0866
17) 13- 17 2.0128 14- 16 1.0869 14- 18 2.0123 17- 19 1.3272
21) 18- 19 1.3273
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.753 1- 4- 10 109.751 1- 11- 12 109.648
4) 1- 13- 14 111.130 1- 13- 15 119.940 1- 13- 17 103.473
7) 2- 3- 9 112.641 2- 3- 12 108.838 2- 3- 14 112.711
10) 2- 4- 6 111.168 2- 4- 10 111.648 3- 2- 4 107.951
13) 3- 2- 5 109.815 3- 2- 8 107.682 3- 14- 16 119.935
16) 3- 14- 18 103.368 4- 1- 7 112.625 4- 1- 11 108.843
19) 4- 1- 13 112.683 4- 2- 3 107.951 4- 2- 5 111.653
22) 4- 2- 8 111.198 5- 2- 3 109.815 5- 2- 4 111.653
25) 5- 2- 8 108.462 6- 4- 10 108.474 7- 1- 4 112.625
28) 7- 1- 11 102.333 7- 1- 13 113.045 8- 2- 3 107.682
31) 8- 2- 4 111.198 8- 2- 5 108.462 9- 3- 12 102.337
34) 9- 3- 14 113.013 10- 4- 6 108.474 11- 1- 4 108.843
37) 11- 1- 7 102.333 11- 1- 13 106.514 12- 3- 9 102.337
40) 12- 3- 14 106.499 13- 1- 4 112.683 13- 1- 7 113.045
43) 13- 1- 11 106.514 13- 14- 16 121.842 13- 14- 18 100.896
46) 13- 17- 19 97.004 14- 3- 9 113.013 14- 3- 12 106.499
49) 14- 13- 15 121.869 14- 13- 17 101.071 14- 18- 19 96.918
52) 15- 13- 14 121.869 15- 13- 17 92.671 16- 14- 18 92.902
55) 17- 13- 14 101.071 17- 13- 15 92.671 18- 14- 16 92.902
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.472 1- 11- 12- 3 -0.435
1- 13- 14- 3 -0.445 1- 4- 2- 5 -121.269
1- 4- 2- 8 117.438 1- 13- 14- 16 -150.970
1- 13- 14- 18 108.646 1- 13- 17- 19 -145.129
2- 4- 1- 7 -173.501 2- 3- 12- 11 -61.881
2- 4- 1- 11 -60.750 2- 3- 14- 13 58.913
2- 4- 1- 13 57.165 2- 3- 14- 16 -149.926
2- 3- 14- 18 -48.570 3- 2- 4- 6 -118.463
3- 2- 4- 10 120.254 3- 14- 13- 15 150.051
3- 14- 13- 17 -109.722 3- 14- 18- 19 146.383
4- 2- 3- 9 174.132 4- 1- 11- 12 62.350
4- 2- 3- 12 61.370 4- 1- 13- 14 -58.390
4- 2- 3- 14 -56.540 4- 1- 13- 15 150.469
4- 1- 13- 17 49.325 5- 2- 4- 6 120.741
5- 2- 3- 9 -63.930 5- 2- 4- 10 -0.543
5- 2- 3- 12 -176.692 5- 2- 3- 14 65.398
6- 4- 1- 7 -53.340 6- 4- 2- 8 -0.553
6- 4- 1- 11 59.411 6- 4- 1- 13 177.326
7- 1- 4- 10 64.594 7- 1- 11- 12 -178.264
7- 1- 13- 14 172.493 7- 1- 13- 15 21.352
7- 1- 13- 17 -79.792 8- 2- 3- 9 53.986
8- 2- 4- 10 -121.836 8- 2- 3- 12 -58.776
8- 2- 3- 14 -176.687 9- 3- 12- 11 178.715
9- 3- 14- 13 -171.952 9- 3- 14- 16 -20.790
9- 3- 14- 18 80.565 10- 4- 1- 11 177.345
10- 4- 1- 13 -64.740 11- 1- 13- 14 60.887
11- 12- 3- 14 59.889 11- 1- 13- 15 -90.254
11- 1- 13- 17 168.602 12- 3- 14- 13 -60.365
12- 11- 1- 13 -59.398 12- 3- 14- 16 90.797
12- 3- 14- 18 -167.848 13- 17- 19- 18 59.574
13- 14- 18- 19 31.304 14- 18- 19- 17 -59.991
14- 13- 17- 19 -30.004 15- 13- 14- 16 -0.475
15- 13- 14- 18 -100.858 15- 13- 17- 19 93.206
16- 14- 13- 17 99.753 16- 14- 18- 19 -91.907
17- 13- 14- 18 -0.631

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5239 1- 7 1.0935 1- 11 1.4468 1- 13 1.5059
5) 2- 3 1.5239 2- 4 1.5450 2- 5 1.0913 2- 8 1.0930
9) 3- 9 1.0935 3- 12 1.4468 3- 14 1.5059 4- 6 1.0930
13) 4- 10 1.0913 11- 12 1.4854 13- 14 1.4004 13- 15 1.0863
17) 13- 17 1.9930 14- 16 1.0863 14- 18 1.9930 17- 19 1.3088
21) 18- 19 1.3088
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.575 1- 4- 10 110.034 1- 11- 12 110.043
4) 1- 13- 14 110.948 1- 13- 15 120.133 1- 13- 17 103.840
7) 2- 3- 9 112.697 2- 3- 12 108.790 2- 3- 14 112.471
10) 2- 4- 6 110.992 2- 4- 10 111.854 3- 2- 4 107.808
13) 3- 2- 5 110.034 3- 2- 8 107.575 3- 14- 16 120.132
16) 3- 14- 18 103.840 4- 1- 7 112.697 4- 1- 11 108.789
19) 4- 1- 13 112.471 4- 2- 3 107.808 4- 2- 5 111.854
22) 4- 2- 8 110.992 5- 2- 3 110.034 5- 2- 4 111.854
25) 5- 2- 8 108.491 6- 4- 10 108.491 7- 1- 4 112.697
28) 7- 1- 11 102.410 7- 1- 13 112.956 8- 2- 3 107.575
31) 8- 2- 4 110.992 8- 2- 5 108.491 9- 3- 12 102.410
34) 9- 3- 14 112.956 10- 4- 6 108.491 11- 1- 4 108.789
37) 11- 1- 7 102.410 11- 1- 13 106.764 12- 3- 9 102.410
40) 12- 3- 14 106.763 13- 1- 4 112.471 13- 1- 7 112.956
43) 13- 1- 11 106.764 13- 14- 16 121.722 13- 14- 18 100.680
46) 13- 17- 19 97.269 14- 3- 9 112.956 14- 3- 12 106.763
49) 14- 13- 15 121.722 14- 13- 17 100.680 14- 18- 19 97.269
52) 15- 13- 14 121.722 15- 13- 17 92.952 16- 14- 18 92.953
55) 17- 13- 14 100.680 17- 13- 15 92.952 18- 14- 16 92.953
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.003
1- 13- 14- 3 -0.000 1- 4- 2- 5 -121.098
1- 4- 2- 8 117.577 1- 13- 14- 16 -150.293
1- 13- 14- 18 109.442 1- 13- 17- 19 -145.323
2- 4- 1- 7 -173.543 2- 3- 12- 11 -62.094
2- 4- 1- 11 -60.692 2- 3- 14- 13 59.155
2- 4- 1- 13 57.370 2- 3- 14- 16 -150.015
2- 3- 14- 18 -48.224 3- 2- 4- 6 -117.577
3- 2- 4- 10 121.098 3- 14- 13- 15 150.294
3- 14- 13- 17 -109.442 3- 14- 18- 19 145.323
4- 2- 3- 9 173.544 4- 1- 11- 12 62.099
4- 2- 3- 12 60.692 4- 1- 13- 14 -59.155
4- 2- 3- 14 -57.369 4- 1- 13- 15 150.013
4- 1- 13- 17 48.223 5- 2- 4- 6 121.325
5- 2- 3- 9 -64.229 5- 2- 4- 10 -0.000
5- 2- 3- 12 -177.081 5- 2- 3- 14 64.858
6- 4- 1- 7 -53.780 6- 4- 2- 8 0.000
6- 4- 1- 11 59.072 6- 4- 1- 13 177.134
7- 1- 4- 10 64.229 7- 1- 11- 12 -178.417
7- 1- 13- 14 171.892 7- 1- 13- 15 21.061
7- 1- 13- 17 -80.729 8- 2- 3- 9 53.780
8- 2- 4- 10 -121.325 8- 2- 3- 12 -59.072
8- 2- 3- 14 -177.133 9- 3- 12- 11 178.421
9- 3- 14- 13 -171.893 9- 3- 14- 16 -21.063
9- 3- 14- 18 80.728 10- 4- 1- 11 177.081
10- 4- 1- 13 -64.858 11- 1- 13- 14 60.094
11- 12- 3- 14 59.515 11- 1- 13- 15 -90.737
11- 1- 13- 17 167.473 12- 3- 14- 13 -60.095

12- 11- 1- 13 -59.511 12- 3- 14- 16 90.735
12- 3- 14- 18 -167.474 13- 17- 19- 18 59.670
13- 14- 18- 19 30.415 14- 18- 19- 17 -59.670
14- 13- 17- 19 -30.415 15- 13- 14- 16 0.001
15- 13- 14- 18 -100.265 15- 13- 17- 19 92.644
16- 14- 13- 17 100.266 16- 14- 18- 19 -92.644
17- 13- 14- 18 -0.000

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5362 1- 7 1.0928 1- 11 1.4536 1- 13 1.5079
5) 2- 3 1.5362 2- 4 1.5515 2- 5 1.0929 2- 8 1.0942
9) 3- 9 1.0928 3- 12 1.4536 3- 14 1.5079 4- 6 1.0942
13) 4- 10 1.0929 11- 12 1.4814 13- 14 1.3597 13- 15 1.0842
17) 13- 17 2.5224 14- 16 1.0842 14- 18 2.5224 17- 19 1.2822
21) 18- 19 1.2822
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.007 1- 4- 10 109.869 1- 11- 12 110.189
4) 1- 13- 14 111.906 1- 13- 15 122.222 1- 13- 17 103.598
7) 2- 3- 9 112.791 2- 3- 12 108.291 2- 3- 14 111.804
10) 2- 4- 6 111.106 2- 4- 10 111.614 3- 2- 4 107.681
13) 3- 2- 5 109.867 3- 2- 8 108.012 3- 14- 16 122.224
16) 3- 14- 18 103.594 4- 1- 7 112.791 4- 1- 11 108.290
19) 4- 1- 13 111.810 4- 2- 3 107.681 4- 2- 5 111.612
22) 4- 2- 8 111.107 5- 2- 3 109.867 5- 2- 4 111.612
25) 5- 2- 8 108.495 6- 4- 10 108.495 7- 1- 4 112.791
28) 7- 1- 11 102.882 7- 1- 13 113.454 8- 2- 3 108.012
31) 8- 2- 4 111.107 8- 2- 5 108.495 9- 3- 12 102.881
34) 9- 3- 14 113.455 10- 4- 6 108.495 11- 1- 4 108.290
37) 11- 1- 7 102.882 11- 1- 13 106.918 12- 3- 9 102.881
40) 12- 3- 14 106.923 13- 1- 4 111.810 13- 1- 7 113.454
43) 13- 1- 11 106.918 13- 14- 16 124.580 13- 14- 18 99.193
46) 13- 17- 19 95.932 14- 3- 9 113.455 14- 3- 12 106.923
49) 14- 13- 15 124.580 14- 13- 17 99.190 14- 18- 19 95.933
52) 15- 13- 14 124.580 15- 13- 17 79.903 16- 14- 18 79.898
55) 17- 13- 14 99.190 17- 13- 15 79.903 18- 14- 16 79.898
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 0.028 1- 11- 12- 3 0.026
1- 13- 14- 3 0.016 1- 4- 2- 5 -120.633
1- 4- 2- 8 118.123 1- 13- 14- 16 -167.203
1- 13- 14- 18 108.782 1- 13- 17- 19 -144.093
2- 4- 1- 7 -174.057 2- 3- 12- 11 -62.472
2- 4- 1- 11 -60.881 2- 3- 14- 13 59.096
2- 4- 1- 13 56.660 2- 3- 14- 16 -133.338
2- 3- 14- 18 -46.829 3- 2- 4- 6 -118.062
3- 2- 4- 10 120.694 3- 14- 13- 15 167.226
3- 14- 13- 17 -108.753 3- 14- 18- 19 144.060
4- 2- 3- 9 174.021 4- 1- 11- 12 62.443
4- 2- 3- 12 60.844 4- 1- 13- 14 -59.110
4- 2- 3- 14 -56.700 4- 1- 13- 15 133.332
4- 1- 13- 17 46.815 5- 2- 4- 6 121.277
5- 2- 3- 9 -64.227 5- 2- 4- 10 0.033
5- 2- 3- 12 -177.404 5- 2- 3- 14 65.051
6- 4- 1- 7 -53.988 6- 4- 2- 8 0.034
6- 4- 1- 11 59.189 6- 4- 1- 13 176.730
7- 1- 4- 10 64.186 7- 1- 11- 12 -177.946
7- 1- 13- 14 171.956 7- 1- 13- 15 4.398

7- 1- 13- 17 -82.119 8- 2- 3- 9 53.949
8- 2- 4- 10 -121.210 8- 2- 3- 12 -59.228
8- 2- 3- 14 -176.772 9- 3- 12- 11 177.916
9- 3- 14- 13 -171.974 9- 3- 14- 16 -4.408
9- 3- 14- 18 82.101 10- 4- 1- 11 177.363
10- 4- 1- 13 -65.096 11- 1- 13- 14 59.252
11- 12- 3- 14 58.157 11- 1- 13- 15 -108.306
11- 1- 13- 17 165.177 12- 3- 14- 13 -59.267
12- 11- 1- 13 -58.190 12- 3- 14- 16 108.300
12- 3- 14- 18 -165.192 13- 17- 19- 18 62.385
13- 14- 18- 19 28.723 14- 18- 19- 17 -62.377
14- 13- 17- 19 -28.754 15- 13- 14- 16 0.007
15- 13- 14- 18 -84.008 15- 13- 17- 19 94.968
16- 14- 13- 17 84.028 16- 14- 18- 19 -94.999
17- 13- 14- 18 0.012

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5345 1- 7 1.0923 1- 11 1.4625 1- 13 1.5067
5) 2- 3 1.5346 2- 4 1.5506 2- 5 1.0927 2- 8 1.0940
9) 3- 9 1.0923 3- 12 1.4625 3- 14 1.5065 4- 6 1.0941
13) 4- 10 1.0928 11- 12 1.4832 13- 14 1.3609 13- 15 1.0837
17) 13- 17 2.5196 14- 16 1.0837 14- 18 2.5168 17- 19 1.2833
21) 18- 19 1.2836
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.066 1- 4- 10 109.731 1- 11- 12 110.089
4) 1- 13- 14 111.968 1- 13- 15 122.127 1- 13- 17 103.959
7) 2- 3- 9 112.873 2- 3- 12 108.164 2- 3- 14 111.999
10) 2- 4- 6 111.202 2- 4- 10 111.697 3- 2- 4 107.786
13) 3- 2- 5 109.695 3- 2- 8 108.115 3- 14- 16 122.137
16) 3- 14- 18 103.891 4- 1- 7 112.872 4- 1- 11 108.151
19) 4- 1- 13 112.052 4- 2- 3 107.786 4- 2- 5 111.688
22) 4- 2- 8 111.198 5- 2- 3 109.695 5- 2- 4 111.688
25) 5- 2- 8 108.294 6- 4- 10 108.289 7- 1- 4 112.872
28) 7- 1- 11 102.731 7- 1- 13 113.537 8- 2- 3 108.115
31) 8- 2- 4 111.198 8- 2- 5 108.294 9- 3- 12 102.741
34) 9- 3- 14 113.540 10- 4- 6 108.289 11- 1- 4 108.151
37) 11- 1- 7 102.731 11- 1- 13 106.730 12- 3- 9 102.741
40) 12- 3- 14 106.767 13- 1- 4 112.052 13- 1- 7 113.537
43) 13- 1- 11 106.730 13- 14- 16 124.538 13- 14- 18 99.346
46) 13- 17- 19 95.728 14- 3- 9 113.540 14- 3- 12 106.767
49) 14- 13- 15 124.533 14- 13- 17 99.048 14- 18- 19 95.763
52) 15- 13- 14 124.533 15- 13- 17 80.016 16- 14- 18 79.727
55) 17- 13- 14 99.048 17- 13- 15 80.016 18- 14- 16 79.727
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 0.263 1- 11- 12- 3 0.241
1- 13- 14- 3 0.176 1- 4- 2- 5 -120.299
1- 4- 2- 8 118.599 1- 13- 14- 16 -166.724
1- 13- 14- 18 109.369 1- 13- 17- 19 -144.683
2- 4- 1- 7 -174.115 2- 3- 12- 11 -62.597
2- 4- 1- 11 -61.161 2- 3- 14- 13 58.678
2- 4- 1- 13 56.204 2- 3- 14- 16 -134.061
2- 3- 14- 18 -47.592 3- 2- 4- 6 -118.018
3- 2- 4- 10 120.877 3- 14- 13- 15 166.994
3- 14- 13- 17 -108.949 3- 14- 18- 19 144.153

```
4- 2- 3- 9 173.795 4- 1- 11- 12 62.329
4- 2- 3- 12 60.821 4- 1- 13- 14 -58.853
4- 2- 3- 14 -56.566 4- 1- 13- 15 133.963
4- 1- 13- 17 47.108 5- 2- 4- 6 121.421
5- 2- 3- 9 -64.399 5- 2- 4- 10 0.315
5- 2- 3- 12 -177.373 5- 2- 3- 14 65.240
6- 4- 1- 7 -53.839 6- 4- 2- 8 0.318
6- 4- 1- 11 59.116 6- 4- 1- 13 176.480
7- 1- 4- 10 64.044 7- 1- 11- 12 -178.106
7- 1- 13- 14 171.811 7- 1- 13- 15 4.627
7- 1- 13- 17 -82.227 8- 2- 3- 9 53.498
8- 2- 4- 10 -120.787 8- 2- 3- 12 -59.477
8- 2- 3- 14 -176.863 9- 3- 12- 11 177.826
9- 3- 14- 13 -172.031 9- 3- 14- 16 -4.769
9- 3- 14- 18 81.700 10- 4- 1- 11 176.999
10- 4- 1- 13 -65.637 11- 1- 13- 14 59.358
11- 12- 3- 14 58.105 11- 1- 13- 15 -107.826
11- 1- 13- 17 165.320 12- 3- 14- 13 -59.542
12- 11- 1- 13 -58.410 12- 3- 14- 16 107.719
12- 3- 14- 18 -165.812 13- 17- 19- 18 62.852
13- 14- 18- 19 28.604 14- 18- 19- 17 -62.698
14- 13- 17- 19 -29.221 15- 13- 14- 16 0.095
15- 13- 14- 18 -83.812 15- 13- 17- 19 94.477
16- 14- 13- 17 84.152 16- 14- 18- 19 -95.045
17- 13- 14- 18 0.245
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Optimised structures for the transition state for primary ozonide 14b.formation at all levels reported.

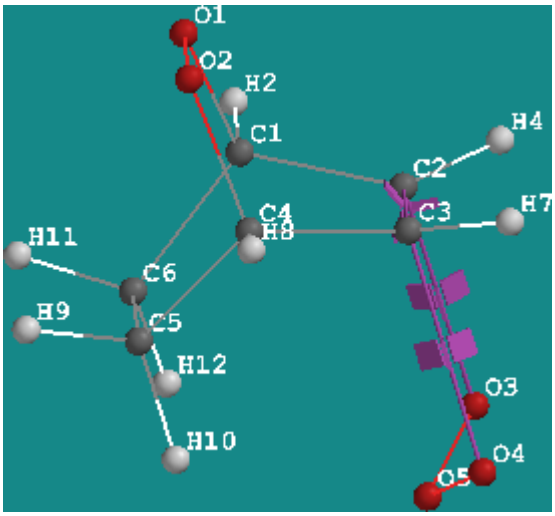

Figure S10: Optimised geometry for primary ozonide TS formation **14b**.

HF/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5273 1- 7 1.0793 1- 11 1.4274 1- 13 1.5114
5) 2- 3 1.5273 2- 4 1.5477 2- 5 1.0817 2- 8 1.0828
9) 3- 9 1.0793 3- 12 1.4274 3- 14 1.5114 4- 6 1.0828
13) 4- 10 1.0817 11- 12 1.4122 13- 14 1.3633 13- 15 1.0708
17) 13- 17 2.2064 14- 16 1.0708 14- 18 2.2064 17- 19 1.2370
21) 18- 19 1.2370
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.896 1- 4- 10 110.602 1- 11- 12 111.562
4) 1- 13- 14 111.301 1- 13- 15 121.398 1- 13- 17 107.986
7) 2- 3- 9 112.650 2- 3- 12 107.459 2- 3- 14 112.560
10) 2- 4- 6 110.762 2- 4- 10 112.285 3- 2- 4 107.404
13) 3- 2- 5 110.602 3- 2- 8 107.896 3- 14- 16 121.398
16) 3- 14- 18 107.986 4- 1- 7 112.650 4- 1- 11 107.459
19) 4- 1- 13 112.560 4- 2- 3 107.404 4- 2- 5 112.285
22) 4- 2- 8 110.762 5- 2- 3 110.602 5- 2- 4 112.285
25) 5- 2- 8 107.821 6- 4- 10 107.821 7- 1- 4 112.650
28) 7- 1- 11 103.984 7- 1- 13 112.916 8- 2- 3 107.896
31) 8- 2- 4 110.762 8- 2- 5 107.821 9- 3- 12 103.984
34) 9- 3- 14 112.916 10- 4- 6 107.821 11- 1- 4 107.459
37) 11- 1- 7 103.984 11- 1- 13 106.545 12- 3- 9 103.984
40) 12- 3- 14 106.545 13- 1- 4 112.560 13- 1- 7 112.916
43) 13- 1- 11 106.545 13- 14- 16 123.337 13- 14- 18 99.160
46) 13- 17- 19 99.182 14- 3- 9 112.916 14- 3- 12 106.545
49) 14- 13- 15 123.337 14- 13- 17 99.160 14- 18- 19 99.182
52) 15- 13- 14 123.337 15- 13- 17 83.922 16- 14- 18 83.922
55) 17- 13- 14 99.160 17- 13- 15 83.922 18- 14- 16 83.922
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 14- 3 -0.000 1- 4- 2- 5 -121.802
1- 4- 2- 8 117.596 1- 13- 14- 16 -157.789
1- 13- 14- 18 113.489 1- 13- 17- 19 -88.038
2- 4- 1- 7 -173.783 2- 3- 12- 11 -62.520
2- 4- 1- 11 -59.846 2- 3- 14- 13 59.361
2- 4- 1- 13 57.149 2- 3- 14- 16 -142.354
2- 3- 14- 18 -48.470 3- 2- 4- 6 -117.596
3- 2- 4- 10 121.802 3- 14- 13- 15 157.789
3- 14- 13- 17 -113.489 3- 14- 18- 19 88.038
4- 2- 3- 9 173.783 4- 1- 11- 12 62.520
4- 2- 3- 12 59.846 4- 1- 13- 14 -59.361
4- 2- 3- 14 -57.149 4- 1- 13- 15 142.354
4- 1- 13- 17 48.470 5- 2- 4- 6 120.602
5- 2- 3- 9 -63.370 5- 2- 4- 10 -0.000
5- 2- 3- 12 -177.307 5- 2- 3- 14 65.698
6- 4- 1- 7 -54.337 6- 4- 2- 8 -0.000
6- 4- 1- 11 59.600 6- 4- 1- 13 176.595
7- 1- 4- 10 63.370 7- 1- 11- 12 -177.853
7- 1- 13- 14 171.709 7- 1- 13- 15 13.425
7- 1- 13- 17 -80.459 8- 2- 3- 9 54.337
8- 2- 4- 10 -120.602 8- 2- 3- 12 -59.600
8- 2- 3- 14 -176.595 9- 3- 12- 11 177.853
9- 3- 14- 13 -171.709 9- 3- 14- 16 -13.425
9- 3- 14- 18 80.459 10- 4- 1- 11 177.307
10- 4- 1- 13 -65.698 11- 1- 13- 14 58.176
11- 12- 3- 14 58.341 11- 1- 13- 15 -100.109
11- 1- 13- 17 166.007 12- 3- 14- 13 -58.176

12- 11- 1- 13 -58.341 12- 3- 14- 16 100.109
12- 3- 14- 18 -166.007 13- 17- 19- 18 -57.429
13- 14- 18- 19 -28.015 14- 18- 19- 17 57.429
14- 13- 17- 19 28.015 15- 13- 14- 16 -0.000
15- 13- 14- 18 -88.722 15- 13- 17- 19 150.879
16- 14- 13- 17 88.722 16- 14- 18- 19 -150.879
17- 13- 14- 18 -0.000

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5261 1- 7 1.0788 1- 11 1.4355 1- 13 1.5104
5) 2- 3 1.5261 2- 4 1.5466 2- 5 1.0813 2- 8 1.0825
9) 3- 9 1.0788 3- 12 1.4355 3- 14 1.5104 4- 6 1.0825
13) 4- 10 1.0813 11- 12 1.4131 13- 14 1.3635 13- 15 1.0706
17) 13- 17 2.2126 14- 16 1.0706 14- 18 2.2126 17- 19 1.2374
21) 18- 19 1.2374
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.922 1- 4- 10 110.462 1- 11- 12 111.488
4) 1- 13- 14 111.380 1- 13- 15 121.382 1- 13- 17 107.874
7) 2- 3- 9 112.774 2- 3- 12 107.377 2- 3- 14 112.762
10) 2- 4- 6 110.855 2- 4- 10 112.324 3- 2- 4 107.505
13) 3- 2- 5 110.462 3- 2- 8 107.922 3- 14- 16 121.382
16) 3- 14- 18 107.874 4- 1- 7 112.774 4- 1- 11 107.377
19) 4- 1- 13 112.762 4- 2- 3 107.505 4- 2- 5 112.324
22) 4- 2- 8 110.855 5- 2- 3 110.462 5- 2- 4 112.324
25) 5- 2- 8 107.701 6- 4- 10 107.701 7- 1- 4 112.774
28) 7- 1- 11 103.836 7- 1- 13 112.987 8- 2- 3 107.922
31) 8- 2- 4 110.855 8- 2- 5 107.701 9- 3- 12 103.836
34) 9- 3- 14 112.987 10- 4- 6 107.701 11- 1- 4 107.377
37) 11- 1- 7 103.836 11- 1- 13 106.310 12- 3- 9 103.836
40) 12- 3- 14 106.310 13- 1- 4 112.762 13- 1- 7 112.987
43) 13- 1- 11 106.310 13- 14- 16 123.340 13- 14- 18 99.134
46) 13- 17- 19 99.154 14- 3- 9 112.987 14- 3- 12 106.310
49) 14- 13- 15 123.340 14- 13- 17 99.134 14- 18- 19 99.154
52) 15- 13- 14 123.340 15- 13- 17 83.885 16- 14- 18 83.885
55) 17- 13- 14 99.134 17- 13- 15 83.885 18- 14- 16 83.885
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 14- 3 -0.000 1- 4- 2- 5 -121.720
1- 4- 2- 8 117.739 1- 13- 14- 16 -157.963
1- 13- 14- 18 113.377 1- 13- 17- 19 -88.012
2- 4- 1- 7 -173.698 2- 3- 12- 11 -62.490
2- 4- 1- 11 -59.924 2- 3- 14- 13 59.032
2- 4- 1- 13 56.847 2- 3- 14- 16 -142.509
2- 3- 14- 18 -48.748 3- 2- 4- 6 -117.739
3- 2- 4- 10 121.720 3- 14- 13- 15 157.963
3- 14- 13- 17 -113.377 3- 14- 18- 19 88.012
4- 2- 3- 9 173.698 4- 1- 11- 12 62.490
4- 2- 3- 12 59.924 4- 1- 13- 14 -59.032
4- 2- 3- 14 -56.847 4- 1- 13- 15 142.509
4- 1- 13- 17 48.748 5- 2- 4- 6 120.541
5- 2- 3- 9 -63.428 5- 2- 4- 10 -0.000
5- 2- 3- 12 -177.202 5- 2- 3- 14 66.027
6- 4- 1- 7 -54.072 6- 4- 2- 8 -0.000
6- 4- 1- 11 59.702 6- 4- 1- 13 176.473

7- 1- 4- 10 63.428 7- 1- 11- 12 -177.854
7- 1- 13- 14 171.624 7- 1- 13- 15 13.164
7- 1- 13- 17 -80.597 8- 2- 3- 9 54.072
8- 2- 4- 10 -120.541 8- 2- 3- 12 -59.702
8- 2- 3- 14 -176.473 9- 3- 12- 11 177.854
9- 3- 14- 13 -171.624 9- 3- 14- 16 -13.164
9- 3- 14- 18 80.597 10- 4- 1- 11 177.202
10- 4- 1- 13 -66.027 11- 1- 13- 14 58.371
11- 12- 3- 14 58.440 11- 1- 13- 15 -100.088
11- 1- 13- 17 166.151 12- 3- 14- 13 -58.371
12- 11- 1- 13 -58.440 12- 3- 14- 16 100.088
12- 3- 14- 18 -166.151 13- 17- 19- 18 -57.566
13- 14- 18- 19 -28.079 14- 18- 19- 17 57.566
14- 13- 17- 19 28.079 15- 13- 14- 16 -0.000
15- 13- 14- 18 -88.660 15- 13- 17- 19 150.941
16- 14- 13- 17 88.660 16- 14- 18- 19 -150.941
17- 13- 14- 18 -0.000

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5232 1- 7 1.0942 1- 11 1.4564 1- 13 1.5028
5) 2- 3 1.5232 2- 4 1.5437 2- 5 1.0933 2- 8 1.0935
9) 3- 9 1.0942 3- 12 1.4564 3- 14 1.5028 4- 6 1.0935
13) 4- 10 1.0933 11- 12 1.5057 13- 14 1.3958 13- 15 1.0866
17) 13- 17 2.0191 14- 16 1.0866 14- 18 2.0191 17- 19 1.3279
21) 18- 19 1.3279
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.477 1- 4- 10 110.051 1- 11- 12 109.627
4) 1- 13- 14 111.229 1- 13- 15 120.069 1- 13- 17 107.037
7) 2- 3- 9 112.545 2- 3- 12 108.421 2- 3- 14 113.152
10) 2- 4- 6 111.098 2- 4- 10 112.145 3- 2- 4 107.981
13) 3- 2- 5 110.051 3- 2- 8 107.477 3- 14- 16 120.069
16) 3- 14- 18 107.037 4- 1- 7 112.545 4- 1- 11 108.421
19) 4- 1- 13 113.152 4- 2- 3 107.981 4- 2- 5 112.145
22) 4- 2- 8 111.098 5- 2- 3 110.051 5- 2- 4 112.145
25) 5- 2- 8 107.992 6- 4- 10 107.992 7- 1- 4 112.545
28) 7- 1- 11 102.409 7- 1- 13 113.070 8- 2- 3 107.477
31) 8- 2- 4 111.098 8- 2- 5 107.992 9- 3- 12 102.409
34) 9- 3- 14 113.070 10- 4- 6 107.992 11- 1- 4 108.421
37) 11- 1- 7 102.409 11- 1- 13 106.364 12- 3- 9 102.409
40) 12- 3- 14 106.364 13- 1- 4 113.152 13- 1- 7 113.070
43) 13- 1- 11 106.364 13- 14- 16 121.682 13- 14- 18 100.999
46) 13- 17- 19 98.105 14- 3- 9 113.070 14- 3- 12 106.364
49) 14- 13- 15 121.682 14- 13- 17 100.999 14- 18- 19 98.105
52) 15- 13- 14 121.682 15- 13- 17 89.318 16- 14- 18 89.318
55) 17- 13- 14 100.999 17- 13- 15 89.318 18- 14- 16 89.318
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 14- 3 -0.000 1- 4- 2- 5 -121.416
1- 4- 2- 8 117.623 1- 13- 14- 16 -150.622
1- 13- 14- 18 113.310 1- 13- 17- 19 -86.562
2- 4- 1- 7 -173.846 2- 3- 12- 11 -62.341
2- 4- 1- 11 -61.295 2- 3- 14- 13 58.246
2- 4- 1- 13 56.440 2- 3- 14- 16 -150.595
2- 3- 14- 18 -51.212 3- 2- 4- 6 -117.623
3- 2- 4- 10 121.416 3- 14- 13- 15 150.622
3- 14- 13- 17 -113.310 3- 14- 18- 19 86.562

4- 2- 3- 9 173.846 4- 1- 11- 12 62.341
4- 2- 3- 12 61.295 4- 1- 13- 14 -58.246
4- 2- 3- 14 -56.440 4- 1- 13- 15 150.595
4- 1- 13- 17 51.212 5- 2- 4- 6 120.961
5- 2- 3- 9 -63.449 5- 2- 4- 10 -0.000
5- 2- 3- 12 -175.999 5- 2- 3- 14 66.266
6- 4- 1- 7 -53.915 6- 4- 2- 8 -0.000
6- 4- 1- 11 58.636 6- 4- 1- 13 176.371
7- 1- 4- 10 63.449 7- 1- 11- 12 -178.511
7- 1- 13- 14 172.307 7- 1- 13- 15 21.148
7- 1- 13- 17 -78.235 8- 2- 3- 9 53.915
8- 2- 4- 10 -120.961 8- 2- 3- 12 -58.636
8- 2- 3- 14 -176.371 9- 3- 12- 11 178.511
9- 3- 14- 13 -172.307 9- 3- 14- 16 -21.148
9- 3- 14- 18 78.235 10- 4- 1- 11 175.999
10- 4- 1- 13 -66.266 11- 1- 13- 14 60.685
11- 12- 3- 14 59.644 11- 1- 13- 15 -90.474
11- 1- 13- 17 170.142 12- 3- 14- 13 -60.685
12- 11- 1- 13 -59.644 12- 3- 14- 16 90.474
12- 3- 14- 18 -170.142 13- 17- 19- 18 -57.727
13- 14- 18- 19 -29.885 14- 18- 19- 17 57.727
14- 13- 17- 19 29.885 15- 13- 14- 16 -0.000
15- 13- 14- 18 -96.068 15- 13- 17- 19 152.077
16- 14- 13- 17 96.068 16- 14- 18- 19 -152.077
17- 13- 14- 18 -0.000

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5245 1- 7 1.0932 1- 11 1.4490 1- 13 1.5053
5) 2- 3 1.5245 2- 4 1.5456 2- 5 1.0919 2- 8 1.0927
9) 3- 9 1.0932 3- 12 1.4490 3- 14 1.5053 4- 6 1.0927
13) 4- 10 1.0919 11- 12 1.4865 13- 14 1.3994 13- 15 1.0860
17) 13- 17 1.9989 14- 16 1.0860 14- 18 1.9989 17- 19 1.3099
21) 18- 19 1.3099
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.351 1- 4- 10 110.377 1- 11- 12 110.020
4) 1- 13- 14 111.008 1- 13- 15 120.243 1- 13- 17 107.349
7) 2- 3- 9 112.606 2- 3- 12 108.403 2- 3- 14 112.876
10) 2- 4- 6 110.874 2- 4- 10 112.338 3- 2- 4 107.819
13) 3- 2- 5 110.377 3- 2- 8 107.351 3- 14- 16 120.243
16) 3- 14- 18 107.349 4- 1- 7 112.606 4- 1- 11 108.403
19) 4- 1- 13 112.876 4- 2- 3 107.819 4- 2- 5 112.338
22) 4- 2- 8 110.874 5- 2- 3 110.377 5- 2- 4 112.338
25) 5- 2- 8 107.976 6- 4- 10 107.976 7- 1- 4 112.606
28) 7- 1- 11 102.449 7- 1- 13 113.006 8- 2- 3 107.351
31) 8- 2- 4 110.874 8- 2- 5 107.976 9- 3- 12 102.449
34) 9- 3- 14 113.006 10- 4- 6 107.976 11- 1- 4 108.403
37) 11- 1- 7 102.449 11- 1- 13 106.677 12- 3- 9 102.449
40) 12- 3- 14 106.677 13- 1- 4 112.876 13- 1- 7 113.006
43) 13- 1- 11 106.677 13- 14- 16 121.498 13- 14- 18 100.721
46) 13- 17- 19 98.412 14- 3- 9 113.006 14- 3- 12 106.677
49) 14- 13- 15 121.498 14- 13- 17 100.721 14- 18- 19 98.412
52) 15- 13- 14 121.498 15- 13- 17 89.717 16- 14- 18 89.717
55) 17- 13- 14 100.721 17- 13- 15 89.717 18- 14- 16 89.717
Dihedrals
I J K L Theta I J K L Theta

1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 14- 3 -0.000 1- 4- 2- 5 -121.836
1- 4- 2- 8 117.247 1- 13- 14- 16 -150.237
1- 13- 14- 18 113.442 1- 13- 17- 19 -86.611
2- 4- 1- 7 -173.547 2- 3- 12- 11 -62.323
2- 4- 1- 11 -60.926 2- 3- 14- 13 58.813
2- 4- 1- 13 57.020 2- 3- 14- 16 -150.525
2- 3- 14- 18 -50.380 3- 2- 4- 6 -117.247
3- 2- 4- 10 121.836 3- 14- 13- 15 150.237
3- 14- 13- 17 -113.442 3- 14- 18- 19 86.611
4- 2- 3- 9 173.547 4- 1- 11- 12 62.323
4- 2- 3- 12 60.926 4- 1- 13- 14 -58.813
4- 2- 3- 14 -57.020 4- 1- 13- 15 150.525
4- 1- 13- 17 50.380 5- 2- 4- 6 120.917
5- 2- 3- 9 -63.410 5- 2- 4- 10 -0.000
5- 2- 3- 12 -176.031 5- 2- 3- 14 66.023
6- 4- 1- 7 -54.040 6- 4- 2- 8 -0.000
6- 4- 1- 11 58.582 6- 4- 1- 13 176.528
7- 1- 4- 10 63.410 7- 1- 11- 12 -178.447
7- 1- 13- 14 171.959 7- 1- 13- 15 21.297
7- 1- 13- 17 -78.848 8- 2- 3- 9 54.040
8- 2- 4- 10 -120.917 8- 2- 3- 12 -58.582
8- 2- 3- 14 -176.528 9- 3- 12- 11 178.447
9- 3- 14- 13 -171.959 9- 3- 14- 16 -21.297
9- 3- 14- 18 78.848 10- 4- 1- 11 176.031
10- 4- 1- 13 -66.023 11- 1- 13- 14 60.140
11- 12- 3- 14 59.504 11- 1- 13- 15 -90.522
11- 1- 13- 17 169.333 12- 3- 14- 13 -60.140
12- 11- 1- 13 -59.504 12- 3- 14- 16 90.522
12- 3- 14- 18 -169.333 13- 17- 19- 18 -57.500
13- 14- 18- 19 -29.583 14- 18- 19- 17 57.500
14- 13- 17- 19 29.583 15- 13- 14- 16 -0.000
15- 13- 14- 18 -96.322 15- 13- 17- 19 151.644
16- 14- 13- 17 96.322 16- 14- 18- 19 -151.644
17- 13- 14- 18 -0.000

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5359 1- 7 1.0926 1- 11 1.4548 1- 13 1.5084
5) 2- 3 1.5359 2- 4 1.5529 2- 5 1.0937 2- 8 1.0940
9) 3- 9 1.0926 3- 12 1.4548 3- 14 1.5084 4- 6 1.0940
13) 4- 10 1.0937 11- 12 1.4817 13- 14 1.3647 13- 15 1.0829
17) 13- 17 2.4437 14- 16 1.0829 14- 18 2.4437 17- 19 1.2864
21) 18- 19 1.2864
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.954 1- 4- 10 110.091 1- 11- 12 110.218
4) 1- 13- 14 111.843 1- 13- 15 122.249 1- 13- 17 107.523
7) 2- 3- 9 112.714 2- 3- 12 108.088 2- 3- 14 112.219
10) 2- 4- 6 110.929 2- 4- 10 112.200 3- 2- 4 107.708
13) 3- 2- 5 110.091 3- 2- 8 107.954 3- 14- 16 122.249
16) 3- 14- 18 107.523 4- 1- 7 112.714 4- 1- 11 108.088
19) 4- 1- 13 112.219 4- 2- 3 107.708 4- 2- 5 112.200
22) 4- 2- 8 110.929 5- 2- 3 110.091 5- 2- 4 112.200
25) 5- 2- 8 107.885 6- 4- 10 107.885 7- 1- 4 112.714
28) 7- 1- 11 102.899 7- 1- 13 113.447 8- 2- 3 107.954
31) 8- 2- 4 110.929 8- 2- 5 107.885 9- 3- 12 102.899
34) 9- 3- 14 113.447 10- 4- 6 107.885 11- 1- 4 108.088
37) 11- 1- 7 102.899 11- 1- 13 106.713 12- 3- 9 102.899

40) 12- 3- 14 106.713 13- 1- 4 112.219 13- 1- 7 113.447
43) 13- 1- 11 106.713 13- 14- 16 124.014 13- 14- 18 99.400
46) 13- 17- 19 97.914 14- 3- 9 113.447 14- 3- 12 106.713
49) 14- 13- 15 124.014 14- 13- 17 99.400 14- 18- 19 97.914
52) 15- 13- 14 124.014 15- 13- 17 78.272 16- 14- 18 78.272
55) 17- 13- 14 99.400 17- 13- 15 78.272 18- 14- 16 78.272
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 14- 3 -0.000 1- 4- 2- 5 -121.317
1- 4- 2- 8 117.940 1- 13- 14- 16 -164.590
1- 13- 14- 18 113.275 1- 13- 17- 19 -88.653
2- 4- 1- 7 -173.963 2- 3- 12- 11 -62.531
2- 4- 1- 11 -60.927 2- 3- 14- 13 58.822
2- 4- 1- 13 56.474 2- 3- 14- 16 -136.275
2- 3- 14- 18 -49.303 3- 2- 4- 6 -117.940
3- 2- 4- 10 121.317 3- 14- 13- 15 164.590
3- 14- 13- 17 -113.275 3- 14- 18- 19 88.653
4- 2- 3- 9 173.963 4- 1- 11- 12 62.531
4- 2- 3- 12 60.927 4- 1- 13- 14 -58.822
4- 2- 3- 14 -56.474 4- 1- 13- 15 136.275
4- 1- 13- 17 49.303 5- 2- 4- 6 120.743
5- 2- 3- 9 -63.414 5- 2- 4- 10 -0.000
5- 2- 3- 12 -176.450 5- 2- 3- 14 66.149
6- 4- 1- 7 -54.120 6- 4- 2- 8 -0.000
6- 4- 1- 11 58.916 6- 4- 1- 13 176.317
7- 1- 4- 10 63.414 7- 1- 11- 12 -178.029
7- 1- 13- 14 171.996 7- 1- 13- 15 7.092
7- 1- 13- 17 -79.880 8- 2- 3- 9 54.120
8- 2- 4- 10 -120.743 8- 2- 3- 12 -58.916
8- 2- 3- 14 -176.317 9- 3- 12- 11 178.029
9- 3- 14- 13 -171.996 9- 3- 14- 16 -7.092
9- 3- 14- 18 79.880 10- 4- 1- 11 176.450
10- 4- 1- 13 -66.149 11- 1- 13- 14 59.396
11- 12- 3- 14 58.361 11- 1- 13- 15 -105.508
11- 1- 13- 17 167.520 12- 3- 14- 13 -59.396
12- 11- 1- 13 -58.361 12- 3- 14- 16 105.508
12- 3- 14- 18 -167.520 13- 17- 19- 18 -58.640
13- 14- 18- 19 -27.946 14- 18- 19- 17 58.640
14- 13- 17- 19 27.946 15- 13- 14- 16 -0.000
15- 13- 14- 18 -82.135 15- 13- 17- 19 150.952
16- 14- 13- 17 82.135 16- 14- 18- 19 -150.952
17- 13- 14- 18 -0.000

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5343 1- 7 1.0921 1- 11 1.4637 1- 13 1.5073
5) 2- 3 1.5343 2- 4 1.5517 2- 5 1.0933 2- 8 1.0937
9) 3- 9 1.0921 3- 12 1.4637 3- 14 1.5073 4- 6 1.0937
13) 4- 10 1.0933 11- 12 1.4832 13- 14 1.3650 13- 15 1.0827
17) 13- 17 2.4593 14- 16 1.0827 14- 18 2.4593 17- 19 1.2868
21) 18- 19 1.2868
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.019 1- 4- 10 109.919 1- 11- 12 110.132
4) 1- 13- 14 111.927 1- 13- 15 122.215 1- 13- 17 107.608
7) 2- 3- 9 112.844 2- 3- 12 108.024 2- 3- 14 112.380

10) 2- 4- 6 111.056 2- 4- 10 112.245 3- 2- 4 107.819
13) 3- 2- 5 109.919 3- 2- 8 108.019 3- 14- 16 122.215
16) 3- 14- 18 107.608 4- 1- 7 112.844 4- 1- 11 108.024
19) 4- 1- 13 112.380 4- 2- 3 107.819 4- 2- 5 112.245
22) 4- 2- 8 111.056 5- 2- 3 109.919 5- 2- 4 112.245
25) 5- 2- 8 107.708 6- 4- 10 107.708 7- 1- 4 112.844
28) 7- 1- 11 102.762 7- 1- 13 113.512 8- 2- 3 108.019
31) 8- 2- 4 111.056 8- 2- 5 107.708 9- 3- 12 102.762
34) 9- 3- 14 113.512 10- 4- 6 107.708 11- 1- 4 108.024
37) 11- 1- 7 102.762 11- 1- 13 106.495 12- 3- 9 102.762
40) 12- 3- 14 106.495 13- 1- 4 112.380 13- 1- 7 113.512
43) 13- 1- 11 106.495 13- 14- 16 124.018 13- 14- 18 99.347
46) 13- 17- 19 97.832 14- 3- 9 113.512 14- 3- 12 106.495
49) 14- 13- 15 124.018 14- 13- 17 99.347 14- 18- 19 97.832
52) 15- 13- 14 124.018 15- 13- 17 78.045 16- 14- 18 78.045
55) 17- 13- 14 99.347 17- 13- 15 78.045 18- 14- 16 78.045
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 14- 3 -0.000 1- 4- 2- 5 -121.205
1- 4- 2- 8 118.158 1- 13- 14- 16 -164.800
1- 13- 14- 18 113.374 1- 13- 17- 19 -88.669
2- 4- 1- 7 -173.904 2- 3- 12- 11 -62.482
2- 4- 1- 11 -61.003 2- 3- 14- 13 58.500
2- 4- 1- 13 56.183 2- 3- 14- 16 -136.383
2- 3- 14- 18 -49.645 3- 2- 4- 6 -118.158
3- 2- 4- 10 121.205 3- 14- 13- 15 164.800
3- 14- 13- 17 -113.374 3- 14- 18- 19 88.669
4- 2- 3- 9 173.904 4- 1- 11- 12 62.482
4- 2- 3- 12 61.003 4- 1- 13- 14 -58.500
4- 2- 3- 14 -56.183 4- 1- 13- 15 136.383
4- 1- 13- 17 49.645 5- 2- 4- 6 120.637
5- 2- 3- 9 -63.452 5- 2- 4- 10 -0.000
5- 2- 3- 12 -176.354 5- 2- 3- 14 66.460
6- 4- 1- 7 -53.811 6- 4- 2- 8 -0.000
6- 4- 1- 11 59.091 6- 4- 1- 13 176.277
7- 1- 4- 10 63.452 7- 1- 11- 12 -178.026
7- 1- 13- 14 171.931 7- 1- 13- 15 6.815
7- 1- 13- 17 -79.923 8- 2- 3- 9 53.811
8- 2- 4- 10 -120.637 8- 2- 3- 12 -59.091
8- 2- 3- 14 -176.277 9- 3- 12- 11 178.026
9- 3- 14- 13 -171.931 9- 3- 14- 16 -6.815
9- 3- 14- 18 79.923 10- 4- 1- 11 176.354
10- 4- 1- 13 -66.460 11- 1- 13- 14 59.593
11- 12- 3- 14 58.443 11- 1- 13- 15 -105.524
11- 1- 13- 17 167.738 12- 3- 14- 13 -59.593
12- 11- 1- 13 -58.443 12- 3- 14- 16 105.524
12- 3- 14- 18 -167.738 13- 17- 19- 18 -58.911
13- 14- 18- 19 -28.029 14- 18- 19- 17 58.911
14- 13- 17- 19 28.029 15- 13- 14- 16 -0.000
15- 13- 14- 18 -81.826 15- 13- 17- 19 151.033
16- 14- 13- 17 81.826 16- 14- 18- 19 -151.033
17- 13- 14- 18 -0.000

Optimised structures for the transition state for primary ozonide 14c formation at all levels reported.

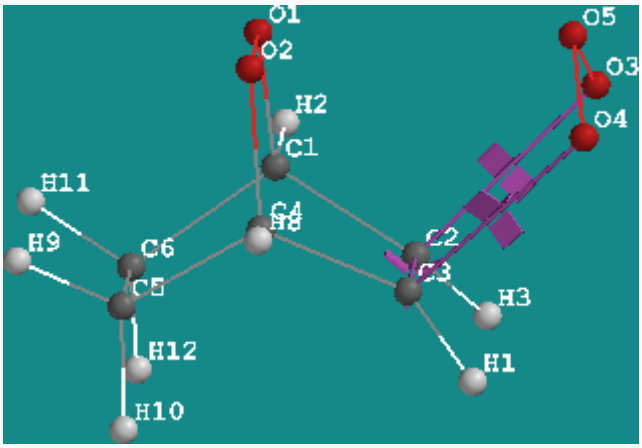

Figure S11: Optimised geometry for primary ozonide TS formation **14c**.

HF/6-31G* (GAS)

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Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5354 1- 7 1.0792 1- 11 1.4151 1- 13 1.5106
5) 2- 3 1.5354 2- 4 1.5494 2- 5 1.0845 2- 8 1.0832
9) 3- 9 1.0792 3- 12 1.4151 3- 15 1.5106 4- 6 1.0832
13) 4- 10 1.0845 11- 12 1.4138 13- 14 1.0713 13- 15 1.3653
17) 13- 17 2.1526 15- 16 1.0713 15- 18 2.1526 17- 19 1.2375
21) 18- 19 1.2375
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.604 1- 4- 10 110.224 1- 11- 12 111.798
4) 1- 13- 14 121.430 1- 13- 15 111.339 1- 13- 17 103.805
7) 2- 3- 9 112.915 2- 3- 12 107.683 2- 3- 15 108.907
10) 2- 4- 6 110.908 2- 4- 10 111.905 3- 2- 4 107.342
13) 3- 2- 5 110.224 3- 2- 8 108.604 3- 15- 16 121.430
16) 3- 15- 18 103.805 4- 1- 7 112.915 4- 1- 11 107.683
19) 4- 1- 13 108.907 4- 2- 3 107.342 4- 2- 5 111.905
22) 4- 2- 8 110.908 5- 2- 3 110.224 5- 2- 4 111.905
25) 5- 2- 8 107.824 6- 4- 10 107.824 7- 1- 4 112.915
28) 7- 1- 11 104.185 7- 1- 13 113.258 8- 2- 3 108.604
31) 8- 2- 4 110.908 8- 2- 5 107.824 9- 3- 12 104.185
34) 9- 3- 15 113.258 10- 4- 6 107.824 11- 1- 4 107.683
37) 11- 1- 7 104.185 11- 1- 13 109.639 12- 3- 9 104.185
40) 12- 3- 15 109.639 13- 1- 4 108.907 13- 1- 7 113.258
43) 13- 1- 11 109.639 13- 15- 16 123.911 13- 15- 18 99.255
46) 13- 17- 19 98.525 14- 13- 15 123.911 14- 13- 17 86.129
49) 15- 3- 9 113.258 15- 3- 12 109.639 15- 13- 14 123.911
52) 15- 13- 17 99.255 15- 18- 19 98.525 16- 15- 18 86.129
55) 17- 13- 14 86.129 17- 13- 15 99.255 18- 15- 16 86.129
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.057
1- 4- 2- 8 118.494 1- 13- 15- 16 159.588
1- 13- 15- 18 -108.858 1- 13- 17- 19 86.001
2- 4- 1- 7 -173.936 2- 3- 12- 11 -62.326
2- 4- 1- 11 -59.479 2- 3- 15- 13 61.832
2- 4- 1- 13 59.342 2- 3- 15- 16 -98.339
2- 3- 15- 18 167.722 3- 2- 4- 6 -118.494
```

3- 2- 4- 10 121.057 3- 15- 13- 14 -159.588
3- 15- 13- 17 108.858 3- 15- 18- 19 -86.001
4- 2- 3- 9 173.936 4- 1- 11- 12 62.326
4- 2- 3- 12 59.479 4- 1- 13- 14 98.339
4- 1- 13- 15 -61.832 4- 2- 3- 15 -59.342
4- 1- 13- 17 -167.722 5- 2- 4- 6 120.449
5- 2- 3- 9 -63.954 5- 2- 4- 10 -0.000
5- 2- 3- 12 -178.411 5- 2- 3- 15 62.767
6- 4- 1- 7 -53.963 6- 4- 2- 8 -0.000
6- 4- 1- 11 60.494 6- 4- 1- 13 179.315
7- 1- 4- 10 63.954 7- 1- 11- 12 -177.534
7- 1- 13- 14 -28.186 7- 1- 13- 15 171.643
7- 1- 13- 17 65.752 8- 2- 3- 9 53.963
8- 2- 4- 10 -120.449 8- 2- 3- 12 -60.494
8- 2- 3- 15 -179.315 9- 3- 12- 11 177.534
9- 3- 15- 13 -171.643 9- 3- 15- 16 28.186
9- 3- 15- 18 -65.752 10- 4- 1- 11 178.411
10- 4- 1- 13 -62.767 11- 1- 13- 14 -144.072
11- 1- 13- 15 55.757 11- 12- 3- 15 56.025
11- 1- 13- 17 -50.133 12- 3- 15- 13 -55.757
12- 11- 1- 13 -56.025 12- 3- 15- 16 144.072
12- 3- 15- 18 50.133 13- 17- 19- 18 58.874
13- 15- 18- 19 28.814 14- 13- 15- 16 -0.000
14- 13- 15- 18 91.554 14- 13- 17- 19 -152.562
15- 18- 19- 17 -58.874 15- 13- 17- 19 -28.814
16- 15- 13- 17 -91.554 16- 15- 18- 19 152.562
17- 13- 15- 18 -0.000

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5340 1- 7 1.0789 1- 11 1.4224 1- 13 1.5095
5) 2- 3 1.5340 2- 4 1.5483 2- 5 1.0835 2- 8 1.0830
9) 3- 9 1.0789 3- 12 1.4224 3- 15 1.5095 4- 6 1.0830
13) 4- 10 1.0835 11- 12 1.4147 13- 14 1.0713 13- 15 1.3643
17) 13- 17 2.1800 15- 16 1.0713 15- 18 2.1800 17- 19 1.2371
21) 18- 19 1.2371
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.595 1- 4- 10 110.014 1- 11- 12 111.721
4) 1- 13- 14 121.453 1- 13- 15 111.433 1- 13- 17 103.853
7) 2- 3- 9 113.026 2- 3- 12 107.721 2- 3- 15 108.961
10) 2- 4- 6 111.035 2- 4- 10 111.951 3- 2- 4 107.435
13) 3- 2- 5 110.014 3- 2- 8 108.595 3- 15- 16 121.453
16) 3- 15- 18 103.853 4- 1- 7 113.026 4- 1- 11 107.721
19) 4- 1- 13 108.961 4- 2- 3 107.435 4- 2- 5 111.951
22) 4- 2- 8 111.035 5- 2- 3 110.014 5- 2- 4 111.951
25) 5- 2- 8 107.771 6- 4- 10 107.771 7- 1- 4 113.026
28) 7- 1- 11 104.075 7- 1- 13 113.338 8- 2- 3 108.595
31) 8- 2- 4 111.035 8- 2- 5 107.771 9- 3- 12 104.075
34) 9- 3- 15 113.338 10- 4- 6 107.771 11- 1- 4 107.721
37) 11- 1- 7 104.075 11- 1- 13 109.444 12- 3- 9 104.075
40) 12- 3- 15 109.444 13- 1- 4 108.961 13- 1- 7 113.338
43) 13- 1- 11 109.444 13- 15- 16 123.950 13- 15- 18 99.180
46) 13- 17- 19 98.447 14- 13- 15 123.950 14- 13- 17 85.738
49) 15- 3- 9 113.338 15- 3- 12 109.444 15- 13- 14 123.950
52) 15- 13- 17 99.180 15- 18- 19 98.447 16- 15- 18 85.738
55) 17- 13- 14 85.738 17- 13- 15 99.180 18- 15- 16 85.738

Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -120.887
1- 4- 2- 8 118.612 1- 13- 15- 16 160.061
1- 13- 15- 18 -108.905 1- 13- 17- 19 86.136
2- 4- 1- 7 -173.903 2- 3- 12- 11 -62.232
2- 4- 1- 11 -59.497 2- 3- 15- 13 61.626
2- 4- 1- 13 59.144 2- 3- 15- 16 -99.008
2- 3- 15- 18 167.489 3- 2- 4- 6 -118.612
3- 2- 4- 10 120.887 3- 15- 13- 14 -160.061
3- 15- 13- 17 108.905 3- 15- 18- 19 -86.136
4- 2- 3- 9 173.903 4- 1- 11- 12 62.232
4- 2- 3- 12 59.497 4- 1- 13- 14 99.008
4- 1- 13- 15 -61.626 4- 2- 3- 15 -59.144
4- 1- 13- 17 -167.489 5- 2- 4- 6 120.501
5- 2- 3- 9 -63.997 5- 2- 4- 10 -0.000
5- 2- 3- 12 -178.403 5- 2- 3- 15 62.956
6- 4- 1- 7 -53.730 6- 4- 2- 8 -0.000
6- 4- 1- 11 60.676 6- 4- 1- 13 179.316
7- 1- 4- 10 63.997 7- 1- 11- 12 -177.539
7- 1- 13- 14 -27.767 7- 1- 13- 15 171.599
7- 1- 13- 17 65.736 8- 2- 3- 9 53.730
8- 2- 4- 10 -120.501 8- 2- 3- 12 -60.676
8- 2- 3- 15 -179.316 9- 3- 12- 11 177.539
9- 3- 15- 13 -171.599 9- 3- 15- 16 27.767
9- 3- 15- 18 -65.736 10- 4- 1- 11 178.403
10- 4- 1- 13 -62.956 11- 1- 13- 14 -143.437
11- 1- 13- 15 55.929 11- 12- 3- 15 56.098
11- 1- 13- 17 -49.934 12- 3- 15- 13 -55.929
12- 11- 1- 13 -56.098 12- 3- 15- 16 143.437
12- 3- 15- 18 49.934 13- 17- 19- 18 59.048
13- 15- 18- 19 28.768 14- 13- 15- 16 -0.000
14- 13- 15- 18 91.034 14- 13- 17- 19 -152.496
15- 18- 19- 17 -59.048 15- 13- 17- 19 -28.768
16- 15- 13- 17 -91.034 16- 15- 18- 19 152.496
17- 13- 15- 18 -0.000

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5342 1- 7 1.0945 1- 11 1.4388 1- 13 1.5053
5) 2- 3 1.5342 2- 4 1.5462 2- 5 1.0955 2- 8 1.0939
9) 3- 9 1.0945 3- 12 1.4388 3- 15 1.5053 4- 6 1.0939
13) 4- 10 1.0955 11- 12 1.5085 13- 14 1.0871 13- 15 1.3988
17) 13- 17 1.9787 15- 16 1.0871 15- 18 1.9787 17- 19 1.3285
21) 18- 19 1.3285
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.054 1- 4- 10 110.040 1- 11- 12 109.827
4) 1- 13- 14 120.299 1- 13- 15 111.139 1- 13- 17 104.510
7) 2- 3- 9 112.957 2- 3- 12 108.449 2- 3- 15 109.362
10) 2- 4- 6 111.080 2- 4- 10 112.001 3- 2- 4 107.806
13) 3- 2- 5 110.040 3- 2- 8 108.054 3- 15- 16 120.299
16) 3- 15- 18 104.510 4- 1- 7 112.957 4- 1- 11 108.449
19) 4- 1- 13 109.362 4- 2- 3 107.806 4- 2- 5 112.001
22) 4- 2- 8 111.080 5- 2- 3 110.040 5- 2- 4 112.001
25) 5- 2- 8 107.795 6- 4- 10 107.795 7- 1- 4 112.957
28) 7- 1- 11 102.469 7- 1- 13 113.138 8- 2- 3 108.054
31) 8- 2- 4 111.080 8- 2- 5 107.795 9- 3- 12 102.469

34) 9- 3- 15 113.138 10- 4- 6 107.795 11- 1- 4 108.449
37) 11- 1- 7 102.469 11- 1- 13 110.186 12- 3- 9 102.469
40) 12- 3- 15 110.186 13- 1- 4 109.362 13- 1- 7 113.138
43) 13- 1- 11 110.186 13- 15- 16 122.292 13- 15- 18 101.006
46) 13- 17- 19 97.733 14- 13- 15 122.292 14- 13- 17 90.301
49) 15- 3- 9 113.138 15- 3- 12 110.186 15- 13- 14 122.292
52) 15- 13- 17 101.006 15- 18- 19 97.733 16- 15- 18 90.301
55) 17- 13- 14 90.301 17- 13- 15 101.006 18- 15- 16 90.301
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.196
1- 4- 2- 8 118.206 1- 13- 15- 16 152.157
1- 13- 15- 18 -110.417 1- 13- 17- 19 84.774
2- 4- 1- 7 -173.999 2- 3- 12- 11 -62.422
2- 4- 1- 11 -61.139 2- 3- 15- 13 61.094
2- 4- 1- 13 59.046 2- 3- 15- 16 -91.695
2- 3- 15- 18 169.243 3- 2- 4- 6 -118.206
3- 2- 4- 10 121.196 3- 15- 13- 14 -152.157
3- 15- 13- 17 110.417 3- 15- 18- 19 -84.774
4- 2- 3- 9 173.999 4- 1- 11- 12 62.422
4- 2- 3- 12 61.139 4- 1- 13- 14 91.695
4- 1- 13- 15 -61.094 4- 2- 3- 15 -59.046
4- 1- 13- 17 -169.243 5- 2- 4- 6 120.598
5- 2- 3- 9 -63.590 5- 2- 4- 10 -0.000
5- 2- 3- 12 -176.451 5- 2- 3- 15 63.364
6- 4- 1- 7 -53.865 6- 4- 2- 8 -0.000
6- 4- 1- 11 58.995 6- 4- 1- 13 179.180
7- 1- 4- 10 63.590 7- 1- 11- 12 -177.917
7- 1- 13- 14 -35.156 7- 1- 13- 15 172.055
7- 1- 13- 17 63.906 8- 2- 3- 9 53.865
8- 2- 4- 10 -120.598 8- 2- 3- 12 -58.995
8- 2- 3- 15 -179.180 9- 3- 12- 11 177.917
9- 3- 15- 13 -172.055 9- 3- 15- 16 35.156
9- 3- 15- 18 -63.906 10- 4- 1- 11 176.451
10- 4- 1- 13 -63.364 11- 1- 13- 14 -149.189
11- 1- 13- 15 58.022 11- 12- 3- 15 57.249
11- 1- 13- 17 -50.127 12- 3- 15- 13 -58.022
12- 11- 1- 13 -57.249 12- 3- 15- 16 149.189
12- 3- 15- 18 50.127 13- 17- 19- 18 58.849
13- 15- 18- 19 30.682 14- 13- 15- 16 -0.000
14- 13- 15- 18 97.426 14- 13- 17- 19 -153.726
15- 18- 19- 17 -58.849 15- 13- 17- 19 -30.682
16- 15- 13- 17 -97.426 16- 15- 18- 19 153.726
17- 13- 15- 18 -0.000

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5356 1- 7 1.0934 1- 11 1.4313 1- 13 1.5074
5) 2- 3 1.5356 2- 4 1.5484 2- 5 1.0945 2- 8 1.0934
9) 3- 9 1.0934 3- 12 1.4313 3- 15 1.5074 4- 6 1.0934
13) 4- 10 1.0945 11- 12 1.4899 13- 14 1.0864 13- 15 1.4022
17) 13- 17 1.9629 15- 16 1.0864 15- 18 1.9629 17- 19 1.3105
21) 18- 19 1.3105
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.021 1- 4- 10 110.146 1- 11- 12 110.221

4) 1- 13- 14 120.429 1- 13- 15 110.932 1- 13- 17 105.165
7) 2- 3- 9 113.121 2- 3- 12 108.567 2- 3- 15 108.974
10) 2- 4- 6 110.960 2- 4- 10 112.104 3- 2- 4 107.645
13) 3- 2- 5 110.146 3- 2- 8 108.021 3- 15- 16 120.429
16) 3- 15- 18 105.165 4- 1- 7 113.121 4- 1- 11 108.567
19) 4- 1- 13 108.974 4- 2- 3 107.645 4- 2- 5 112.104
22) 4- 2- 8 110.960 5- 2- 3 110.146 5- 2- 4 112.104
25) 5- 2- 8 107.899 6- 4- 10 107.899 7- 1- 4 113.121
28) 7- 1- 11 102.548 7- 1- 13 112.988 8- 2- 3 108.021
31) 8- 2- 4 110.960 8- 2- 5 107.899 9- 3- 12 102.548
34) 9- 3- 15 112.988 10- 4- 6 107.899 11- 1- 4 108.567
37) 11- 1- 7 102.548 11- 1- 13 110.419 12- 3- 9 102.548
40) 12- 3- 15 110.419 13- 1- 4 108.974 13- 1- 7 112.988
43) 13- 1- 11 110.419 13- 15- 16 122.208 13- 15- 18 100.718
46) 13- 17- 19 98.124 14- 13- 15 122.208 14- 13- 17 90.285
49) 15- 3- 9 112.988 15- 3- 12 110.419 15- 13- 14 122.208
52) 15- 13- 17 100.718 15- 18- 19 98.124 16- 15- 18 90.285
55) 17- 13- 14 90.285 17- 13- 15 100.718 18- 15- 16 90.285
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.283
1- 4- 2- 8 118.001 1- 13- 15- 16 151.864
1- 13- 15- 18 -110.944 1- 13- 17- 19 85.043
2- 4- 1- 7 -173.812 2- 3- 12- 11 -62.323
2- 4- 1- 11 -60.694 2- 3- 15- 13 61.661
2- 4- 1- 13 59.616 2- 3- 15- 16 -90.775
2- 3- 15- 18 169.718 3- 2- 4- 6 -118.001
3- 2- 4- 10 121.283 3- 15- 13- 14 -151.864
3- 15- 13- 17 110.944 3- 15- 18- 19 -85.043
4- 2- 3- 9 173.812 4- 1- 11- 12 62.323
4- 2- 3- 12 60.694 4- 1- 13- 14 90.775
4- 1- 13- 15 -61.661 4- 2- 3- 15 -59.616
4- 1- 13- 17 -169.718 5- 2- 4- 6 120.717
5- 2- 3- 9 -63.690 5- 2- 4- 10 -0.000
5- 2- 3- 12 -176.807 5- 2- 3- 15 62.883
6- 4- 1- 7 -53.930 6- 4- 2- 8 -0.000
6- 4- 1- 11 59.188 6- 4- 1- 13 179.498
7- 1- 4- 10 63.690 7- 1- 11- 12 -177.734
7- 1- 13- 14 -35.874 7- 1- 13- 15 171.690
7- 1- 13- 17 63.633 8- 2- 3- 9 53.930
8- 2- 4- 10 -120.717 8- 2- 3- 12 -59.188
8- 2- 3- 15 -179.498 9- 3- 12- 11 177.734
9- 3- 15- 13 -171.690 9- 3- 15- 16 35.874
9- 3- 15- 18 -63.633 10- 4- 1- 11 176.807
10- 4- 1- 13 -62.883 11- 1- 13- 14 -150.063
11- 1- 13- 15 57.501 11- 12- 3- 15 57.086
11- 1- 13- 17 -50.556 12- 3- 15- 13 -57.501
12- 11- 1- 13 -57.086 12- 3- 15- 16 150.063
12- 3- 15- 18 50.556 13- 17- 19- 18 58.482
13- 15- 18- 19 30.299 14- 13- 15- 16 -0.000
14- 13- 15- 18 97.193 14- 13- 17- 19 -153.215
15- 18- 19- 17 -58.482 15- 13- 17- 19 -30.299
16- 15- 13- 17 -97.193 16- 15- 18- 19 153.215
17- 13- 15- 18 -0.000

DFT/6-31G* (GAS)

Geometry information
Bond Lengths

I J R I J R I J R I J R
1) 1- 4 1.5458 1- 7 1.0927 1- 11 1.4394 1- 13 1.5102
5) 2- 3 1.5458 2- 4 1.5535 2- 5 1.0957 2- 8 1.0942
9) 3- 9 1.0927 3- 12 1.4394 3- 15 1.5102 4- 6 1.0942
13) 4- 10 1.0957 11- 12 1.4885 13- 14 1.0830 13- 15 1.3708
17) 13- 17 2.2945 15- 16 1.0830 15- 18 2.2945 17- 19 1.2908
21) 18- 19 1.2908
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.144 1- 4- 10 110.275 1- 11- 12 110.319
4) 1- 13- 14 122.161 1- 13- 15 111.710 1- 13- 17 103.139
7) 2- 3- 9 112.768 2- 3- 12 107.961 2- 3- 15 109.068
10) 2- 4- 6 110.968 2- 4- 10 112.040 3- 2- 4 107.599
13) 3- 2- 5 110.275 3- 2- 8 108.144 3- 15- 16 122.161
16) 3- 15- 18 103.139 4- 1- 7 112.768 4- 1- 11 107.961
19) 4- 1- 13 109.068 4- 2- 3 107.599 4- 2- 5 112.040
22) 4- 2- 8 110.968 5- 2- 3 110.275 5- 2- 4 112.040
25) 5- 2- 8 107.759 6- 4- 10 107.759 7- 1- 4 112.768
28) 7- 1- 11 103.159 7- 1- 13 113.540 8- 2- 3 108.144
31) 8- 2- 4 110.968 8- 2- 5 107.759 9- 3- 12 103.159
34) 9- 3- 15 113.540 10- 4- 6 107.759 11- 1- 4 107.961
37) 11- 1- 7 103.159 11- 1- 13 110.071 12- 3- 9 103.159
40) 12- 3- 15 110.071 13- 1- 4 109.068 13- 1- 7 113.540
43) 13- 1- 11 110.071 13- 15- 16 124.252 13- 15- 18 99.807
46) 13- 17- 19 97.276 14- 13- 15 124.252 14- 13- 17 81.936
49) 15- 3- 9 113.540 15- 3- 12 110.071 15- 13- 14 124.252
52) 15- 13- 17 99.807 15- 18- 19 97.276 16- 15- 18 81.936
55) 17- 13- 14 81.936 17- 13- 15 99.807 18- 15- 16 81.936
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.373
1- 4- 2- 8 118.126 1- 13- 15- 16 164.636
1- 13- 15- 18 -108.489 1- 13- 17- 19 86.264
2- 4- 1- 7 -174.238 2- 3- 12- 11 -62.680
2- 4- 1- 11 -60.936 2- 3- 15- 13 61.187
2- 4- 1- 13 58.651 2- 3- 15- 16 -103.820
2- 3- 15- 18 167.520 3- 2- 4- 6 -118.126
3- 2- 4- 10 121.373 3- 15- 13- 14 -164.636
3- 15- 13- 17 108.489 3- 15- 18- 19 -86.264
4- 2- 3- 9 174.238 4- 1- 11- 12 62.680
4- 2- 3- 12 60.936 4- 1- 13- 14 103.820
4- 1- 13- 15 -61.187 4- 2- 3- 15 -58.651
4- 1- 13- 17 -167.520 5- 2- 4- 6 120.500
5- 2- 3- 9 -63.292 5- 2- 4- 10 -0.000
5- 2- 3- 12 -176.594 5- 2- 3- 15 63.819
6- 4- 1- 7 -54.305 6- 4- 2- 8 -0.000
6- 4- 1- 11 58.998 6- 4- 1- 13 178.585
7- 1- 4- 10 63.292 7- 1- 11- 12 -177.744
7- 1- 13- 14 -22.850 7- 1- 13- 15 172.143
7- 1- 13- 17 65.810 8- 2- 3- 9 54.305
8- 2- 4- 10 -120.500 8- 2- 3- 12 -58.998
8- 2- 3- 15 -178.585 9- 3- 12- 11 177.744
9- 3- 15- 13 -172.143 9- 3- 15- 16 22.850
9- 3- 15- 18 -65.810 10- 4- 1- 11 176.594
10- 4- 1- 13 -63.819 11- 1- 13- 14 -137.909
11- 1- 13- 15 57.084 11- 12- 3- 15 56.271
11- 1- 13- 17 -49.248 12- 3- 15- 13 -57.084
12- 11- 1- 13 -56.271 12- 3- 15- 16 137.909
12- 3- 15- 18 49.248 13- 17- 19- 18 59.741
13- 15- 18- 19 28.941 14- 13- 15- 16 -0.000
14- 13- 15- 18 86.875 14- 13- 17- 19 -152.472

15- 18- 19- 17 -59.741 15- 13- 17- 19 -28.941
16- 15- 13- 17 -86.875 16- 15- 18- 19 152.472
17- 13- 15- 18 -0.000

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5436 1- 7 1.0922 1- 11 1.4490 1- 13 1.5082
5) 2- 3 1.5436 2- 4 1.5519 2- 5 1.0945 2- 8 1.0940
9) 3- 9 1.0922 3- 12 1.4490 3- 15 1.5082 4- 6 1.0940
13) 4- 10 1.0945 11- 12 1.4896 13- 14 1.0830 13- 15 1.3673
17) 13- 17 2.3774 15- 16 1.0830 15- 18 2.3774 17- 19 1.2887
21) 18- 19 1.2887
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.176 1- 4- 10 109.989 1- 11- 12 110.211
4) 1- 13- 14 122.289 1- 13- 15 111.866 1- 13- 17 103.107
7) 2- 3- 9 112.871 2- 3- 12 108.051 2- 3- 15 109.205
10) 2- 4- 6 111.160 2- 4- 10 112.084 3- 2- 4 107.703
13) 3- 2- 5 109.989 3- 2- 8 108.176 3- 15- 16 122.289
16) 3- 15- 18 103.107 4- 1- 7 112.871 4- 1- 11 108.051
19) 4- 1- 13 109.205 4- 2- 3 107.703 4- 2- 5 112.084
22) 4- 2- 8 111.160 5- 2- 3 109.989 5- 2- 4 112.084
25) 5- 2- 8 107.667 6- 4- 10 107.667 7- 1- 4 112.871
28) 7- 1- 11 103.040 7- 1- 13 113.659 8- 2- 3 108.176
31) 8- 2- 4 111.160 8- 2- 5 107.667 9- 3- 12 103.040
34) 9- 3- 15 113.659 10- 4- 6 107.667 11- 1- 4 108.051
37) 11- 1- 7 103.040 11- 1- 13 109.704 12- 3- 9 103.040
40) 12- 3- 15 109.704 13- 1- 4 109.205 13- 1- 7 113.659
43) 13- 1- 11 109.704 13- 15- 16 124.408 13- 15- 18 99.562
46) 13- 17- 19 97.038 14- 13- 15 124.408 14- 13- 17 80.578
49) 15- 3- 9 113.659 15- 3- 12 109.704 15- 13- 14 124.408
52) 15- 13- 17 99.562 15- 18- 19 97.038 16- 15- 18 80.578
55) 17- 13- 14 80.578 17- 13- 15 99.562 18- 15- 16 80.578
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.114
1- 4- 2- 8 118.338 1- 13- 15- 16 166.540
1- 13- 15- 18 -108.384 1- 13- 17- 19 86.434
2- 4- 1- 7 -174.226 2- 3- 12- 11 -62.562
2- 4- 1- 11 -60.958 2- 3- 15- 13 60.872
2- 4- 1- 13 58.319 2- 3- 15- 16 -105.998
2- 3- 15- 18 166.966 3- 2- 4- 6 -118.338
3- 2- 4- 10 121.114 3- 15- 13- 14 -166.540
3- 15- 13- 17 108.384 3- 15- 18- 19 -86.434
4- 2- 3- 9 174.226 4- 1- 11- 12 62.562
4- 2- 3- 12 60.958 4- 1- 13- 14 105.998
4- 1- 13- 15 -60.872 4- 2- 3- 15 -58.319
4- 1- 13- 17 -166.966 5- 2- 4- 6 120.547
5- 2- 3- 9 -63.358 5- 2- 4- 10 -0.000
5- 2- 3- 12 -176.626 5- 2- 3- 15 64.097
6- 4- 1- 7 -53.986 6- 4- 2- 8 -0.000
6- 4- 1- 11 59.282 6- 4- 1- 13 178.559
7- 1- 4- 10 63.358 7- 1- 11- 12 -177.763
7- 1- 13- 14 -21.011 7- 1- 13- 15 172.119
7- 1- 13- 17 66.025 8- 2- 3- 9 53.986
8- 2- 4- 10 -120.547 8- 2- 3- 12 -59.282
8- 2- 3- 15 -178.559 9- 3- 12- 11 177.763
9- 3- 15- 13 -172.119 9- 3- 15- 16 21.011

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9- 3- 15- 18 -66.025 10- 4- 1- 11 176.626
10- 4- 1- 13 -64.097 11- 1- 13- 14 -135.754
11- 1- 13- 15 57.376 11- 12- 3- 15 56.399
11- 1- 13- 17 -48.718 12- 3- 15- 13 -57.376
12- 11- 1- 13 -56.399 12- 3- 15- 16 135.754
12- 3- 15- 18 48.718 13- 17- 19- 18 60.360
13- 15- 18- 19 28.844 14- 13- 15- 16 -0.000
14- 13- 15- 18 85.075 14- 13- 17- 19 -152.412
15- 18- 19- 17 -60.360 15- 13- 17- 19 -28.844
16- 15- 13- 17 -85.075 16- 15- 18- 19 152.412
17- 13- 15- 18 -0.000
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Optimised structures for the transition state for primary ozonide 14d.formation at all levels reported.

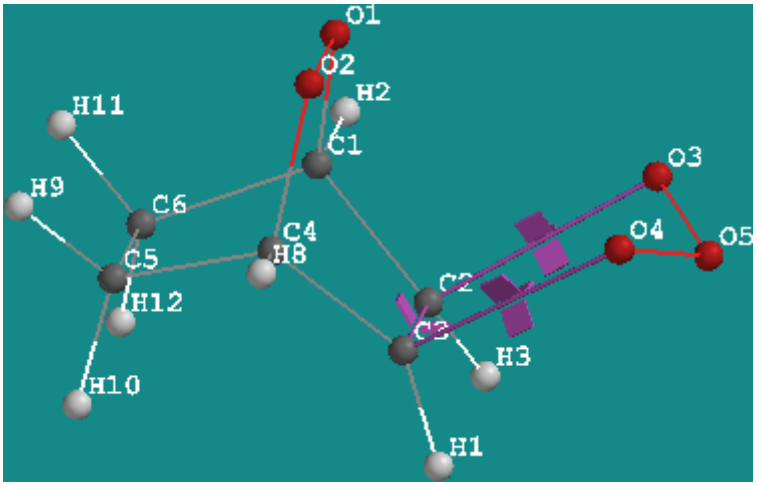

Figure S12: Optimised geometry for primary ozonide TS formation **14d**.

HF/6-31G* (GAS)

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Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5365 1- 7 1.0796 1- 11 1.4118 1- 13 1.5102
5) 2- 3 1.5365 2- 4 1.5502 2- 5 1.0846 2- 8 1.0831
9) 3- 9 1.0796 3- 12 1.4118 3- 15 1.5102 4- 6 1.0831
13) 4- 10 1.0846 11- 12 1.4118 13- 14 1.0720 13- 15 1.3620
17) 13- 17 2.1703 15- 16 1.0720 15- 18 2.1703 17- 19 1.2367
21) 18- 19 1.2367
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.574 1- 4- 10 110.389 1- 11- 12 111.800
4) 1- 13- 14 121.155 1- 13- 15 111.325 1- 13- 17 101.287
7) 2- 3- 9 112.898 2- 3- 12 107.613 2- 3- 15 108.399
10) 2- 4- 6 110.894 2- 4- 10 111.879 3- 2- 4 107.228
13) 3- 2- 5 110.389 3- 2- 8 108.574 3- 15- 16 121.155
16) 3- 15- 18 101.287 4- 1- 7 112.898 4- 1- 11 107.613
19) 4- 1- 13 108.399 4- 2- 3 107.228 4- 2- 5 111.879
22) 4- 2- 8 110.894 5- 2- 3 110.389 5- 2- 4 111.879
25) 5- 2- 8 107.844 6- 4- 10 107.844 7- 1- 4 112.898
28) 7- 1- 11 104.253 7- 1- 13 113.189 8- 2- 3 108.574
31) 8- 2- 4 110.894 8- 2- 5 107.844 9- 3- 12 104.253
34) 9- 3- 15 113.189 10- 4- 6 107.844 11- 1- 4 107.613
37) 11- 1- 7 104.253 11- 1- 13 110.299 12- 3- 9 104.253
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40) 12- 3- 15 110.299 13- 1- 4 108.399 13- 1- 7 113.189
43) 13- 1- 11 110.299 13- 15- 16 124.288 13- 15- 18 99.331
46) 13- 17- 19 97.783 14- 13- 15 124.288 14- 13- 17 88.133
49) 15- 3- 9 113.189 15- 3- 12 110.299 15- 13- 14 124.288
52) 15- 13- 17 99.331 15- 18- 19 97.783 16- 15- 18 88.133
55) 17- 13- 14 88.133 17- 13- 15 99.331 18- 15- 16 88.133
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.171
1- 4- 2- 8 118.381 1- 13- 15- 16 159.781
1- 13- 15- 18 -106.086 1- 13- 17- 19 142.864
2- 4- 1- 7 -174.064 2- 3- 12- 11 -62.506
2- 4- 1- 11 -59.577 2- 3- 15- 13 62.295
2- 4- 1- 13 59.709 2- 3- 15- 16 -98.213
2- 3- 15- 18 167.092 3- 2- 4- 6 -118.381
3- 2- 4- 10 121.171 3- 15- 13- 14 -159.781
3- 15- 13- 17 106.086 3- 15- 18- 19 -142.864
4- 2- 3- 9 174.064 4- 1- 11- 12 62.506
4- 2- 3- 12 59.577 4- 1- 13- 14 98.213
4- 1- 13- 15 -62.295 4- 2- 3- 15 -59.709
4- 1- 13- 17 -167.092 5- 2- 4- 6 120.448
5- 2- 3- 9 -63.830 5- 2- 4- 10 -0.000
5- 2- 3- 12 -178.317 5- 2- 3- 15 62.396
6- 4- 1- 7 -54.190 6- 4- 2- 8 -0.000
6- 4- 1- 11 60.297 6- 4- 1- 13 179.584
7- 1- 4- 10 63.830 7- 1- 11- 12 -177.372
7- 1- 13- 14 -27.843 7- 1- 13- 15 171.649
7- 1- 13- 17 66.851 8- 2- 3- 9 54.190
8- 2- 4- 10 -120.448 8- 2- 3- 12 -60.297
8- 2- 3- 15 -179.584 9- 3- 12- 11 177.372
9- 3- 15- 13 -171.649 9- 3- 15- 16 27.843
9- 3- 15- 18 -66.851 10- 4- 1- 11 178.317
10- 4- 1- 13 -62.396 11- 1- 13- 14 -144.204
11- 1- 13- 15 55.288 11- 12- 3- 15 55.560
11- 1- 13- 17 -49.509 12- 3- 15- 13 -55.288
12- 11- 1- 13 -55.560 12- 3- 15- 16 144.204
12- 3- 15- 18 49.509 13- 17- 19- 18 -59.658
13- 15- 18- 19 -28.747 14- 13- 15- 16 -0.000
14- 13- 15- 18 94.133 14- 13- 17- 19 -95.714
15- 18- 19- 17 59.658 15- 13- 17- 19 28.747
16- 15- 13- 17 -94.133 16- 15- 18- 19 95.714
17- 13- 15- 18 -0.000

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5350 1- 7 1.0793 1- 11 1.4201 1- 13 1.5086
5) 2- 3 1.5350 2- 4 1.5491 2- 5 1.0836 2- 8 1.0829
9) 3- 9 1.0793 3- 12 1.4201 3- 15 1.5086 4- 6 1.0829
13) 4- 10 1.0836 11- 12 1.4128 13- 14 1.0719 13- 15 1.3614
17) 13- 17 2.1946 15- 16 1.0719 15- 18 2.1946 17- 19 1.2365
21) 18- 19 1.2365
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.588 1- 4- 10 110.158 1- 11- 12 111.710
4) 1- 13- 14 121.146 1- 13- 15 111.422 1- 13- 17 101.704
7) 2- 3- 9 112.993 2- 3- 12 107.620 2- 3- 15 108.509

10) 2- 4- 6 111.019 2- 4- 10 111.927 3- 2- 4 107.326
13) 3- 2- 5 110.158 3- 2- 8 108.588 3- 15- 16 121.146
16) 3- 15- 18 101.704 4- 1- 7 112.993 4- 1- 11 107.620
19) 4- 1- 13 108.509 4- 2- 3 107.326 4- 2- 5 111.927
22) 4- 2- 8 111.019 5- 2- 3 110.158 5- 2- 4 111.927
25) 5- 2- 8 107.788 6- 4- 10 107.788 7- 1- 4 112.993
28) 7- 1- 11 104.102 7- 1- 13 113.310 8- 2- 3 108.588
31) 8- 2- 4 111.019 8- 2- 5 107.788 9- 3- 12 104.102
34) 9- 3- 15 113.310 10- 4- 6 107.788 11- 1- 4 107.620
37) 11- 1- 7 104.102 11- 1- 13 110.088 12- 3- 9 104.102
40) 12- 3- 15 110.088 13- 1- 4 108.509 13- 1- 7 113.310
43) 13- 1- 11 110.088 13- 15- 16 124.302 13- 15- 18 99.249
46) 13- 17- 19 97.710 14- 13- 15 124.302 14- 13- 17 87.555
49) 15- 3- 9 113.310 15- 3- 12 110.088 15- 13- 14 124.302
52) 15- 13- 17 99.249 15- 18- 19 97.710 16- 15- 18 87.555
55) 17- 13- 14 87.555 17- 13- 15 99.249 18- 15- 16 87.555
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -120.978
1- 4- 2- 8 118.527 1- 13- 15- 16 160.091
1- 13- 15- 18 -106.539 1- 13- 17- 19 143.081
2- 4- 1- 7 -173.986 2- 3- 12- 11 -62.433
2- 4- 1- 11 -59.625 2- 3- 15- 13 62.049
2- 4- 1- 13 59.476 2- 3- 15- 16 -98.762
2- 3- 15- 18 166.977 3- 2- 4- 6 -118.527
3- 2- 4- 10 120.978 3- 15- 13- 14 -160.091
3- 15- 13- 17 106.539 3- 15- 18- 19 -143.081
4- 2- 3- 9 173.986 4- 1- 11- 12 62.433
4- 2- 3- 12 59.625 4- 1- 13- 14 98.762
4- 1- 13- 15 -62.049 4- 2- 3- 15 -59.476
4- 1- 13- 17 -166.977 5- 2- 4- 6 120.495
5- 2- 3- 9 -63.927 5- 2- 4- 10 -0.000
5- 2- 3- 12 -178.287 5- 2- 3- 15 62.612
6- 4- 1- 7 -53.899 6- 4- 2- 8 -0.000
6- 4- 1- 11 60.461 6- 4- 1- 13 179.562
7- 1- 4- 10 63.927 7- 1- 11- 12 -177.409
7- 1- 13- 14 -27.593 7- 1- 13- 15 171.595
7- 1- 13- 17 66.668 8- 2- 3- 9 53.899
8- 2- 4- 10 -120.495 8- 2- 3- 12 -60.461
8- 2- 3- 15 -179.562 9- 3- 12- 11 177.409
9- 3- 15- 13 -171.595 9- 3- 15- 16 27.593
9- 3- 15- 18 -66.668 10- 4- 1- 11 178.287
10- 4- 1- 13 -62.612 11- 1- 13- 14 -143.701
11- 1- 13- 15 55.487 11- 12- 3- 15 55.654
11- 1- 13- 17 -49.440 12- 3- 15- 13 -55.487
12- 11- 1- 13 -55.654 12- 3- 15- 16 143.701
12- 3- 15- 18 49.440 13- 17- 19- 18 -59.906
13- 15- 18- 19 -28.773 14- 13- 15- 16 -0.000
14- 13- 15- 18 93.370 14- 13- 17- 19 -95.597
15- 18- 19- 17 59.906 15- 13- 17- 19 28.773
16- 15- 13- 17 -93.370 16- 15- 18- 19 95.597
17- 13- 15- 18 -0.000

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5352 1- 7 1.0950 1- 11 1.4357 1- 13 1.5050
5) 2- 3 1.5352 2- 4 1.5469 2- 5 1.0954 2- 8 1.0938
9) 3- 9 1.0950 3- 12 1.4357 3- 15 1.5050 4- 6 1.0938

13) 4- 10 1.0954 11- 12 1.5049 13- 14 1.0872 13- 15 1.3952
17) 13- 17 1.9911 15- 16 1.0872 15- 18 1.9911 17- 19 1.3282
21) 18- 19 1.3282
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.017 1- 4- 10 110.230 1- 11- 12 109.838
4) 1- 13- 14 120.019 1- 13- 15 111.111 1- 13- 17 101.640
7) 2- 3- 9 112.920 2- 3- 12 108.390 2- 3- 15 108.852
10) 2- 4- 6 111.053 2- 4- 10 111.965 3- 2- 4 107.680
13) 3- 2- 5 110.230 3- 2- 8 108.017 3- 15- 16 120.019
16) 3- 15- 18 101.640 4- 1- 7 112.920 4- 1- 11 108.390
19) 4- 1- 13 108.852 4- 2- 3 107.680 4- 2- 5 111.965
22) 4- 2- 8 111.053 5- 2- 3 110.230 5- 2- 4 111.965
25) 5- 2- 8 107.834 6- 4- 10 107.834 7- 1- 4 112.920
28) 7- 1- 11 102.511 7- 1- 13 113.092 8- 2- 3 108.017
31) 8- 2- 4 111.053 8- 2- 5 107.834 9- 3- 12 102.511
34) 9- 3- 15 113.092 10- 4- 6 107.834 11- 1- 4 108.390
37) 11- 1- 7 102.511 11- 1- 13 110.869 12- 3- 9 102.511
40) 12- 3- 15 110.869 13- 1- 4 108.852 13- 1- 7 113.092
43) 13- 1- 11 110.869 13- 15- 16 122.717 13- 15- 18 101.154
46) 13- 17- 19 97.025 14- 13- 15 122.717 14- 13- 17 92.584
49) 15- 3- 9 113.092 15- 3- 12 110.869 15- 13- 14 122.717
52) 15- 13- 17 101.154 15- 18- 19 97.025 16- 15- 18 92.584
55) 17- 13- 14 92.584 17- 13- 15 101.154 18- 15- 16 92.584
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.326
1- 4- 2- 8 118.070 1- 13- 15- 16 152.305
1- 13- 15- 18 -107.251 1- 13- 17- 19 145.064
2- 4- 1- 7 -174.085 2- 3- 12- 11 -62.601
2- 4- 1- 11 -61.228 2- 3- 15- 13 61.587
2- 4- 1- 13 59.450 2- 3- 15- 16 -91.566
2- 3- 15- 18 168.519 3- 2- 4- 6 -118.070
3- 2- 4- 10 121.326 3- 15- 13- 14 -152.305
3- 15- 13- 17 107.251 3- 15- 18- 19 -145.064
4- 2- 3- 9 174.085 4- 1- 11- 12 62.601
4- 2- 3- 12 61.228 4- 1- 13- 14 91.566
4- 1- 13- 15 -61.587 4- 2- 3- 15 -59.450
4- 1- 13- 17 -168.519 5- 2- 4- 6 120.604
5- 2- 3- 9 -63.512 5- 2- 4- 10 -0.000
5- 2- 3- 12 -176.369 5- 2- 3- 15 62.953
6- 4- 1- 7 -54.074 6- 4- 2- 8 -0.000
6- 4- 1- 11 58.783 6- 4- 1- 13 179.461
7- 1- 4- 10 63.512 7- 1- 11- 12 -177.784
7- 1- 13- 14 -34.800 7- 1- 13- 15 172.047
7- 1- 13- 17 65.114 8- 2- 3- 9 54.074
8- 2- 4- 10 -120.604 8- 2- 3- 12 -58.783
8- 2- 3- 15 -179.461 9- 3- 12- 11 177.784
9- 3- 15- 13 -172.047 9- 3- 15- 16 34.800
9- 3- 15- 18 -65.114 10- 4- 1- 11 176.369
10- 4- 1- 13 -62.953 11- 1- 13- 14 -149.294
11- 1- 13- 15 57.553 11- 12- 3- 15 56.816
11- 1- 13- 17 -49.379 12- 3- 15- 13 -57.553
12- 11- 1- 13 -56.816 12- 3- 15- 16 149.294
12- 3- 15- 18 49.379 13- 17- 19- 18 -59.339
13- 15- 18- 19 -30.518 14- 13- 15- 16 -0.000
14- 13- 15- 18 100.444 14- 13- 17- 19 -93.563
15- 18- 19- 17 59.339 15- 13- 17- 19 30.518
16- 15- 13- 17 -100.444 16- 15- 18- 19 93.563
17- 13- 15- 18 -0.000

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5366 1- 7 1.0940 1- 11 1.4280 1- 13 1.5071
5) 2- 3 1.5366 2- 4 1.5491 2- 5 1.0945 2- 8 1.0932
9) 3- 9 1.0940 3- 12 1.4280 3- 15 1.5071 4- 6 1.0932
13) 4- 10 1.0945 11- 12 1.4861 13- 14 1.0867 13- 15 1.3993
17) 13- 17 1.9726 15- 16 1.0867 15- 18 1.9726 17- 19 1.3099
21) 18- 19 1.3099
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.982 1- 4- 10 110.327 1- 11- 12 110.243
4) 1- 13- 14 120.161 1- 13- 15 110.896 1- 13- 17 102.271
7) 2- 3- 9 112.990 2- 3- 12 108.507 2- 3- 15 108.429
10) 2- 4- 6 110.921 2- 4- 10 112.068 3- 2- 4 107.521
13) 3- 2- 5 110.327 3- 2- 8 107.982 3- 15- 16 120.161
16) 3- 15- 18 102.271 4- 1- 7 112.990 4- 1- 11 108.507
19) 4- 1- 13 108.429 4- 2- 3 107.521 4- 2- 5 112.068
22) 4- 2- 8 110.921 5- 2- 3 110.327 5- 2- 4 112.068
25) 5- 2- 8 107.957 6- 4- 10 107.957 7- 1- 4 112.990
28) 7- 1- 11 102.642 7- 1- 13 112.998 8- 2- 3 107.982
31) 8- 2- 4 110.921 8- 2- 5 107.957 9- 3- 12 102.642
34) 9- 3- 15 112.998 10- 4- 6 107.957 11- 1- 4 108.507
37) 11- 1- 7 102.642 11- 1- 13 111.128 12- 3- 9 102.642
40) 12- 3- 15 111.128 13- 1- 4 108.429 13- 1- 7 112.998
43) 13- 1- 11 111.128 13- 15- 16 122.653 13- 15- 18 100.842
46) 13- 17- 19 97.338 14- 13- 15 122.653 14- 13- 17 92.577
49) 15- 3- 9 112.998 15- 3- 12 111.128 15- 13- 14 122.653
52) 15- 13- 17 100.842 15- 18- 19 97.338 16- 15- 18 92.577
55) 17- 13- 14 92.577 17- 13- 15 100.842 18- 15- 16 92.577
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.403
1- 4- 2- 8 117.857 1- 13- 15- 16 152.056
1- 13- 15- 18 -107.743 1- 13- 17- 19 144.670
2- 4- 1- 7 -173.896 2- 3- 12- 11 -62.496
2- 4- 1- 11 -60.772 2- 3- 15- 13 62.168
2- 4- 1- 13 60.037 2- 3- 15- 16 -90.682
2- 3- 15- 18 168.971 3- 2- 4- 6 -117.857
3- 2- 4- 10 121.403 3- 15- 13- 14 -152.056
3- 15- 13- 17 107.743 3- 15- 18- 19 -144.670
4- 2- 3- 9 173.896 4- 1- 11- 12 62.496
4- 2- 3- 12 60.772 4- 1- 13- 14 90.682
4- 1- 13- 15 -62.168 4- 2- 3- 15 -60.037
4- 1- 13- 17 -168.971 5- 2- 4- 6 120.740
5- 2- 3- 9 -63.618 5- 2- 4- 10 -0.000
5- 2- 3- 12 -176.742 5- 2- 3- 15 62.449
6- 4- 1- 7 -54.150 6- 4- 2- 8 -0.000
6- 4- 1- 11 58.973 6- 4- 1- 13 179.783
7- 1- 4- 10 63.618 7- 1- 11- 12 -177.691
7- 1- 13- 14 -35.380 7- 1- 13- 15 171.770
7- 1- 13- 17 64.967 8- 2- 3- 9 54.150
8- 2- 4- 10 -120.740 8- 2- 3- 12 -58.973
8- 2- 3- 15 -179.783 9- 3- 12- 11 177.691
9- 3- 15- 13 -171.770 9- 3- 15- 16 35.380
9- 3- 15- 18 -64.967 10- 4- 1- 11 176.742
10- 4- 1- 13 -62.449 11- 1- 13- 14 -150.145

11- 1- 13- 15 57.005 11- 12- 3- 15 56.630
11- 1- 13- 17 -49.798 12- 3- 15- 13 -57.005
12- 11- 1- 13 -56.630 12- 3- 15- 16 150.145
12- 3- 15- 18 49.798 13- 17- 19- 18 -59.209
13- 15- 18- 19 -30.258 14- 13- 15- 16 -0.000
14- 13- 15- 18 100.201 14- 13- 17- 19 -93.696
15- 18- 19- 17 59.209 15- 13- 17- 19 30.258
16- 15- 13- 17 -100.201 16- 15- 18- 19 93.696
17- 13- 15- 18 -0.000

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5466 1- 7 1.0929 1- 11 1.4370 1- 13 1.5100
5) 2- 3 1.5466 2- 4 1.5542 2- 5 1.0955 2- 8 1.0941
9) 3- 9 1.0929 3- 12 1.4370 3- 15 1.5100 4- 6 1.0941
13) 4- 10 1.0955 11- 12 1.4845 13- 14 1.0840 13- 15 1.3664
17) 13- 17 2.3388 15- 16 1.0840 15- 18 2.3388 17- 19 1.2890
21) 18- 19 1.2890
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.149 1- 4- 10 110.304 1- 11- 12 110.328
4) 1- 13- 14 121.949 1- 13- 15 111.699 1- 13- 17 101.154
7) 2- 3- 9 112.748 2- 3- 12 107.982 2- 3- 15 108.706
10) 2- 4- 6 110.995 2- 4- 10 112.038 3- 2- 4 107.473
13) 3- 2- 5 110.304 3- 2- 8 108.149 3- 15- 16 121.949
16) 3- 15- 18 101.154 4- 1- 7 112.748 4- 1- 11 107.982
19) 4- 1- 13 108.706 4- 2- 3 107.473 4- 2- 5 112.038
22) 4- 2- 8 110.995 5- 2- 3 110.304 5- 2- 4 112.038
25) 5- 2- 8 107.826 6- 4- 10 107.826 7- 1- 4 112.748
28) 7- 1- 11 103.213 7- 1- 13 113.453 8- 2- 3 108.149
31) 8- 2- 4 110.995 8- 2- 5 107.826 9- 3- 12 103.213
34) 9- 3- 15 113.453 10- 4- 6 107.826 11- 1- 4 107.982
37) 11- 1- 7 103.213 11- 1- 13 110.518 12- 3- 9 103.213
40) 12- 3- 15 110.518 13- 1- 4 108.706 13- 1- 7 113.453
43) 13- 1- 11 110.518 13- 15- 16 124.832 13- 15- 18 99.799
46) 13- 17- 19 96.587 14- 13- 15 124.832 14- 13- 17 82.497
49) 15- 3- 9 113.453 15- 3- 12 110.518 15- 13- 14 124.832
52) 15- 13- 17 99.799 15- 18- 19 96.587 16- 15- 18 82.497
55) 17- 13- 14 82.497 17- 13- 15 99.799 18- 15- 16 82.497
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.324
1- 4- 2- 8 118.072 1- 13- 15- 16 166.104
1- 13- 15- 18 -106.260 1- 13- 17- 19 143.348
2- 4- 1- 7 -174.353 2- 3- 12- 11 -62.814
2- 4- 1- 11 -60.983 2- 3- 15- 13 61.581
2- 4- 1- 13 58.948 2- 3- 15- 16 -104.985
2- 3- 15- 18 166.958 3- 2- 4- 6 -118.072
3- 2- 4- 10 121.324 3- 15- 13- 14 -166.104
3- 15- 13- 17 106.260 3- 15- 18- 19 -143.348
4- 2- 3- 9 174.353 4- 1- 11- 12 62.814
4- 2- 3- 12 60.983 4- 1- 13- 14 104.985
4- 1- 13- 15 -61.581 4- 2- 3- 15 -58.948
4- 1- 13- 17 -166.958 5- 2- 4- 6 120.604
5- 2- 3- 9 -63.242 5- 2- 4- 10 -0.000
5- 2- 3- 12 -176.612 5- 2- 3- 15 63.457

6- 4- 1- 7 -54.455 6- 4- 2- 8 -0.000
6- 4- 1- 11 58.916 6- 4- 1- 13 178.847
7- 1- 4- 10 63.242 7- 1- 11- 12 -177.596
7- 1- 13- 14 -21.307 7- 1- 13- 15 172.127
7- 1- 13- 17 66.750 8- 2- 3- 9 54.455
8- 2- 4- 10 -120.604 8- 2- 3- 12 -58.916
8- 2- 3- 15 -178.847 9- 3- 12- 11 177.596
9- 3- 15- 13 -172.127 9- 3- 15- 16 21.307
9- 3- 15- 18 -66.750 10- 4- 1- 11 176.612
10- 4- 1- 13 -63.457 11- 1- 13- 14 -136.673
11- 1- 13- 15 56.761 11- 12- 3- 15 55.969
11- 1- 13- 17 -48.616 12- 3- 15- 13 -56.761
12- 11- 1- 13 -55.969 12- 3- 15- 16 136.673
12- 3- 15- 18 48.616 13- 17- 19- 18 -60.486
13- 15- 18- 19 -28.735 14- 13- 15- 16 -0.000
14- 13- 15- 18 87.636 14- 13- 17- 19 -95.451
15- 18- 19- 17 60.486 15- 13- 17- 19 28.735
16- 15- 13- 17 -87.636 16- 15- 18- 19 95.451
17- 13- 15- 18 -0.000

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5441 1- 7 1.0925 1- 11 1.4479 1- 13 1.5074
5) 2- 3 1.5441 2- 4 1.5525 2- 5 1.0944 2- 8 1.0939
9) 3- 9 1.0925 3- 12 1.4479 3- 15 1.5074 4- 6 1.0939
13) 4- 10 1.0944 11- 12 1.4863 13- 14 1.0838 13- 15 1.3624
17) 13- 17 2.4409 15- 16 1.0838 15- 18 2.4409 17- 19 1.2867
21) 18- 19 1.2867
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.233 1- 4- 10 109.974 1- 11- 12 110.188
4) 1- 13- 14 122.053 1- 13- 15 111.874 1- 13- 17 102.117
7) 2- 3- 9 112.827 2- 3- 12 108.049 2- 3- 15 108.945
10) 2- 4- 6 111.181 2- 4- 10 112.086 3- 2- 4 107.587
13) 3- 2- 5 109.974 3- 2- 8 108.233 3- 15- 16 122.053
16) 3- 15- 18 102.117 4- 1- 7 112.827 4- 1- 11 108.049
19) 4- 1- 13 108.945 4- 2- 3 107.587 4- 2- 5 112.086
22) 4- 2- 8 111.181 5- 2- 3 109.974 5- 2- 4 112.086
25) 5- 2- 8 107.721 6- 4- 10 107.721 7- 1- 4 112.827
28) 7- 1- 11 103.037 7- 1- 13 113.631 8- 2- 3 108.233
31) 8- 2- 4 111.181 8- 2- 5 107.721 9- 3- 12 103.037
34) 9- 3- 15 113.631 10- 4- 6 107.721 11- 1- 4 108.049
37) 11- 1- 7 103.037 11- 1- 13 110.081 12- 3- 9 103.037
40) 12- 3- 15 110.081 13- 1- 4 108.945 13- 1- 7 113.631
43) 13- 1- 11 110.081 13- 15- 16 124.970 13- 15- 18 99.474
46) 13- 17- 19 96.189 14- 13- 15 124.970 14- 13- 17 80.205
49) 15- 3- 9 113.631 15- 3- 12 110.081 15- 13- 14 124.970
52) 15- 13- 17 99.474 15- 18- 19 96.189 16- 15- 18 80.205
55) 17- 13- 14 80.205 17- 13- 15 99.474 18- 15- 16 80.205
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -0.000 1- 11- 12- 3 -0.000
1- 13- 15- 3 -0.000 1- 4- 2- 5 -121.020
1- 4- 2- 8 118.348 1- 13- 15- 16 168.143
1- 13- 15- 18 -107.237 1- 13- 17- 19 143.757
2- 4- 1- 7 -174.290 2- 3- 12- 11 -62.716
2- 4- 1- 11 -61.050 2- 3- 15- 13 61.180

2- 4- 1- 13 58.532 2- 3- 15- 16 -107.362
2- 3- 15- 18 166.702 3- 2- 4- 6 -118.348
3- 2- 4- 10 121.020 3- 15- 13- 14 -168.143
3- 15- 13- 17 107.237 3- 15- 18- 19 -143.757
4- 2- 3- 9 174.290 4- 1- 11- 12 62.716
4- 2- 3- 12 61.050 4- 1- 13- 14 107.362
4- 1- 13- 15 -61.180 4- 2- 3- 15 -58.532
4- 1- 13- 17 -166.702 5- 2- 4- 6 120.632
5- 2- 3- 9 -63.375 5- 2- 4- 10 -0.000
5- 2- 3- 12 -176.614 5- 2- 3- 15 63.804
6- 4- 1- 7 -54.059 6- 4- 2- 8 -0.000
6- 4- 1- 11 59.181 6- 4- 1- 13 178.762
7- 1- 4- 10 63.375 7- 1- 11- 12 -177.662
7- 1- 13- 14 -19.359 7- 1- 13- 15 172.099
7- 1- 13- 17 66.578 8- 2- 3- 9 54.059
8- 2- 4- 10 -120.632 8- 2- 3- 12 -59.181
8- 2- 3- 15 -178.762 9- 3- 12- 11 177.662
9- 3- 15- 13 -172.099 9- 3- 15- 16 19.359
9- 3- 15- 18 -66.578 10- 4- 1- 11 176.614
10- 4- 1- 13 -63.804 11- 1- 13- 14 -134.327
11- 1- 13- 15 57.131 11- 12- 3- 15 56.146
11- 1- 13- 17 -48.390 12- 3- 15- 13 -57.131
12- 11- 1- 13 -56.146 12- 3- 15- 16 134.327
12- 3- 15- 18 48.390 13- 17- 19- 18 -61.598
13- 15- 18- 19 -28.786 14- 13- 15- 16 -0.000
14- 13- 15- 18 84.620 14- 13- 17- 19 -95.329
15- 18- 19- 17 61.598 15- 13- 17- 19 28.786
16- 15- 13- 17 -84.620 16- 15- 18- 19 95.329
17- 13- 15- 18 -0.000

Optimised structures for the transition state for primary ozonide 16a.ring-opening at all levels reported.

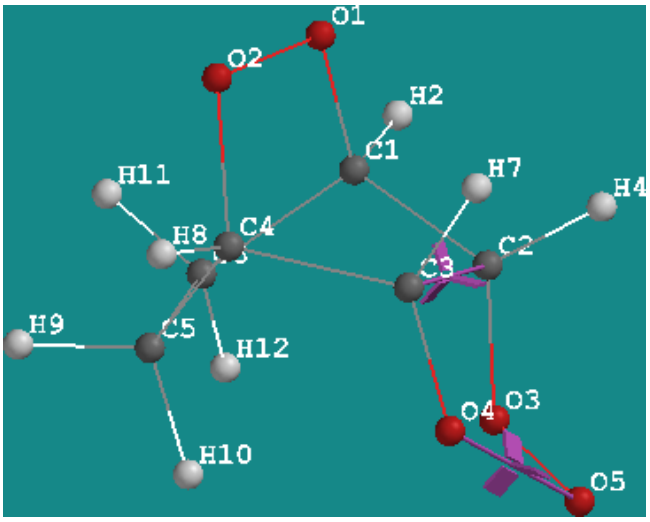

Figure S13: Optimised geometry for primary ozonide TS ring-opening **16a**.

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5242 1- 7 1.0827 1- 11 1.4100 1- 13 1.5130
5) 2- 3 1.5253 2- 4 1.5425 2- 5 1.0821 2- 8 1.0829
9) 3- 9 1.0819 3- 12 1.4169 3- 14 1.5327 4- 6 1.0827
13) 4- 10 1.0822 11- 12 1.4085 13- 14 1.9339 13- 15 1.0750
17) 13- 17 1.2952 14- 16 1.0866 14- 18 1.2525 17- 19 1.2896
21) 18- 19 1.9483
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.268 1- 4- 10 110.214 1- 11- 12 112.169
4) 1- 13- 14 103.898 1- 13- 15 120.111 1- 13- 17 115.599
7) 2- 3- 9 111.865 2- 3- 12 109.372 2- 3- 14 114.337
10) 2- 4- 6 110.898 2- 4- 10 111.765 3- 2- 4 107.742
13) 3- 2- 5 109.563 3- 2- 8 109.560 3- 14- 16 113.513
16) 3- 14- 18 120.293 4- 1- 7 112.433 4- 1- 11 111.006
19) 4- 1- 13 111.581 4- 2- 3 107.742 4- 2- 5 111.898
22) 4- 2- 8 110.246 5- 2- 3 109.563 5- 2- 4 111.898
25) 5- 2- 8 107.819 6- 4- 10 107.955 7- 1- 4 112.433
28) 7- 1- 11 104.315 7- 1- 13 111.469 8- 2- 3 109.560
31) 8- 2- 4 110.246 8- 2- 5 107.819 9- 3- 12 103.106
34) 9- 3- 14 108.877 10- 4- 6 107.955 11- 1- 4 111.006
37) 11- 1- 7 104.315 11- 1- 13 105.588 12- 3- 9 103.106
40) 12- 3- 14 108.648 13- 1- 4 111.581 13- 1- 7 111.469
43) 13- 1- 11 105.588 13- 14- 16 99.002 13- 14- 18 102.533
46) 13- 17- 19 112.405 14- 3- 9 108.877 14- 3- 12 108.648
49) 14- 13- 15 96.766 14- 13- 17 97.252 14- 18- 19 103.841
52) 15- 13- 14 96.766 15- 13- 17 116.542 16- 14- 18 117.634
55) 17- 13- 14 97.252 17- 13- 15 116.542 18- 14- 16 117.634
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 19.713 1- 11- 12- 3 25.668
1- 13- 14- 3 16.977 1- 4- 2- 5 -100.786
1- 4- 2- 8 139.229 1- 13- 14- 16 -98.446
1- 13- 14- 18 140.470 1- 13- 17- 19 -163.154
```

2- 4- 1- 7 179.315 2- 3- 12- 11 -70.751
2- 4- 1- 11 -64.257 2- 3- 14- 13 53.146
2- 4- 1- 13 53.222 2- 3- 14- 16 156.536
2- 3- 14- 18 -56.326 3- 2- 4- 6 -97.944
3- 2- 4- 10 141.541 3- 14- 13- 15 140.329
3- 14- 13- 17 -101.721 3- 14- 18- 19 113.076
4- 2- 3- 9 155.455 4- 1- 11- 12 40.636
4- 2- 3- 12 41.871 4- 1- 13- 14 -71.785
4- 2- 3- 14 -80.204 4- 1- 13- 15 -178.272
4- 1- 13- 17 33.448 5- 2- 4- 6 141.558
5- 2- 3- 9 -82.590 5- 2- 4- 10 21.043
5- 2- 3- 12 163.827 5- 2- 3- 14 41.751
6- 4- 1- 7 -60.743 6- 4- 2- 8 21.572
6- 4- 1- 11 55.685 6- 4- 1- 13 173.164
7- 1- 4- 10 56.545 7- 1- 11- 12 161.958
7- 1- 13- 14 161.594 7- 1- 13- 15 55.107
7- 1- 13- 17 -93.173 8- 2- 3- 9 35.504
8- 2- 4- 10 -98.943 8- 2- 3- 12 -78.080
8- 2- 3- 14 159.845 9- 3- 12- 11 170.093
9- 3- 14- 13 179.065 9- 3- 14- 16 -77.546
9- 3- 14- 18 69.593 10- 4- 1- 11 172.973
10- 4- 1- 13 -69.548 11- 1- 13- 14 48.916
11- 12- 3- 14 54.679 11- 1- 13- 15 -57.571
11- 1- 13- 17 154.149 12- 3- 14- 13 -69.325
12- 11- 1- 13 -80.440 12- 3- 14- 16 34.065
12- 3- 14- 18 -178.796 13- 17- 19- 18 56.345
13- 14- 18- 19 6.204 14- 18- 19- 17 -34.217
14- 13- 17- 19 -53.918 15- 13- 14- 16 24.906
15- 13- 14- 18 -96.177 15- 13- 17- 19 47.403
16- 14- 13- 17 142.857 16- 14- 18- 19 -101.092
17- 13- 14- 18 21.773

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5226 1- 7 1.0816 1- 11 1.4162 1- 13 1.5144
5) 2- 3 1.5242 2- 4 1.5418 2- 5 1.0822 2- 8 1.0823
9) 3- 9 1.0817 3- 12 1.4201 3- 14 1.5334 4- 6 1.0822
13) 4- 10 1.0814 11- 12 1.4095 13- 14 1.9074 13- 15 1.0752
17) 13- 17 1.3004 14- 16 1.0864 14- 18 1.2587 17- 19 1.2917
21) 18- 19 1.9446
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.315 1- 4- 10 110.175 1- 11- 12 112.119
4) 1- 13- 14 104.231 1- 13- 15 119.867 1- 13- 17 115.256
7) 2- 3- 9 112.064 2- 3- 12 109.348 2- 3- 14 114.612
10) 2- 4- 6 110.977 2- 4- 10 111.769 3- 2- 4 107.858
13) 3- 2- 5 109.501 3- 2- 8 109.365 3- 14- 16 113.433
16) 3- 14- 18 120.271 4- 1- 7 112.696 4- 1- 11 110.953
19) 4- 1- 13 111.757 4- 2- 3 107.858 4- 2- 5 111.979
22) 4- 2- 8 110.397 5- 2- 3 109.501 5- 2- 4 111.979
25) 5- 2- 8 107.719 6- 4- 10 107.895 7- 1- 4 112.696
28) 7- 1- 11 104.314 7- 1- 13 111.258 8- 2- 3 109.365
31) 8- 2- 4 110.397 8- 2- 5 107.719 9- 3- 12 103.177
34) 9- 3- 14 108.812 10- 4- 6 107.895 11- 1- 4 110.953
37) 11- 1- 7 104.314 11- 1- 13 105.366 12- 3- 9 103.177
40) 12- 3- 14 108.145 13- 1- 4 111.757 13- 1- 7 111.258
43) 13- 1- 11 105.366 13- 14- 16 99.227 13- 14- 18 103.131

46) 13- 17- 19 112.212 14- 3- 9 108.812 14- 3- 12 108.145
49) 14- 13- 15 97.539 14- 13- 17 97.558 14- 18- 19 103.429
52) 15- 13- 14 97.539 15- 13- 17 116.344 16- 14- 18 116.930
55) 17- 13- 14 97.558 17- 13- 15 116.344 18- 14- 16 116.930
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 19.127 1- 11- 12- 3 24.972
1- 13- 14- 3 17.055 1- 4- 2- 5 -101.420
1- 4- 2- 8 138.564 1- 13- 14- 16 -98.474
1- 13- 14- 18 140.925 1- 13- 17- 19 -163.617
2- 4- 1- 7 179.268 2- 3- 12- 11 -70.642
2- 4- 1- 11 -64.173 2- 3- 14- 13 52.614
2- 4- 1- 13 53.107 2- 3- 14- 16 156.506
2- 3- 14- 18 -57.953 3- 2- 4- 6 -98.616
3- 2- 4- 10 140.889 3- 14- 13- 15 140.545
3- 14- 13- 17 -101.478 3- 14- 18- 19 113.518
4- 2- 3- 9 156.338 4- 1- 11- 12 41.237
4- 2- 3- 12 42.571 4- 1- 13- 14 -71.676
4- 2- 3- 14 -79.023 4- 1- 13- 15 -179.237
4- 1- 13- 17 33.969 5- 2- 4- 6 140.838
5- 2- 3- 9 -81.573 5- 2- 4- 10 20.343
5- 2- 3- 12 164.660 5- 2- 3- 14 43.066
6- 4- 1- 7 -60.686 6- 4- 2- 8 20.822
6- 4- 1- 11 55.873 6- 4- 1- 13 173.153
7- 1- 4- 10 56.537 7- 1- 11- 12 162.845
7- 1- 13- 14 161.380 7- 1- 13- 15 53.819
7- 1- 13- 17 -92.975 8- 2- 3- 9 36.248
8- 2- 4- 10 -99.674 8- 2- 3- 12 -77.519
8- 2- 3- 14 160.887 9- 3- 12- 11 169.946
9- 3- 14- 13 178.953 9- 3- 14- 16 -77.155
9- 3- 14- 18 68.385 10- 4- 1- 11 173.096
10- 4- 1- 13 -69.624 11- 1- 13- 14 48.920
11- 12- 3- 14 54.779 11- 1- 13- 15 -58.641
11- 1- 13- 17 154.565 12- 3- 14- 13 -69.635
12- 11- 1- 13 -79.886 12- 3- 14- 16 34.257
12- 3- 14- 18 179.797 13- 17- 19- 18 55.776
13- 14- 18- 19 5.554 14- 18- 19- 17 -33.500
14- 13- 17- 19 -53.937 15- 13- 14- 16 25.016
15- 13- 14- 18 -95.585 15- 13- 17- 19 48.385
16- 14- 13- 17 142.992 16- 14- 18- 19 -102.095
17- 13- 14- 18 22.391

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5231 1- 7 1.0966 1- 11 1.4365 1- 13 1.5136
5) 2- 3 1.5205 2- 4 1.5406 2- 5 1.0946 2- 8 1.0934
9) 3- 9 1.0963 3- 12 1.4381 3- 14 1.5418 4- 6 1.0934
13) 4- 10 1.0941 11- 12 1.5015 13- 14 1.7664 13- 15 1.0909
17) 13- 17 1.3719 14- 16 1.1065 14- 18 1.3026 17- 19 1.3341
21) 18- 19 2.1891
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.078 1- 4- 10 110.506 1- 11- 12 109.343
4) 1- 13- 14 107.309 1- 13- 15 119.718 1- 13- 17 111.575
7) 2- 3- 9 112.944 2- 3- 12 110.300 2- 3- 14 112.953
10) 2- 4- 6 111.195 2- 4- 10 111.901 3- 2- 4 107.172
13) 3- 2- 5 108.549 3- 2- 8 110.314 3- 14- 16 110.817

16) 3- 14- 18 117.649 4- 1- 7 113.074 4- 1- 11 111.211
19) 4- 1- 13 111.121 4- 2- 3 107.172 4- 2- 5 112.240
22) 4- 2- 8 110.637 5- 2- 3 108.549 5- 2- 4 112.240
25) 5- 2- 8 107.918 6- 4- 10 108.026 7- 1- 4 113.074
28) 7- 1- 11 103.052 7- 1- 13 112.332 8- 2- 3 110.314
31) 8- 2- 4 110.637 8- 2- 5 107.918 9- 3- 12 102.665
34) 9- 3- 14 108.121 10- 4- 6 108.026 11- 1- 4 111.211
37) 11- 1- 7 103.052 11- 1- 13 105.512 12- 3- 9 102.665
40) 12- 3- 14 109.323 13- 1- 4 111.121 13- 1- 7 112.332
43) 13- 1- 11 105.512 13- 14- 16 100.261 13- 14- 18 107.337
46) 13- 17- 19 110.632 14- 3- 9 108.121 14- 3- 12 109.323
49) 14- 13- 15 101.531 14- 13- 17 101.938 14- 18- 19 98.874
52) 15- 13- 14 101.531 15- 13- 17 112.481 16- 14- 18 117.699
55) 17- 13- 14 101.938 17- 13- 15 112.481 18- 14- 16 117.699

Dihedrals

I J K L Theta I J K L Theta
1- 4- 2- 3 22.401 1- 11- 12- 3 25.581
1- 13- 14- 3 18.892 1- 4- 2- 5 -96.682
1- 4- 2- 8 142.709 1- 13- 14- 16 -94.519
1- 13- 14- 18 142.020 1- 13- 17- 19 -175.898
2- 4- 1- 7 175.464 2- 3- 12- 11 -72.600
2- 4- 1- 11 -69.155 2- 3- 14- 13 51.236
2- 4- 1- 13 48.069 2- 3- 14- 16 156.205
2- 3- 14- 18 -64.280 3- 2- 4- 6 -94.826
3- 2- 4- 10 144.269 3- 14- 13- 15 145.300
3- 14- 13- 17 -98.467 3- 14- 18- 19 116.451
4- 2- 3- 9 157.531 4- 1- 11- 12 42.211
4- 2- 3- 12 43.298 4- 1- 13- 14 -71.632
4- 2- 3- 14 -79.372 4- 1- 13- 15 173.597
4- 1- 13- 17 39.236 5- 2- 4- 6 146.091
5- 2- 3- 9 -81.034 5- 2- 4- 10 25.186
5- 2- 3- 12 164.733 5- 2- 3- 14 42.063
6- 4- 1- 7 -64.682 6- 4- 2- 8 25.482
6- 4- 1- 11 50.700 6- 4- 1- 13 167.923
7- 1- 4- 10 52.740 7- 1- 11- 12 163.646
7- 1- 13- 14 160.569 7- 1- 13- 15 45.798
7- 1- 13- 17 -88.563 8- 2- 3- 9 37.017
8- 2- 4- 10 -95.423 8- 2- 3- 12 -77.216
8- 2- 3- 14 160.114 9- 3- 12- 11 166.794
9- 3- 14- 13 176.971 9- 3- 14- 16 -78.060
9- 3- 14- 18 61.455 10- 4- 1- 11 168.121
10- 4- 1- 13 -74.656 11- 1- 13- 14 49.015
11- 12- 3- 14 52.173 11- 1- 13- 15 -65.756
11- 1- 13- 17 159.883 12- 3- 14- 13 -71.976
12- 11- 1- 13 -78.377 12- 3- 14- 16 32.992
12- 3- 14- 18 172.507 13- 17- 19- 18 56.108
13- 14- 18- 19 5.186 14- 18- 19- 17 -35.177
14- 13- 17- 19 -61.654 15- 13- 14- 16 31.889
15- 13- 14- 18 -91.572 15- 13- 17- 19 46.322
16- 14- 13- 17 148.122 16- 14- 18- 19 -106.816
17- 13- 14- 18 24.661

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5243 1- 7 1.0953 1- 11 1.4291 1- 13 1.5196
5) 2- 3 1.5163 2- 4 1.5414 2- 5 1.0912 2- 8 1.0934
9) 3- 9 1.0946 3- 12 1.4135 3- 14 1.5867 4- 6 1.0927
13) 4- 10 1.0931 11- 12 1.4839 13- 14 1.6183 13- 15 1.0945
17) 13- 17 1.4016 14- 16 1.1070 14- 18 1.3154 17- 19 1.3328
21) 18- 19 2.4878
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 109.348 1- 4- 10 109.893 1- 11- 12 108.813
4) 1- 13- 14 112.142 1- 13- 15 113.736 1- 13- 17 107.109
7) 2- 3- 9 113.180 2- 3- 12 112.898 2- 3- 14 111.855
10) 2- 4- 6 111.179 2- 4- 10 111.891 3- 2- 4 108.576
13) 3- 2- 5 109.014 3- 2- 8 107.421 3- 14- 16 107.839
16) 3- 14- 18 111.634 4- 1- 7 113.465 4- 1- 11 109.731
19) 4- 1- 13 110.410 4- 2- 3 108.576 4- 2- 5 111.865
22) 4- 2- 8 110.966 5- 2- 3 109.014 5- 2- 4 111.865
25) 5- 2- 8 108.881 6- 4- 10 108.257 7- 1- 4 113.465
28) 7- 1- 11 103.329 7- 1- 13 111.151 8- 2- 3 107.421
31) 8- 2- 4 110.966 8- 2- 5 108.881 9- 3- 12 103.505
34) 9- 3- 14 106.810 10- 4- 6 108.257 11- 1- 4 109.731
37) 11- 1- 7 103.329 11- 1- 13 108.429 12- 3- 9 103.505
40) 12- 3- 14 108.045 13- 1- 4 110.410 13- 1- 7 111.151
43) 13- 1- 11 108.429 13- 14- 16 107.590 13- 14- 18 113.520
46) 13- 17- 19 111.251 14- 3- 9 106.810 14- 3- 12 108.045
49) 14- 13- 15 104.369 14- 13- 17 109.053 14- 18- 19 83.321
52) 15- 13- 14 104.369 15- 13- 17 110.397 16- 14- 18 115.747
55) 17- 13- 14 109.053 17- 13- 15 110.397 18- 14- 16 115.747
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -14.178 1- 11- 12- 3 -22.314
1- 13- 14- 3 -14.859 1- 4- 2- 5 -134.522
1- 4- 2- 8 103.663 1- 13- 14- 16 -126.959
1- 13- 14- 18 103.623 1- 13- 17- 19 -169.486
2- 4- 1- 7 -165.231 2- 3- 12- 11 -44.607
2- 4- 1- 11 -50.227 2- 3- 14- 13 71.512
2- 4- 1- 13 69.232 2- 3- 14- 16 -176.585
2- 3- 14- 18 -48.373 3- 2- 4- 6 -133.058
3- 2- 4- 10 105.759 3- 14- 13- 15 108.705
3- 14- 13- 17 -133.319 3- 14- 18- 19 145.974
4- 2- 3- 9 -177.870 4- 1- 11- 12 73.589
4- 2- 3- 12 64.961 4- 1- 13- 14 -51.772
4- 2- 3- 14 -57.160 4- 1- 13- 15 -169.912
4- 1- 13- 17 67.832 5- 2- 4- 6 106.597
5- 2- 3- 9 -55.773 5- 2- 4- 10 -14.585
5- 2- 3- 12 -172.942 5- 2- 3- 14 64.937
6- 4- 1- 7 -45.155 6- 4- 2- 8 -15.217
6- 4- 1- 11 69.849 6- 4- 1- 13 -170.691
7- 1- 4- 10 73.541 7- 1- 11- 12 -165.099
7- 1- 13- 14 -178.607 7- 1- 13- 15 63.254
7- 1- 13- 17 -59.003 8- 2- 3- 9 62.058
8- 2- 4- 10 -136.400 8- 2- 3- 12 -55.111
8- 2- 3- 14 -177.232 9- 3- 12- 11 -167.351
9- 3- 14- 13 -164.141 9- 3- 14- 16 -52.238
9- 3- 14- 18 75.973 10- 4- 1- 11 -171.455
10- 4- 1- 13 -51.996 11- 1- 13- 14 68.471
11- 12- 3- 14 79.629 11- 1- 13- 15 -49.668
11- 1- 13- 17 -171.925 12- 3- 14- 13 -53.348

12- 11- 1- 13 -47.077 12- 3- 14- 16 58.555
12- 3- 14- 18 -173.234 13- 17- 19- 18 54.288
13- 14- 18- 19 34.990 14- 18- 19- 17 -57.305
14- 13- 17- 19 -47.917 15- 13- 14- 16 -3.396
15- 13- 14- 18 -132.814 15- 13- 17- 19 66.195
16- 14- 13- 17 114.581 16- 14- 18- 19 -90.166
17- 13- 14- 18 -14.837

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5318 1- 7 1.0970 1- 11 1.4319 1- 13 1.5159
5) 2- 3 1.5303 2- 4 1.5485 2- 5 1.0942 2- 8 1.0937
9) 3- 9 1.0967 3- 12 1.4299 3- 14 1.5540 4- 6 1.0938
13) 4- 10 1.0937 11- 12 1.4850 13- 14 1.9403 13- 15 1.0875
17) 13- 17 1.3309 14- 16 1.1054 14- 18 1.2690 17- 19 1.3291
21) 18- 19 2.0890
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.147 1- 4- 10 110.194 1- 11- 12 111.084
4) 1- 13- 14 105.306 1- 13- 15 120.461 1- 13- 17 114.830
7) 2- 3- 9 112.109 2- 3- 12 111.263 2- 3- 14 113.865
10) 2- 4- 6 111.221 2- 4- 10 111.652 3- 2- 4 108.149
13) 3- 2- 5 108.507 3- 2- 8 110.048 3- 14- 16 111.946
16) 3- 14- 18 120.119 4- 1- 7 112.317 4- 1- 11 111.319
19) 4- 1- 13 111.760 4- 2- 3 108.149 4- 2- 5 111.834
22) 4- 2- 8 110.426 5- 2- 3 108.507 5- 2- 4 111.834
25) 5- 2- 8 107.857 6- 4- 10 107.939 7- 1- 4 112.317
28) 7- 1- 11 102.958 7- 1- 13 111.797 8- 2- 3 110.048
31) 8- 2- 4 110.426 8- 2- 5 107.857 9- 3- 12 102.060
34) 9- 3- 14 107.800 10- 4- 6 107.939 11- 1- 4 111.319
37) 11- 1- 7 102.958 11- 1- 13 106.189 12- 3- 9 102.060
40) 12- 3- 14 109.032 13- 1- 4 111.760 13- 1- 7 111.797
43) 13- 1- 11 106.189 13- 14- 16 98.870 13- 14- 18 103.920
46) 13- 17- 19 111.997 14- 3- 9 107.800 14- 3- 12 109.032
49) 14- 13- 15 96.013 14- 13- 17 98.660 14- 18- 19 102.241
52) 15- 13- 14 96.013 15- 13- 17 115.802 16- 14- 18 119.007
55) 17- 13- 14 98.660 17- 13- 15 115.802 18- 14- 16 119.007
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 19.599 1- 11- 12- 3 21.060
1- 13- 14- 3 15.410 1- 4- 2- 5 -99.819
1- 4- 2- 8 140.066 1- 13- 14- 16 -98.174
1- 13- 14- 18 138.848 1- 13- 17- 19 -168.060
2- 4- 1- 7 179.186 2- 3- 12- 11 -68.002
2- 4- 1- 11 -65.956 2- 3- 14- 13 54.298
2- 4- 1- 13 52.600 2- 3- 14- 16 156.809
2- 3- 14- 18 -56.246 3- 2- 4- 6 -98.066
3- 2- 4- 10 141.294 3- 14- 13- 15 139.282
3- 14- 13- 17 -103.411 3- 14- 18- 19 115.568
4- 2- 3- 9 156.572 4- 1- 11- 12 44.043
4- 2- 3- 12 42.989 4- 1- 13- 14 -70.485
4- 2- 3- 14 -80.708 4- 1- 13- 15 -177.161
4- 1- 13- 17 36.892 5- 2- 4- 6 142.515
5- 2- 3- 9 -81.930 5- 2- 4- 10 21.875
5- 2- 3- 12 164.486 5- 2- 3- 14 40.790
6- 4- 1- 7 -60.585 6- 4- 2- 8 22.401
6- 4- 1- 11 54.273 6- 4- 1- 13 172.829

7- 1- 4- 10 56.604 7- 1- 11- 12 164.577
7- 1- 13- 14 162.648 7- 1- 13- 15 55.971
7- 1- 13- 17 -89.976 8- 2- 3- 9 35.869
8- 2- 4- 10 -98.239 8- 2- 3- 12 -77.714
8- 2- 3- 14 158.589 9- 3- 12- 11 172.255
9- 3- 14- 13 179.348 9- 3- 14- 16 -78.141
9- 3- 14- 18 68.804 10- 4- 1- 11 171.462
10- 4- 1- 13 -69.982 11- 1- 13- 14 51.082
11- 12- 3- 14 58.403 11- 1- 13- 15 -55.594
11- 1- 13- 17 158.459 12- 3- 14- 13 -70.599
12- 11- 1- 13 -77.807 12- 3- 14- 16 31.911
12- 3- 14- 18 178.857 13- 17- 19- 18 57.855
13- 14- 18- 19 8.830 14- 18- 19- 17 -37.541
14- 13- 17- 19 -56.671 15- 13- 14- 16 25.698
15- 13- 14- 18 -97.280 15- 13- 17- 19 44.359
16- 14- 13- 17 143.005 16- 14- 18- 19 -99.776
17- 13- 14- 18 20.027

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5290 1- 7 1.0956 1- 11 1.4379 1- 13 1.5182
5) 2- 3 1.5285 2- 4 1.5480 2- 5 1.0941 2- 8 1.0932
9) 3- 9 1.0962 3- 12 1.4326 3- 14 1.5562 4- 6 1.0931
13) 4- 10 1.0928 11- 12 1.4869 13- 14 1.8962 13- 15 1.0879
17) 13- 17 1.3380 14- 16 1.1048 14- 18 1.2783 17- 19 1.3319
21) 18- 19 2.0842
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.252 1- 4- 10 110.170 1- 11- 12 111.030
4) 1- 13- 14 105.920 1- 13- 15 119.863 1- 13- 17 114.321
7) 2- 3- 9 112.310 2- 3- 12 111.272 2- 3- 14 114.382
10) 2- 4- 6 111.319 2- 4- 10 111.700 3- 2- 4 108.320
13) 3- 2- 5 108.586 3- 2- 8 109.693 3- 14- 16 111.599
16) 3- 14- 18 120.067 4- 1- 7 112.628 4- 1- 11 111.251
19) 4- 1- 13 111.992 4- 2- 3 108.320 4- 2- 5 111.975
22) 4- 2- 8 110.579 5- 2- 3 108.586 5- 2- 4 111.975
25) 5- 2- 8 107.654 6- 4- 10 107.826 7- 1- 4 112.628
28) 7- 1- 11 102.969 7- 1- 13 111.434 8- 2- 3 109.693
31) 8- 2- 4 110.579 8- 2- 5 107.654 9- 3- 12 102.209
34) 9- 3- 14 107.635 10- 4- 6 107.826 11- 1- 4 111.251
37) 11- 1- 7 102.969 11- 1- 13 106.013 12- 3- 9 102.209
40) 12- 3- 14 108.243 13- 1- 4 111.992 13- 1- 7 111.434
43) 13- 1- 11 106.013 13- 14- 16 99.344 13- 14- 18 104.976
46) 13- 17- 19 111.798 14- 3- 9 107.635 14- 3- 12 108.243
49) 14- 13- 15 97.232 14- 13- 17 99.203 14- 18- 19 101.506
52) 15- 13- 14 97.232 15- 13- 17 115.485 16- 14- 18 118.011
55) 17- 13- 14 99.203 17- 13- 15 115.485 18- 14- 16 118.011
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 18.295 1- 11- 12- 3 19.473
1- 13- 14- 3 15.391 1- 4- 2- 5 -101.419
1- 4- 2- 8 138.526 1- 13- 14- 16 -98.114
1- 13- 14- 18 139.426 1- 13- 17- 19 -168.734
2- 4- 1- 7 179.245 2- 3- 12- 11 -67.582
2- 4- 1- 11 -65.731 2- 3- 14- 13 53.642
2- 4- 1- 13 52.710 2- 3- 14- 16 156.937
2- 3- 14- 18 -58.688 3- 2- 4- 6 -99.488

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3- 2- 4- 10 139.916 3- 14- 13- 15 139.318
3- 14- 13- 17 -103.299 3- 14- 18- 19 116.443
4- 2- 3- 9 158.227 4- 1- 11- 12 45.439
4- 2- 3- 12 44.332 4- 1- 13- 14 -70.380
4- 2- 3- 14 -78.713 4- 1- 13- 15 -178.724
4- 1- 13- 17 37.765 5- 2- 4- 6 140.799
5- 2- 3- 9 -79.956 5- 2- 4- 10 20.202
5- 2- 3- 12 166.149 5- 2- 3- 14 43.104
6- 4- 1- 7 -60.411 6- 4- 2- 8 20.744
6- 4- 1- 11 54.612 6- 4- 1- 13 173.054
7- 1- 4- 10 56.691 7- 1- 11- 12 166.315
7- 1- 13- 14 162.441 7- 1- 13- 15 54.097
7- 1- 13- 17 -89.415 8- 2- 3- 9 37.444
8- 2- 4- 10 -99.853 8- 2- 3- 12 -76.451
8- 2- 3- 14 160.504 9- 3- 12- 11 172.349
9- 3- 14- 13 179.193 9- 3- 14- 16 -77.512
9- 3- 14- 18 66.862 10- 4- 1- 11 171.714
10- 4- 1- 13 -69.844 11- 1- 13- 14 51.126
11- 12- 3- 14 58.915 11- 1- 13- 15 -57.218
11- 1- 13- 17 159.270 12- 3- 14- 13 -71.025
12- 11- 1- 13 -76.542 12- 3- 14- 16 32.270
12- 3- 14- 18 176.644 13- 17- 19- 18 56.903
13- 14- 18- 19 8.035 14- 18- 19- 17 -36.521
14- 13- 17- 19 -56.515 15- 13- 14- 16 25.813
15- 13- 14- 18 -96.647 15- 13- 17- 19 46.106
16- 14- 13- 17 143.196 16- 14- 18- 19 -101.396
17- 13- 14- 18 20.737
```

Optimised structures for the transition state for primary ozonide 16b.ring-opening at all levels reported.

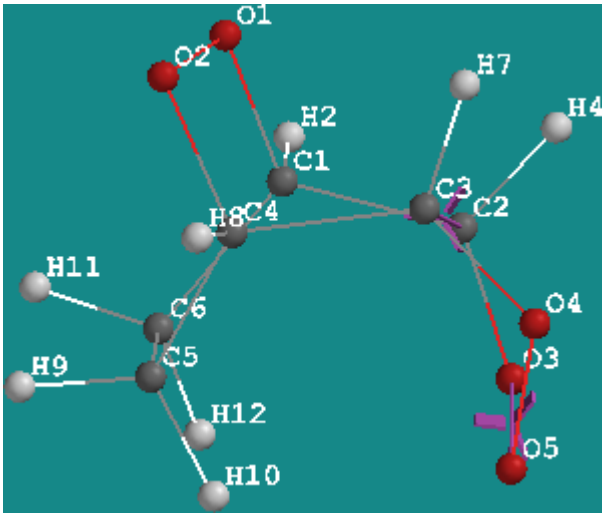

Figure S14: Optimised geometry for primary ozonide TS ring-opening **16b**.

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5184 1- 7 1.0827 1- 11 1.4178 1- 13 1.5322
5) 2- 3 1.5249 2- 4 1.5412 2- 5 1.0776 2- 8 1.0834
9) 3- 9 1.0845 3- 12 1.4110 3- 14 1.5232 4- 6 1.0830
```

13) 4- 10 1.0806 11- 12 1.4112 13- 14 1.9288 13- 15 1.0867
17) 13- 17 1.2555 14- 16 1.0757 14- 18 1.2977 17- 19 1.9476
21) 18- 19 1.2863
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.138 1- 4- 10 109.642 1- 11- 12 112.128
4) 1- 13- 14 98.551 1- 13- 15 115.459 1- 13- 17 118.629
7) 2- 3- 9 111.487 2- 3- 12 108.410 2- 3- 14 118.852
10) 2- 4- 6 110.893 2- 4- 10 111.561 3- 2- 4 107.679
13) 3- 2- 5 110.886 3- 2- 8 107.118 3- 14- 16 112.782
16) 3- 14- 18 124.463 4- 1- 7 111.998 4- 1- 11 111.159
19) 4- 1- 13 112.041 4- 2- 3 107.679 4- 2- 5 112.313
22) 4- 2- 8 110.378 5- 2- 3 110.886 5- 2- 4 112.313
25) 5- 2- 8 108.347 6- 4- 10 108.280 7- 1- 4 111.998
28) 7- 1- 11 103.115 7- 1- 13 109.016 8- 2- 3 107.118
31) 8- 2- 4 110.378 8- 2- 5 108.347 9- 3- 12 104.396
34) 9- 3- 14 107.339 10- 4- 6 108.280 11- 1- 4 111.159
37) 11- 1- 7 103.115 11- 1- 13 109.113 12- 3- 9 104.396
40) 12- 3- 14 105.255 13- 1- 4 112.041 13- 1- 7 109.016
43) 13- 1- 11 109.113 13- 14- 16 109.293 13- 14- 18 96.321
46) 13- 17- 19 104.129 14- 3- 9 107.339 14- 3- 12 105.255
49) 14- 13- 15 97.780 14- 13- 17 102.946 14- 18- 19 113.672
52) 15- 13- 14 97.780 15- 13- 17 117.407 16- 14- 18 110.430
55) 17- 13- 14 102.946 17- 13- 15 117.407 18- 14- 16 110.430
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 14.552 1- 11- 12- 3 23.254
1- 13- 14- 3 22.578 1- 4- 2- 5 -107.812
1- 4- 2- 8 131.164 1- 13- 14- 16 -96.296
1- 13- 14- 18 149.444 1- 13- 17- 19 -107.633
2- 4- 1- 7 -177.262 2- 3- 12- 11 -72.292
2- 4- 1- 11 -62.505 2- 3- 14- 13 46.285
2- 4- 1- 13 59.872 2- 3- 14- 16 162.591
2- 3- 14- 18 -59.039 3- 2- 4- 6 -103.930
3- 2- 4- 10 135.284 3- 14- 13- 15 139.918
3- 14- 13- 17 -99.544 3- 14- 18- 19 52.730
4- 2- 3- 9 162.302 4- 1- 11- 12 43.393
4- 2- 3- 12 47.932 4- 1- 13- 14 -77.592
4- 2- 3- 14 -72.068 4- 1- 13- 15 179.512
4- 1- 13- 17 32.296 5- 2- 4- 6 133.707
5- 2- 3- 9 -74.458 5- 2- 4- 10 12.920
5- 2- 3- 12 171.172 5- 2- 3- 14 51.172
6- 4- 1- 7 -57.043 6- 4- 2- 8 12.682
6- 4- 1- 11 57.714 6- 4- 1- 13 -179.909
7- 1- 4- 10 60.821 7- 1- 11- 12 163.564
7- 1- 13- 14 157.869 7- 1- 13- 15 54.973
7- 1- 13- 17 -92.243 8- 2- 3- 9 43.579
8- 2- 4- 10 -108.104 8- 2- 3- 12 -70.790
8- 2- 3- 14 169.210 9- 3- 12- 11 168.761
9- 3- 14- 13 173.883 9- 3- 14- 16 -69.811
9- 3- 14- 18 68.559 10- 4- 1- 11 175.578
10- 4- 1- 13 -62.046 11- 1- 13- 14 45.942
11- 12- 3- 14 55.873 11- 1- 13- 15 -56.955
11- 1- 13- 17 155.830 12- 3- 14- 13 -75.316
12- 11- 1- 13 -80.663 12- 3- 14- 16 40.990
12- 3- 14- 18 179.360 13- 17- 19- 18 -27.086
13- 14- 18- 19 -54.756 14- 18- 19- 17 53.913
14- 13- 17- 19 -0.218 15- 13- 14- 16 21.044
15- 13- 14- 18 -93.215 15- 13- 17- 19 105.783
16- 14- 13- 17 141.582 16- 14- 18- 19 -168.084
17- 13- 14- 18 27.322

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5180 1- 7 1.0823 1- 11 1.4206 1- 13 1.5326
5) 2- 3 1.5233 2- 4 1.5408 2- 5 1.0780 2- 8 1.0828
9) 3- 9 1.0838 3- 12 1.4158 3- 14 1.5234 4- 6 1.0827
13) 4- 10 1.0805 11- 12 1.4123 13- 14 1.9099 13- 15 1.0862
17) 13- 17 1.2607 14- 16 1.0760 14- 18 1.3021 17- 19 1.9447
21) 18- 19 1.2885
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.042 1- 4- 10 109.665 1- 11- 12 112.096
4) 1- 13- 14 98.933 1- 13- 15 115.541 1- 13- 17 118.402
7) 2- 3- 9 111.713 2- 3- 12 108.326 2- 3- 14 118.931
10) 2- 4- 6 110.935 2- 4- 10 111.702 3- 2- 4 107.727
13) 3- 2- 5 110.825 3- 2- 8 107.145 3- 14- 16 112.735
16) 3- 14- 18 124.395 4- 1- 7 112.110 4- 1- 11 111.046
19) 4- 1- 13 112.286 4- 2- 3 107.727 4- 2- 5 112.388
22) 4- 2- 8 110.433 5- 2- 3 110.825 5- 2- 4 112.388
25) 5- 2- 8 108.204 6- 4- 10 108.096 7- 1- 4 112.110
28) 7- 1- 11 103.116 7- 1- 13 108.933 8- 2- 3 107.145
31) 8- 2- 4 110.433 8- 2- 5 108.204 9- 3- 12 104.414
34) 9- 3- 14 107.227 10- 4- 6 108.096 11- 1- 4 111.046
37) 11- 1- 7 103.116 11- 1- 13 108.920 12- 3- 9 104.414
40) 12- 3- 14 105.101 13- 1- 4 112.286 13- 1- 7 108.933
43) 13- 1- 11 108.920 13- 14- 16 109.282 13- 14- 18 96.608
46) 13- 17- 19 103.799 14- 3- 9 107.227 14- 3- 12 105.101
49) 14- 13- 15 98.034 14- 13- 17 103.429 14- 18- 19 113.651
52) 15- 13- 14 98.034 15- 13- 17 116.912 16- 14- 18 110.033
55) 17- 13- 14 103.429 17- 13- 15 116.912 18- 14- 16 110.033
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 13.930 1- 11- 12- 3 22.427
1- 13- 14- 3 22.066 1- 4- 2- 5 -108.436
1- 4- 2- 8 130.632 1- 13- 14- 16 -96.974
1- 13- 14- 18 149.080 1- 13- 17- 19 -108.024
2- 4- 1- 7 -177.201 2- 3- 12- 11 -72.044
2- 4- 1- 11 -62.444 2- 3- 14- 13 46.357
2- 4- 1- 13 59.776 2- 3- 14- 16 162.879
2- 3- 14- 18 -59.645 3- 2- 4- 6 -104.501
3- 2- 4- 10 134.822 3- 14- 13- 15 139.645
3- 14- 13- 17 -100.113 3- 14- 18- 19 53.853
4- 2- 3- 9 162.972 4- 1- 11- 12 44.033
4- 2- 3- 12 48.506 4- 1- 13- 14 -77.016
4- 2- 3- 14 -71.272 4- 1- 13- 15 179.575
4- 1- 13- 17 33.610 5- 2- 4- 6 133.133
5- 2- 3- 9 -73.703 5- 2- 4- 10 12.456
5- 2- 3- 12 171.831 5- 2- 3- 14 52.053
6- 4- 1- 7 -56.948 6- 4- 2- 8 12.201
6- 4- 1- 11 57.808 6- 4- 1- 13 -179.972
7- 1- 4- 10 60.653 7- 1- 11- 12 164.281
7- 1- 13- 14 158.192 7- 1- 13- 15 54.782
7- 1- 13- 17 -91.183 8- 2- 3- 9 44.144
8- 2- 4- 10 -108.476 8- 2- 3- 12 -70.321

8- 2- 3- 14 169.900 9- 3- 12- 11 168.778
9- 3- 14- 13 174.232 9- 3- 14- 16 -69.245
9- 3- 14- 18 68.231 10- 4- 1- 11 175.410
10- 4- 1- 13 -62.370 11- 1- 13- 14 46.403
11- 12- 3- 14 56.068 11- 1- 13- 15 -57.007
11- 1- 13- 17 157.029 12- 3- 14- 13 -75.059
12- 11- 1- 13 -80.122 12- 3- 14- 16 41.463
12- 3- 14- 18 178.939 13- 17- 19- 18 -27.267
13- 14- 18- 19 -54.383 14- 18- 19- 17 53.535
14- 13- 17- 19 0.072 15- 13- 14- 16 20.604
15- 13- 14- 18 -93.342 15- 13- 17- 19 106.472
16- 14- 13- 17 140.847 16- 14- 18- 19 -167.716
17- 13- 14- 18 26.901

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5136 1- 7 1.1002 1- 11 1.4459 1- 13 1.5269
5) 2- 3 1.5315 2- 4 1.5340 2- 5 1.0886 2- 8 1.0941
9) 3- 9 1.1018 3- 12 1.4409 3- 14 1.5025 4- 6 1.0932
13) 4- 10 1.0927 11- 12 1.4956 13- 14 2.3353 13- 15 1.1060
17) 13- 17 1.2456 14- 16 1.0857 14- 18 1.3459 17- 19 2.4276
21) 18- 19 1.2777
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.124 1- 4- 10 109.367 1- 11- 12 110.330
4) 1- 13- 14 90.911 1- 13- 15 114.994 1- 13- 17 122.426
7) 2- 3- 9 110.224 2- 3- 12 108.522 2- 3- 14 119.968
10) 2- 4- 6 111.080 2- 4- 10 111.100 3- 2- 4 108.461
13) 3- 2- 5 110.405 3- 2- 8 107.540 3- 14- 16 118.887
16) 3- 14- 18 125.520 4- 1- 7 111.785 4- 1- 11 112.117
19) 4- 1- 13 112.118 4- 2- 3 108.461 4- 2- 5 111.805
22) 4- 2- 8 110.018 5- 2- 3 110.405 5- 2- 4 111.805
25) 5- 2- 8 108.523 6- 4- 10 108.461 7- 1- 4 111.785
28) 7- 1- 11 102.362 7- 1- 13 107.723 8- 2- 3 107.540
31) 8- 2- 4 110.018 8- 2- 5 108.523 9- 3- 12 102.600
34) 9- 3- 14 108.555 10- 4- 6 108.461 11- 1- 4 112.117
37) 11- 1- 7 102.362 11- 1- 13 110.240 12- 3- 9 102.600
40) 12- 3- 14 105.492 13- 1- 4 112.118 13- 1- 7 107.723
43) 13- 1- 11 110.240 13- 14- 16 112.322 13- 14- 18 90.487
46) 13- 17- 19 104.472 14- 3- 9 108.555 14- 3- 12 105.492
49) 14- 13- 15 89.615 14- 13- 17 100.354 14- 18- 19 120.459
52) 15- 13- 14 89.615 15- 13- 17 121.279 16- 14- 18 108.759
55) 17- 13- 14 100.354 17- 13- 15 121.279 18- 14- 16 108.759
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 26.297 1- 11- 12- 3 36.137
1- 13- 14- 3 28.808 1- 4- 2- 5 -95.671
1- 4- 2- 8 143.670 1- 13- 14- 16 -94.944
1- 13- 14- 18 154.499 1- 13- 17- 19 -101.478
2- 4- 1- 7 -179.956 2- 3- 12- 11 -75.204
2- 4- 1- 11 -65.669 2- 3- 14- 13 42.854
2- 4- 1- 13 58.960 2- 3- 14- 16 161.400
2- 3- 14- 18 -50.919 3- 2- 4- 6 -92.516
3- 2- 4- 10 146.654 3- 14- 13- 15 143.800
3- 14- 13- 17 -94.426 3- 14- 18- 19 25.857
4- 2- 3- 9 150.885 4- 1- 11- 12 32.123
4- 2- 3- 12 39.255 4- 1- 13- 14 -80.947
4- 2- 3- 14 -81.966 4- 1- 13- 15 -170.947
4- 1- 13- 17 21.942 5- 2- 4- 6 145.516

5- 2- 3- 9 -86.295 5- 2- 4- 10 24.686
5- 2- 3- 12 162.075 5- 2- 3- 14 40.853
6- 4- 1- 7 -59.300 6- 4- 2- 8 24.857
6- 4- 1- 11 54.987 6- 4- 1- 13 179.616
7- 1- 4- 10 58.620 7- 1- 11- 12 152.070
7- 1- 13- 14 155.655 7- 1- 13- 15 65.654
7- 1- 13- 17 -101.456 8- 2- 3- 9 31.938
8- 2- 4- 10 -95.973 8- 2- 3- 12 -79.692
8- 2- 3- 14 159.086 9- 3- 12- 11 168.151
9- 3- 14- 13 170.767 9- 3- 14- 16 -70.687
9- 3- 14- 18 76.994 10- 4- 1- 11 172.906
10- 4- 1- 13 -62.464 11- 1- 13- 14 44.716
11- 12- 3- 14 54.553 11- 1- 13- 15 -45.285
11- 1- 13- 17 147.605 12- 3- 14- 13 -79.853
12- 11- 1- 13 -93.540 12- 3- 14- 16 38.692
12- 3- 14- 18 -173.626 13- 17- 19- 18 -24.787
13- 14- 18- 19 -69.941 14- 18- 19- 17 64.952
14- 13- 17- 19 -3.706 15- 13- 14- 16 20.047
15- 13- 14- 18 -90.510 15- 13- 17- 19 92.206
16- 14- 13- 17 141.822 16- 14- 18- 19 176.229
17- 13- 14- 18 31.265

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5149 1- 7 1.0992 1- 11 1.4382 1- 13 1.5317
5) 2- 3 1.5327 2- 4 1.5360 2- 5 1.0874 2- 8 1.0936
9) 3- 9 1.1008 3- 12 1.4328 3- 14 1.5056 4- 6 1.0924
13) 4- 10 1.0916 11- 12 1.4770 13- 14 2.2884 13- 15 1.1065
17) 13- 17 1.2383 14- 16 1.0851 14- 18 1.3447 17- 19 2.4308
21) 18- 19 1.2617
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.143 1- 4- 10 109.634 1- 11- 12 110.456
4) 1- 13- 14 91.152 1- 13- 15 114.834 1- 13- 17 122.521
7) 2- 3- 9 110.376 2- 3- 12 108.482 2- 3- 14 119.683
10) 2- 4- 6 111.046 2- 4- 10 111.183 3- 2- 4 108.061
13) 3- 2- 5 110.652 3- 2- 8 107.584 3- 14- 16 118.474
16) 3- 14- 18 125.055 4- 1- 7 111.914 4- 1- 11 111.974
19) 4- 1- 13 111.741 4- 2- 3 108.061 4- 2- 5 111.785
22) 4- 2- 8 110.128 5- 2- 3 110.652 5- 2- 4 111.785
25) 5- 2- 8 108.548 6- 4- 10 108.625 7- 1- 4 111.914
28) 7- 1- 11 102.381 7- 1- 13 107.653 8- 2- 3 107.584
31) 8- 2- 4 110.128 8- 2- 5 108.548 9- 3- 12 102.856
34) 9- 3- 14 108.482 10- 4- 6 108.625 11- 1- 4 111.974
37) 11- 1- 7 102.381 11- 1- 13 110.733 12- 3- 9 102.856
40) 12- 3- 14 105.563 13- 1- 4 111.741 13- 1- 7 107.653
43) 13- 1- 11 110.733 13- 14- 16 112.616 13- 14- 18 91.729
46) 13- 17- 19 103.834 14- 3- 9 108.482 14- 3- 12 105.563
49) 14- 13- 15 89.946 14- 13- 17 100.904 14- 18- 19 120.295
52) 15- 13- 14 89.946 15- 13- 17 121.069 16- 14- 18 108.513
55) 17- 13- 14 100.904 17- 13- 15 121.069 18- 14- 16 108.513
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 26.113 1- 11- 12- 3 35.952
1- 13- 14- 3 29.405 1- 4- 2- 5 -95.881
1- 4- 2- 8 143.368 1- 13- 14- 16 -94.286
1- 13- 14- 18 154.816 1- 13- 17- 19 -102.453

2- 4- 1- 7 179.605 2- 3- 12- 11 -75.668
2- 4- 1- 11 -66.094 2- 3- 14- 13 42.478
2- 4- 1- 13 58.787 2- 3- 14- 16 161.581
2- 3- 14- 18 -53.154 3- 2- 4- 6 -92.396
3- 2- 4- 10 146.531 3- 14- 13- 15 144.244
3- 14- 13- 17 -94.063 3- 14- 18- 19 27.753
4- 2- 3- 9 151.430 4- 1- 11- 12 32.901
4- 2- 3- 12 39.442 4- 1- 13- 14 -81.834
4- 2- 3- 14 -81.632 4- 1- 13- 15 -172.308
4- 1- 13- 17 21.888 5- 2- 4- 6 145.610
5- 2- 3- 9 -85.882 5- 2- 4- 10 24.538
5- 2- 3- 12 162.130 5- 2- 3- 14 41.056
6- 4- 1- 7 -60.053 6- 4- 2- 8 24.858
6- 4- 1- 11 54.248 6- 4- 1- 13 179.129
7- 1- 4- 10 58.224 7- 1- 11- 12 152.941
7- 1- 13- 14 154.899 7- 1- 13- 15 64.425
7- 1- 13- 17 -101.379 8- 2- 3- 9 32.546
8- 2- 4- 10 -96.214 8- 2- 3- 12 -79.442
8- 2- 3- 14 159.484 9- 3- 12- 11 167.406
9- 3- 14- 13 170.291 9- 3- 14- 16 -70.606
9- 3- 14- 18 74.659 10- 4- 1- 11 172.525
10- 4- 1- 13 -62.594 11- 1- 13- 14 43.734
11- 12- 3- 14 53.759 11- 1- 13- 15 -46.739
11- 1- 13- 17 147.456 12- 3- 14- 13 -80.038
12- 11- 1- 13 -92.536 12- 3- 14- 16 39.065
12- 3- 14- 18 -175.669 13- 17- 19- 18 -24.563
13- 14- 18- 19 -69.558 14- 18- 19- 17 63.567
14- 13- 17- 19 -3.993 15- 13- 14- 16 20.552
15- 13- 14- 18 -90.346 15- 13- 17- 19 92.607
16- 14- 13- 17 142.245 16- 14- 18- 19 175.870
17- 13- 14- 18 31.347

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5244 1- 7 1.0976 1- 11 1.4337 1- 13 1.5489
5) 2- 3 1.5301 2- 4 1.5486 2- 5 1.0901 2- 8 1.0943
9) 3- 9 1.0992 3- 12 1.4308 3- 14 1.5303 4- 6 1.0938
13) 4- 10 1.0920 11- 12 1.4904 13- 14 1.9224 13- 15 1.1054
17) 13- 17 1.2750 14- 16 1.0893 14- 18 1.3326 17- 19 2.0922
21) 18- 19 1.3274
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.464 1- 4- 10 109.241 1- 11- 12 110.757
4) 1- 13- 14 98.669 1- 13- 15 114.353 1- 13- 17 118.660
7) 2- 3- 9 111.507 2- 3- 12 109.691 2- 3- 14 118.599
10) 2- 4- 6 111.193 2- 4- 10 111.254 3- 2- 4 108.028
13) 3- 2- 5 109.653 3- 2- 8 107.489 3- 14- 16 112.456
16) 3- 14- 18 124.565 4- 1- 7 112.191 4- 1- 11 112.043
19) 4- 1- 13 111.468 4- 2- 3 108.028 4- 2- 5 112.123
22) 4- 2- 8 110.705 5- 2- 3 109.653 5- 2- 4 112.123
25) 5- 2- 8 108.732 6- 4- 10 108.525 7- 1- 4 112.191
28) 7- 1- 11 101.973 7- 1- 13 108.350 8- 2- 3 107.489
31) 8- 2- 4 110.705 8- 2- 5 108.732 9- 3- 12 103.258
34) 9- 3- 14 107.058 10- 4- 6 108.525 11- 1- 4 112.043
37) 11- 1- 7 101.973 11- 1- 13 110.389 12- 3- 9 103.258
40) 12- 3- 14 105.497 13- 1- 4 111.468 13- 1- 7 108.350
43) 13- 1- 11 110.389 13- 14- 16 109.752 13- 14- 18 97.919

46) 13- 17- 19 102.561 14- 3- 9 107.058 14- 3- 12 105.497
49) 14- 13- 15 96.629 14- 13- 17 104.542 14- 18- 19 113.174
52) 15- 13- 14 96.629 15- 13- 17 118.079 16- 14- 18 108.931
55) 17- 13- 14 104.542 17- 13- 15 118.079 18- 14- 16 108.931
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 13.698 1- 11- 12- 3 19.897
1- 13- 14- 3 22.601 1- 4- 2- 5 -107.240
1- 4- 2- 8 131.142 1- 13- 14- 16 -96.309
1- 13- 14- 18 150.239 1- 13- 17- 19 -107.744
2- 4- 1- 7 -177.920 2- 3- 12- 11 -70.656
2- 4- 1- 11 -63.912 2- 3- 14- 13 46.023
2- 4- 1- 13 60.360 2- 3- 14- 16 162.964
2- 3- 14- 18 -61.715 3- 2- 4- 6 -105.261
3- 2- 4- 10 133.645 3- 14- 13- 15 138.554
3- 14- 13- 17 -100.135 3- 14- 18- 19 51.031
4- 2- 3- 9 163.581 4- 1- 11- 12 46.138
4- 2- 3- 12 49.827 4- 1- 13- 14 -77.806
4- 2- 3- 14 -71.393 4- 1- 13- 15 -179.178
4- 1- 13- 17 34.082 5- 2- 4- 6 133.801
5- 2- 3- 9 -73.954 5- 2- 4- 10 12.707
5- 2- 3- 12 172.291 5- 2- 3- 14 51.071
6- 4- 1- 7 -57.244 6- 4- 2- 8 12.183
6- 4- 1- 11 56.764 6- 4- 1- 13 -178.964
7- 1- 4- 10 60.876 7- 1- 11- 12 166.296
7- 1- 13- 14 158.274 7- 1- 13- 15 56.902
7- 1- 13- 17 -89.838 8- 2- 3- 9 44.084
8- 2- 4- 10 -108.911 8- 2- 3- 12 -69.671
8- 2- 3- 14 169.110 9- 3- 12- 11 170.373
9- 3- 14- 13 173.185 9- 3- 14- 16 -69.874
9- 3- 14- 18 65.447 10- 4- 1- 11 174.884
10- 4- 1- 13 -60.844 11- 1- 13- 14 47.392
11- 12- 3- 14 58.159 11- 1- 13- 15 -53.980
11- 1- 13- 17 159.280 12- 3- 14- 13 -77.303
12- 11- 1- 13 -78.733 12- 3- 14- 16 39.638
12- 3- 14- 18 174.959 13- 17- 19- 18 -29.081
13- 14- 18- 19 -58.254 14- 18- 19- 17 55.184
14- 13- 17- 19 0.873 15- 13- 14- 16 19.644
15- 13- 14- 18 -93.808 15- 13- 17- 19 106.749
16- 14- 13- 17 140.956 16- 14- 18- 19 -172.360
17- 13- 14- 18 27.504

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5239 1- 7 1.0970 1- 11 1.4358 1- 13 1.5498
5) 2- 3 1.5279 2- 4 1.5481 2- 5 1.0903 2- 8 1.0935
9) 3- 9 1.0982 3- 12 1.4353 3- 14 1.5314 4- 6 1.0934
13) 4- 10 1.0918 11- 12 1.4924 13- 14 1.8887 13- 15 1.1041
17) 13- 17 1.2837 14- 16 1.0893 14- 18 1.3389 17- 19 2.0823
21) 18- 19 1.3299
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.363 1- 4- 10 109.297 1- 11- 12 110.659
4) 1- 13- 14 99.313 1- 13- 15 114.407 1- 13- 17 118.263
7) 2- 3- 9 111.823 2- 3- 12 109.595 2- 3- 14 118.636
10) 2- 4- 6 111.208 2- 4- 10 111.466 3- 2- 4 108.035
13) 3- 2- 5 109.694 3- 2- 8 107.479 3- 14- 16 112.231

16) 3- 14- 18 124.416 4- 1- 7 112.321 4- 1- 11 111.874
19) 4- 1- 13 111.794 4- 2- 3 108.035 4- 2- 5 112.251
22) 4- 2- 8 110.780 5- 2- 3 109.694 5- 2- 4 112.251
25) 5- 2- 8 108.491 6- 4- 10 108.278 7- 1- 4 112.321
28) 7- 1- 11 102.013 7- 1- 13 108.178 8- 2- 3 107.479
31) 8- 2- 4 110.780 8- 2- 5 108.491 9- 3- 12 103.308
34) 9- 3- 14 106.849 10- 4- 6 108.278 11- 1- 4 111.874
37) 11- 1- 7 102.013 11- 1- 13 110.197 12- 3- 9 103.308
40) 12- 3- 14 105.378 13- 1- 4 111.794 13- 1- 7 108.178
43) 13- 1- 11 110.197 13- 14- 16 109.879 13- 14- 18 98.357
46) 13- 17- 19 101.956 14- 3- 9 106.849 14- 3- 12 105.378
49) 14- 13- 15 97.092 14- 13- 17 105.361 14- 18- 19 113.080
52) 15- 13- 14 97.092 15- 13- 17 117.284 16- 14- 18 108.339
55) 17- 13- 14 105.361 17- 13- 15 117.284 18- 14- 16 108.339
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 12.563 1- 11- 12- 3 18.437
1- 13- 14- 3 21.632 1- 4- 2- 5 -108.509
1- 4- 2- 8 130.040 1- 13- 14- 16 -97.452
1- 13- 14- 18 149.513 1- 13- 17- 19 -108.237
2- 4- 1- 7 -177.818 2- 3- 12- 11 -70.218
2- 4- 1- 11 -63.785 2- 3- 14- 13 46.358
2- 4- 1- 13 60.354 2- 3- 14- 16 163.756
2- 3- 14- 18 -62.450 3- 2- 4- 6 -106.318
3- 2- 4- 10 132.747 3- 14- 13- 15 137.887
3- 14- 13- 17 -101.233 3- 14- 18- 19 52.950
4- 2- 3- 9 164.782 4- 1- 11- 12 47.333
4- 2- 3- 12 50.844 4- 1- 13- 14 -76.916
4- 2- 3- 14 -70.161 4- 1- 13- 15 -179.144
4- 1- 13- 17 36.221 5- 2- 4- 6 132.609
5- 2- 3- 9 -72.568 5- 2- 4- 10 11.674
5- 2- 3- 12 173.494 5- 2- 3- 14 52.489
6- 4- 1- 7 -57.148 6- 4- 2- 8 11.159
6- 4- 1- 11 56.886 6- 4- 1- 13 -178.976
7- 1- 4- 10 60.650 7- 1- 11- 12 167.588
7- 1- 13- 14 158.903 7- 1- 13- 15 56.674
7- 1- 13- 17 -87.960 8- 2- 3- 9 45.199
8- 2- 4- 10 -109.776 8- 2- 3- 12 -68.739
8- 2- 3- 14 170.256 9- 3- 12- 11 170.462
9- 3- 14- 13 173.796 9- 3- 14- 16 -68.805
9- 3- 14- 18 64.989 10- 4- 1- 11 174.683
10- 4- 1- 13 -61.178 11- 1- 13- 14 48.157
11- 12- 3- 14 58.502 11- 1- 13- 15 -54.071
11- 1- 13- 17 161.294 12- 3- 14- 13 -76.769
12- 11- 1- 13 -77.694 12- 3- 14- 16 40.630
12- 3- 14- 18 174.424 13- 17- 19- 18 -29.561
13- 14- 18- 19 -57.541 14- 18- 19- 17 54.663
14- 13- 17- 19 1.531 15- 13- 14- 16 18.803
15- 13- 14- 18 -94.231 15- 13- 17- 19 108.135
16- 14- 13- 17 139.682 16- 14- 18- 19 -171.793
17- 13- 14- 18 26.648

Optimised structures for the transition state for primary ozonide 16c ring-opening at all levels reported.

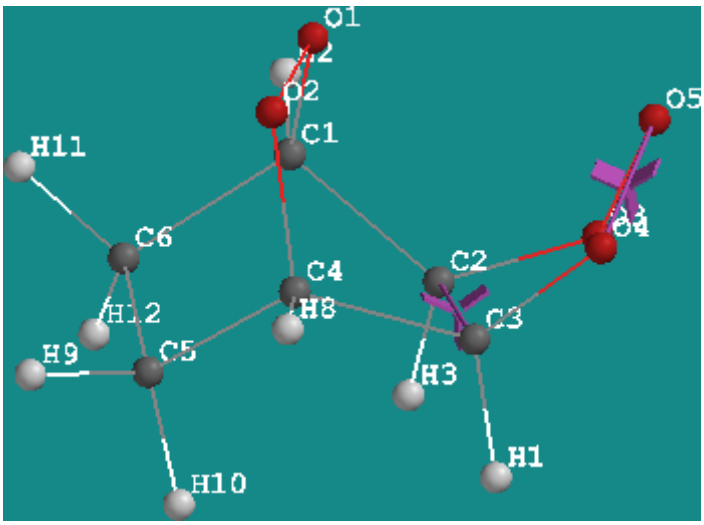

Figure S15: Optimised geometry for primary ozonide TS ring-opening **16c**.

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5270 1- 7 1.0846 1- 11 1.3974 1- 13 1.5237
5) 2- 3 1.5303 2- 4 1.5439 2- 5 1.0864 2- 8 1.0825
9) 3- 9 1.0824 3- 12 1.4042 3- 15 1.5328 4- 6 1.0819
13) 4- 10 1.0844 11- 12 1.4044 13- 14 1.0770 13- 15 1.9679
17) 13- 17 1.2961 15- 16 1.0886 15- 18 1.2471 17- 19 1.2783
21) 18- 19 1.9622
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.687 1- 4- 10 110.824 1- 11- 12 112.129
4) 1- 13- 14 114.806 1- 13- 15 98.600 1- 13- 17 124.119
7) 2- 3- 9 111.743 2- 3- 12 108.426 2- 3- 15 112.647
10) 2- 4- 6 110.739 2- 4- 10 112.099 3- 2- 4 107.097
13) 3- 2- 5 110.362 3- 2- 8 109.994 3- 15- 16 114.684
16) 3- 15- 18 119.340 4- 1- 7 112.601 4- 1- 11 110.239
19) 4- 1- 13 108.053 4- 2- 3 107.097 4- 2- 5 111.793
22) 4- 2- 8 110.510 5- 2- 3 110.362 5- 2- 4 111.793
25) 5- 2- 8 107.108 6- 4- 10 107.669 7- 1- 4 112.601
28) 7- 1- 11 104.127 7- 1- 13 108.285 8- 2- 3 109.994
31) 8- 2- 4 110.510 8- 2- 5 107.108 9- 3- 12 104.100
34) 9- 3- 15 108.631 10- 4- 6 107.669 11- 1- 4 110.239
37) 11- 1- 7 104.127 11- 1- 13 113.580 12- 3- 9 104.100
40) 12- 3- 15 110.974 13- 1- 4 108.053 13- 1- 7 108.285
43) 13- 1- 11 113.580 13- 15- 16 97.263 13- 15- 18 102.352
46) 13- 17- 19 113.937 14- 13- 15 111.231 14- 13- 17 109.256
49) 15- 3- 9 108.631 15- 3- 12 110.974 15- 13- 14 111.231
52) 15- 13- 17 95.739 15- 18- 19 104.447 16- 15- 18 117.728
55) 17- 13- 14 109.256 17- 13- 15 95.739 18- 15- 16 117.728
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 20.127 1- 11- 12- 3 26.845
1- 13- 15- 3 22.784 1- 4- 2- 5 -100.873
1- 4- 2- 8 139.929 1- 13- 15- 16 139.334
1- 13- 15- 18 -100.131 1- 13- 17- 19 49.371
2- 4- 1- 7 178.368 2- 3- 12- 11 -73.181
2- 4- 1- 11 -65.831 2- 3- 15- 13 49.775
2- 4- 1- 13 58.822 2- 3- 15- 16 -52.643
2- 3- 15- 18 159.603 3- 2- 4- 6 -97.408
```

3- 2- 4- 10 142.325 3- 15- 13- 14 -98.145
3- 15- 13- 17 148.612 3- 15- 18- 19 -106.513
4- 2- 3- 9 157.327 4- 1- 11- 12 41.528
4- 2- 3- 12 43.165 4- 1- 13- 14 39.054
4- 1- 13- 15 -79.199 4- 2- 3- 15 -80.052
4- 1- 13- 17 177.819 5- 2- 4- 6 141.592
5- 2- 3- 9 -80.772 5- 2- 4- 10 21.325
5- 2- 3- 12 165.067 5- 2- 3- 15 41.849
6- 4- 1- 7 -62.138 6- 4- 2- 8 22.394
6- 4- 1- 11 53.663 6- 4- 1- 13 178.316
7- 1- 4- 10 55.386 7- 1- 11- 12 162.536
7- 1- 13- 14 -83.182 7- 1- 13- 15 158.565
7- 1- 13- 17 55.583 8- 2- 3- 9 37.195
8- 2- 4- 10 -97.873 8- 2- 3- 12 -76.967
8- 2- 3- 15 159.816 9- 3- 12- 11 167.722
9- 3- 15- 13 174.126 9- 3- 15- 16 71.708
9- 3- 15- 18 -76.046 10- 4- 1- 11 171.187
10- 4- 1- 13 -64.160 11- 1- 13- 14 161.688
11- 1- 13- 15 43.434 11- 12- 3- 15 51.039
11- 1- 13- 17 -59.548 12- 3- 15- 13 -72.010
12- 11- 1- 13 -79.893 12- 3- 15- 16 -174.428
12- 3- 15- 18 37.818 13- 17- 19- 18 55.476
13- 15- 18- 19 1.548 14- 13- 15- 16 18.406
14- 13- 15- 18 138.940 14- 13- 17- 19 -169.960
15- 18- 19- 17 -29.182 15- 13- 17- 19 -55.085
16- 15- 13- 17 -94.837 16- 15- 18- 19 106.696
17- 13- 15- 18 25.697

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5252 1- 7 1.0837 1- 11 1.4063 1- 13 1.5226
5) 2- 3 1.5274 2- 4 1.5429 2- 5 1.0852 2- 8 1.0820
9) 3- 9 1.0822 3- 12 1.4115 3- 15 1.5324 4- 6 1.0816
13) 4- 10 1.0830 11- 12 1.4063 13- 14 1.0770 13- 15 1.9342
17) 13- 17 1.3019 15- 16 1.0870 15- 18 1.2565 17- 19 1.2831
21) 18- 19 1.9569
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.755 1- 4- 10 110.527 1- 11- 12 111.972
4) 1- 13- 14 114.542 1- 13- 15 99.265 1- 13- 17 124.188
7) 2- 3- 9 111.986 2- 3- 12 108.590 2- 3- 15 112.812
10) 2- 4- 6 111.003 2- 4- 10 112.094 3- 2- 4 107.231
13) 3- 2- 5 110.097 3- 2- 8 109.769 3- 15- 16 114.943
16) 3- 15- 18 118.900 4- 1- 7 112.754 4- 1- 11 110.325
19) 4- 1- 13 108.159 4- 2- 3 107.231 4- 2- 5 111.936
22) 4- 2- 8 110.689 5- 2- 3 110.097 5- 2- 4 111.936
25) 5- 2- 8 107.132 6- 4- 10 107.645 7- 1- 4 112.754
28) 7- 1- 11 104.122 7- 1- 13 108.202 8- 2- 3 109.769
31) 8- 2- 4 110.689 8- 2- 5 107.132 9- 3- 12 104.003
34) 9- 3- 15 108.509 10- 4- 6 107.645 11- 1- 4 110.325
37) 11- 1- 7 104.122 11- 1- 13 113.314 12- 3- 9 104.003
40) 12- 3- 15 110.593 13- 1- 4 108.159 13- 1- 7 108.202
43) 13- 1- 11 113.314 13- 15- 16 97.773 13- 15- 18 103.010
46) 13- 17- 19 113.706 14- 13- 15 110.793 14- 13- 17 108.921
49) 15- 3- 9 108.509 15- 3- 12 110.593 15- 13- 14 110.793
52) 15- 13- 17 96.262 15- 18- 19 103.954 16- 15- 18 116.936
55) 17- 13- 14 108.921 17- 13- 15 96.262 18- 15- 16 116.936

Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 19.182 1- 11- 12- 3 25.557
1- 13- 15- 3 22.489 1- 4- 2- 5 -101.664
1- 4- 2- 8 138.894 1- 13- 15- 16 139.565
1- 13- 15- 18 -100.383 1- 13- 17- 19 50.792
2- 4- 1- 7 178.365 2- 3- 12- 11 -72.811
2- 4- 1- 11 -65.690 2- 3- 15- 13 49.655
2- 4- 1- 13 58.758 2- 3- 15- 16 -53.696
2- 3- 15- 18 160.470 3- 2- 4- 6 -98.583
3- 2- 4- 10 141.003 3- 15- 13- 14 -98.315
3- 15- 13- 17 148.693 3- 15- 18- 19 -107.593
4- 2- 3- 9 158.390 4- 1- 11- 12 42.460
4- 2- 3- 12 44.116 4- 1- 13- 14 39.145
4- 1- 13- 15 -78.882 4- 2- 3- 15 -78.843
4- 1- 13- 17 176.971 5- 2- 4- 6 140.571
5- 2- 3- 9 -79.608 5- 2- 4- 10 20.156
5- 2- 3- 12 166.118 5- 2- 3- 15 43.160
6- 4- 1- 7 -61.793 6- 4- 2- 8 21.130
6- 4- 1- 11 54.152 6- 4- 1- 13 178.600
7- 1- 4- 10 55.578 7- 1- 11- 12 163.693
7- 1- 13- 14 -83.290 7- 1- 13- 15 158.683
7- 1- 13- 17 54.536 8- 2- 3- 9 38.090
8- 2- 4- 10 -99.285 8- 2- 3- 12 -76.184
8- 2- 3- 15 160.858 9- 3- 12- 11 167.785
9- 3- 15- 13 174.344 9- 3- 15- 16 70.993
9- 3- 15- 18 -74.842 10- 4- 1- 11 171.523
10- 4- 1- 13 -64.029 11- 1- 13- 14 161.788
11- 1- 13- 15 43.761 11- 12- 3- 15 51.476
11- 1- 13- 17 -60.386 12- 3- 15- 13 -72.180
12- 11- 1- 13 -78.974 12- 3- 15- 16 -175.531
12- 3- 15- 18 38.635 13- 17- 19- 18 54.840
13- 15- 18- 19 1.390 14- 13- 15- 16 18.761
14- 13- 15- 18 138.812 14- 13- 17- 19 -169.420
15- 18- 19- 17 -28.945 15- 13- 17- 19 -54.893
16- 15- 13- 17 -94.231 16- 15- 18- 19 107.239
17- 13- 15- 18 25.820

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5285 1- 7 1.0963 1- 11 1.4163 1- 13 1.5470
5) 2- 3 1.5223 2- 4 1.5435 2- 5 1.0956 2- 8 1.0929
9) 3- 9 1.0958 3- 12 1.4329 3- 15 1.5339 4- 6 1.0932
13) 4- 10 1.0967 11- 12 1.5039 13- 14 1.0973 13- 15 1.5908
17) 13- 17 1.4055 15- 16 1.1110 15- 18 1.3604 17- 19 1.3827
21) 18- 19 2.7015
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.387 1- 4- 10 110.247 1- 11- 12 109.944
4) 1- 13- 14 109.122 1- 13- 15 105.469 1- 13- 17 113.007
7) 2- 3- 9 113.440 2- 3- 12 109.877 2- 3- 15 111.756
10) 2- 4- 6 111.339 2- 4- 10 112.205 3- 2- 4 107.360
13) 3- 2- 5 110.673 3- 2- 8 108.218 3- 15- 16 109.951
16) 3- 15- 18 115.418 4- 1- 7 112.968 4- 1- 11 110.581
19) 4- 1- 13 109.278 4- 2- 3 107.360 4- 2- 5 111.803
22) 4- 2- 8 111.029 5- 2- 3 110.673 5- 2- 4 111.803
25) 5- 2- 8 107.720 6- 4- 10 107.238 7- 1- 4 112.968
28) 7- 1- 11 102.859 7- 1- 13 108.950 8- 2- 3 108.218
31) 8- 2- 4 111.029 8- 2- 5 107.720 9- 3- 12 102.435

34) 9- 3- 15 109.328 10- 4- 6 107.238 11- 1- 4 110.581
37) 11- 1- 7 102.859 11- 1- 13 112.116 12- 3- 9 102.435
40) 12- 3- 15 109.583 13- 1- 4 109.278 13- 1- 7 108.950
43) 13- 1- 11 112.116 13- 15- 16 102.381 13- 15- 18 114.171
46) 13- 17- 19 110.640 14- 13- 15 112.219 14- 13- 17 102.486
49) 15- 3- 9 109.328 15- 3- 12 109.583 15- 13- 14 112.219
52) 15- 13- 17 114.608 15- 18- 19 81.094 16- 15- 18 106.431
55) 17- 13- 14 102.486 17- 13- 15 114.608 18- 15- 16 106.431
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -13.338 1- 11- 12- 3 -12.307
1- 13- 15- 3 -7.965 1- 4- 2- 5 -134.901
1- 4- 2- 8 104.768 1- 13- 15- 16 107.917
1- 13- 15- 18 -137.505 1- 13- 17- 19 68.506
2- 4- 1- 7 -165.863 2- 3- 12- 11 -54.029
2- 4- 1- 11 -51.197 2- 3- 15- 13 66.862
2- 4- 1- 13 72.678 2- 3- 15- 16 -43.929
2- 3- 15- 18 -164.305 3- 2- 4- 6 -131.837
3- 2- 4- 10 107.957 3- 15- 13- 14 -126.663
3- 15- 13- 17 116.980 3- 15- 18- 19 -92.744
4- 2- 3- 9 -178.228 4- 1- 11- 12 67.570
4- 2- 3- 12 67.798 4- 1- 13- 14 62.316
4- 1- 13- 15 -58.429 4- 2- 3- 15 -54.074
4- 1- 13- 17 175.633 5- 2- 4- 6 106.600
5- 2- 3- 9 -55.960 5- 2- 4- 10 -13.606
5- 2- 3- 12 -169.933 5- 2- 3- 15 68.195
6- 4- 1- 7 -45.475 6- 4- 2- 8 -13.731
6- 4- 1- 11 69.191 6- 4- 1- 13 -166.934
7- 1- 4- 10 71.619 7- 1- 11- 12 -171.549
7- 1- 13- 14 -61.545 7- 1- 13- 15 177.710
7- 1- 13- 17 51.773 8- 2- 3- 9 61.858
8- 2- 4- 10 -133.937 8- 2- 3- 12 -52.115
8- 2- 3- 15 -173.987 9- 3- 12- 11 -174.883
9- 3- 15- 13 -166.708 9- 3- 15- 16 82.502
9- 3- 15- 18 -37.875 10- 4- 1- 11 -173.714
10- 4- 1- 13 -49.840 11- 1- 13- 14 -174.718
11- 1- 13- 15 64.536 11- 12- 3- 15 69.129
11- 1- 13- 17 -61.401 12- 3- 15- 13 -55.179
12- 11- 1- 13 -54.657 12- 3- 15- 16 -165.969
12- 3- 15- 18 73.655 13- 17- 19- 18 53.270
13- 15- 18- 19 32.808 14- 13- 15- 16 -10.782
14- 13- 15- 18 103.797 14- 13- 17- 19 -174.201
15- 18- 19- 17 -56.095 15- 13- 17- 19 -52.370
16- 15- 13- 17 -127.139 16- 15- 18- 19 144.979
17- 13- 15- 18 -12.561

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5307 1- 7 1.0953 1- 11 1.4117 1- 13 1.5474
5) 2- 3 1.5236 2- 4 1.5452 2- 5 1.0946 2- 8 1.0922
9) 3- 9 1.0948 3- 12 1.4251 3- 15 1.5362 4- 6 1.0926
13) 4- 10 1.0958 11- 12 1.4834 13- 14 1.0963 13- 15 1.5777
17) 13- 17 1.4030 15- 16 1.1111 15- 18 1.3583 17- 19 1.3743
21) 18- 19 2.7694
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.745 1- 4- 10 110.375 1- 11- 12 110.302

4) 1- 13- 14 108.800 1- 13- 15 105.169 1- 13- 17 112.865
7) 2- 3- 9 113.829 2- 3- 12 109.795 2- 3- 15 111.277
10) 2- 4- 6 111.334 2- 4- 10 112.116 3- 2- 4 107.013
13) 3- 2- 5 110.962 3- 2- 8 108.152 3- 15- 16 109.655
16) 3- 15- 18 115.569 4- 1- 7 113.313 4- 1- 11 110.464
19) 4- 1- 13 108.711 4- 2- 3 107.013 4- 2- 5 111.901
22) 4- 2- 8 110.847 5- 2- 3 110.962 5- 2- 4 111.901
25) 5- 2- 8 107.922 6- 4- 10 107.310 7- 1- 4 113.313
28) 7- 1- 11 102.920 7- 1- 13 109.059 8- 2- 3 108.152
31) 8- 2- 4 110.847 8- 2- 5 107.922 9- 3- 12 102.654
34) 9- 3- 15 109.354 10- 4- 6 107.310 11- 1- 4 110.464
37) 11- 1- 7 102.920 11- 1- 13 112.346 12- 3- 9 102.654
40) 12- 3- 15 109.560 13- 1- 4 108.711 13- 1- 7 109.059
43) 13- 1- 11 112.346 13- 15- 16 102.731 13- 15- 18 114.944
46) 13- 17- 19 111.127 14- 13- 15 112.067 14- 13- 17 102.151
49) 15- 3- 9 109.354 15- 3- 12 109.560 15- 13- 14 112.067
52) 15- 13- 17 115.796 15- 18- 19 79.211 16- 15- 18 105.088
55) 17- 13- 14 102.151 17- 13- 15 115.796 18- 15- 16 105.088
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -15.757 1- 11- 12- 3 -14.790
1- 13- 15- 3 -9.903 1- 4- 2- 5 -137.508
1- 4- 2- 8 101.963 1- 13- 15- 16 105.928
1- 13- 15- 18 -140.530 1- 13- 17- 19 69.176
2- 4- 1- 7 -163.937 2- 3- 12- 11 -52.601
2- 4- 1- 11 -49.060 2- 3- 15- 13 68.257
2- 4- 1- 13 74.640 2- 3- 15- 16 -42.952
2- 3- 15- 18 -161.462 3- 2- 4- 6 -134.417
3- 2- 4- 10 105.350 3- 15- 13- 14 -127.951
3- 15- 13- 17 115.420 3- 15- 18- 19 -93.007
4- 2- 3- 9 -176.518 4- 1- 11- 12 68.801
4- 2- 3- 12 69.059 4- 1- 13- 14 62.558
4- 1- 13- 15 -57.673 4- 2- 3- 15 -52.409
4- 1- 13- 17 175.194 5- 2- 4- 6 103.832
5- 2- 3- 9 -54.178 5- 2- 4- 10 -16.401
5- 2- 3- 12 -168.601 5- 2- 3- 15 69.931
6- 4- 1- 7 -43.607 6- 4- 2- 8 -16.697
6- 4- 1- 11 71.270 6- 4- 1- 13 -165.031
7- 1- 4- 10 73.858 7- 1- 11- 12 -169.935
7- 1- 13- 14 -61.433 7- 1- 13- 15 178.336
7- 1- 13- 17 51.202 8- 2- 3- 9 64.012
8- 2- 4- 10 -136.930 8- 2- 3- 12 -50.411
8- 2- 3- 15 -171.879 9- 3- 12- 11 -173.992
9- 3- 15- 13 -165.137 9- 3- 15- 16 83.655
9- 3- 15- 18 -34.856 10- 4- 1- 11 -171.265
10- 4- 1- 13 -47.566 11- 1- 13- 14 -174.872
11- 1- 13- 15 64.897 11- 12- 3- 15 69.891
11- 1- 13- 17 -62.237 12- 3- 15- 13 -53.348
12- 11- 1- 13 -52.773 12- 3- 15- 16 -164.556
12- 3- 15- 18 76.934 13- 17- 19- 18 52.552
13- 15- 18- 19 33.827 14- 13- 15- 16 -12.119
14- 13- 15- 18 101.423 14- 13- 17- 19 -174.173
15- 18- 19- 17 -56.722 15- 13- 17- 19 -52.106
16- 15- 13- 17 -128.748 16- 15- 18- 19 145.983
17- 13- 15- 18 -15.206

DFT/6-31G* (GAS)

Geometry information
Bond Lengths

I J R I J R I J R I J R
1) 1- 4 1.5354 1- 7 1.0989 1- 11 1.4158 1- 13 1.5341
5) 2- 3 1.5376 2- 4 1.5498 2- 5 1.0979 2- 8 1.0936
9) 3- 9 1.0966 3- 12 1.4235 3- 15 1.5502 4- 6 1.0930
13) 4- 10 1.0951 11- 12 1.4813 13- 14 1.0908 13- 15 1.9573
17) 13- 17 1.3298 15- 16 1.1084 15- 18 1.2652 17- 19 1.3228
21) 18- 19 2.1017
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.472 1- 4- 10 110.986 1- 11- 12 110.561
4) 1- 13- 14 114.876 1- 13- 15 98.878 1- 13- 17 123.505
7) 2- 3- 9 112.070 2- 3- 12 109.083 2- 3- 15 112.885
10) 2- 4- 6 110.967 2- 4- 10 112.080 3- 2- 4 107.115
13) 3- 2- 5 110.159 3- 2- 8 110.151 3- 15- 16 113.415
16) 3- 15- 18 119.871 4- 1- 7 112.912 4- 1- 11 110.830
19) 4- 1- 13 107.879 4- 2- 3 107.115 4- 2- 5 111.755
22) 4- 2- 8 110.610 5- 2- 3 110.159 5- 2- 4 111.755
25) 5- 2- 8 107.078 6- 4- 10 107.638 7- 1- 4 112.912
28) 7- 1- 11 102.938 7- 1- 13 107.978 8- 2- 3 110.151
31) 8- 2- 4 110.610 8- 2- 5 107.078 9- 3- 12 103.296
34) 9- 3- 15 107.915 10- 4- 6 107.638 11- 1- 4 110.830
37) 11- 1- 7 102.938 11- 1- 13 114.334 12- 3- 9 103.296
40) 12- 3- 15 111.193 13- 1- 4 107.879 13- 1- 7 107.978
43) 13- 1- 11 114.334 13- 15- 16 95.977 13- 15- 18 103.655
46) 13- 17- 19 112.906 14- 13- 15 111.508 14- 13- 17 107.978
49) 15- 3- 9 107.915 15- 3- 12 111.193 15- 13- 14 111.508
52) 15- 13- 17 97.820 15- 18- 19 103.122 16- 15- 18 118.357
55) 17- 13- 14 107.978 17- 13- 15 97.820 18- 15- 16 118.357
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 20.872 1- 11- 12- 3 26.223
1- 13- 15- 3 24.287 1- 4- 2- 5 -99.867
1- 4- 2- 8 140.932 1- 13- 15- 16 139.223
1- 13- 15- 18 -99.653 1- 13- 17- 19 47.721
2- 4- 1- 7 177.178 2- 3- 12- 11 -73.534
2- 4- 1- 11 -67.932 2- 3- 15- 13 48.343
2- 4- 1- 13 57.940 2- 3- 15- 16 -52.305
2- 3- 15- 18 159.959 3- 2- 4- 6 -96.456
3- 2- 4- 10 143.172 3- 15- 13- 14 -96.990
3- 15- 13- 17 150.118 3- 15- 18- 19 -106.743
4- 2- 3- 9 158.193 4- 1- 11- 12 42.427
4- 2- 3- 12 44.436 4- 1- 13- 14 38.773
4- 1- 13- 15 -80.008 4- 2- 3- 15 -79.705
4- 1- 13- 17 174.414 5- 2- 4- 6 142.805
5- 2- 3- 9 -80.061 5- 2- 4- 10 22.433
5- 2- 3- 12 166.182 5- 2- 3- 15 42.042
6- 4- 1- 7 -63.246 6- 4- 2- 8 23.604
6- 4- 1- 11 51.645 6- 4- 1- 13 177.516
7- 1- 4- 10 54.204 7- 1- 11- 12 163.411
7- 1- 13- 14 -83.554 7- 1- 13- 15 157.665
7- 1- 13- 17 52.087 8- 2- 3- 9 37.840
8- 2- 4- 10 -96.768 8- 2- 3- 12 -75.917
8- 2- 3- 15 159.942 9- 3- 12- 11 167.106
9- 3- 15- 13 172.751 9- 3- 15- 16 72.103
9- 3- 15- 18 -75.633 10- 4- 1- 11 169.094
10- 4- 1- 13 -65.034 11- 1- 13- 14 162.549
11- 1- 13- 15 43.768 11- 12- 3- 15 51.599
11- 1- 13- 17 -61.810 12- 3- 15- 13 -74.631
12- 11- 1- 13 -79.751 12- 3- 15- 16 -175.280
12- 3- 15- 18 36.985 13- 17- 19- 18 56.264
13- 15- 18- 19 2.434 14- 13- 15- 16 17.946
14- 13- 15- 18 139.070 14- 13- 17- 19 -174.103

15- 18- 19- 17 -30.978 15- 13- 17- 19 -58.404
16- 15- 13- 17 -94.946 16- 15- 18- 19 107.082
17- 13- 15- 18 26.178

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5324 1- 7 1.0978 1- 11 1.4255 1- 13 1.5337
5) 2- 3 1.5332 2- 4 1.5485 2- 5 1.0962 2- 8 1.0930
9) 3- 9 1.0962 3- 12 1.4330 3- 15 1.5489 4- 6 1.0928
13) 4- 10 1.0935 11- 12 1.4847 13- 14 1.0904 13- 15 1.9016
17) 13- 17 1.3385 15- 16 1.1050 15- 18 1.2800 17- 19 1.3276
21) 18- 19 2.0899
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 107.565 1- 4- 10 110.547 1- 11- 12 110.342
4) 1- 13- 14 114.258 1- 13- 15 99.958 1- 13- 17 123.428
7) 2- 3- 9 112.349 2- 3- 12 109.340 2- 3- 15 113.071
10) 2- 4- 6 111.363 2- 4- 10 112.094 3- 2- 4 107.260
13) 3- 2- 5 109.810 3- 2- 8 109.891 3- 15- 16 113.662
16) 3- 15- 18 119.167 4- 1- 7 112.988 4- 1- 11 111.026
19) 4- 1- 13 108.067 4- 2- 3 107.260 4- 2- 5 111.886
22) 4- 2- 8 110.882 5- 2- 3 109.810 5- 2- 4 111.886
25) 5- 2- 8 107.122 6- 4- 10 107.574 7- 1- 4 112.988
28) 7- 1- 11 103.000 7- 1- 13 107.890 8- 2- 3 109.891
31) 8- 2- 4 110.882 8- 2- 5 107.122 9- 3- 12 103.179
34) 9- 3- 15 107.735 10- 4- 6 107.574 11- 1- 4 111.026
37) 11- 1- 7 103.000 11- 1- 13 113.877 12- 3- 9 103.179
40) 12- 3- 15 110.725 13- 1- 4 108.067 13- 1- 7 107.890
43) 13- 1- 11 113.877 13- 15- 16 96.812 13- 15- 18 104.777
46) 13- 17- 19 112.653 14- 13- 15 111.301 14- 13- 17 107.443
49) 15- 3- 9 107.735 15- 3- 12 110.725 15- 13- 14 111.301
52) 15- 13- 17 98.605 15- 18- 19 102.228 16- 15- 18 117.149
55) 17- 13- 14 107.443 17- 13- 15 98.605 18- 15- 16 117.149
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 19.239 1- 11- 12- 3 24.212
1- 13- 15- 3 23.555 1- 4- 2- 5 -101.243
1- 4- 2- 8 139.229 1- 13- 15- 16 139.134
1- 13- 15- 18 -100.417 1- 13- 17- 19 50.184
2- 4- 1- 7 177.208 2- 3- 12- 11 -72.966
2- 4- 1- 11 -67.651 2- 3- 15- 13 48.431
2- 4- 1- 13 57.907 2- 3- 15- 16 -53.655
2- 3- 15- 18 161.749 3- 2- 4- 6 -98.423
3- 2- 4- 10 140.999 3- 15- 13- 14 -97.521
3- 15- 13- 17 149.872 3- 15- 18- 19 -108.189
4- 2- 3- 9 159.909 4- 1- 11- 12 43.933
4- 2- 3- 12 45.983 4- 1- 13- 14 39.540
4- 1- 13- 15 -79.385 4- 2- 3- 15 -77.876
4- 1- 13- 17 173.283 5- 2- 4- 6 141.095
5- 2- 3- 9 -78.301 5- 2- 4- 10 20.518
5- 2- 3- 12 167.773 5- 2- 3- 15 43.914
6- 4- 1- 7 -62.696 6- 4- 2- 8 21.567
6- 4- 1- 11 52.444 6- 4- 1- 13 178.003
7- 1- 4- 10 54.489 7- 1- 11- 12 165.141
7- 1- 13- 14 -82.938 7- 1- 13- 15 158.138
7- 1- 13- 17 50.806 8- 2- 3- 9 39.288
8- 2- 4- 10 -99.010 8- 2- 3- 12 -74.638

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8- 2- 3- 15 161.503 9- 3- 12- 11 167.292
9- 3- 15- 13 173.192 9- 3- 15- 16 71.106
9- 3- 15- 18 -73.490 10- 4- 1- 11 169.630
10- 4- 1- 13 -64.811 11- 1- 13- 14 163.397
11- 1- 13- 15 44.472 11- 12- 3- 15 52.262
11- 1- 13- 17 -62.860 12- 3- 15- 13 -74.664
12- 11- 1- 13 -78.309 12- 3- 15- 16 -176.750
12- 3- 15- 18 38.654 13- 17- 19- 18 55.318
13- 15- 18- 19 2.568 14- 13- 15- 16 18.057
14- 13- 15- 18 138.507 14- 13- 17- 19 -173.477
15- 18- 19- 17 -30.925 15- 13- 17- 19 -57.841
16- 15- 13- 17 -94.549 16- 15- 18- 19 108.419
17- 13- 15- 18 25.900
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Optimised structures for the transition state for primary ozonide 16d ring-opening at all levels reported.

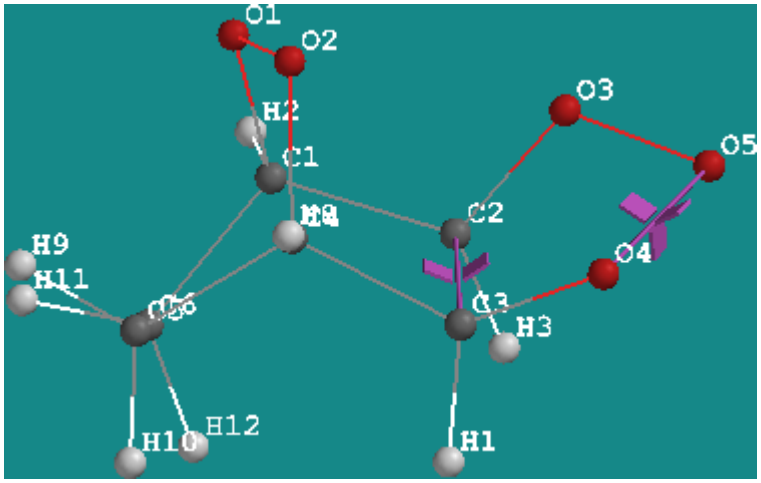

Figure S16: Optimised geometry for primary ozonide TS ring-opening **16d**.

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5319 1- 7 1.0828 1- 11 1.4039 1- 13 1.5073
5) 2- 3 1.5251 2- 4 1.5439 2- 5 1.0841 2- 8 1.0823
9) 3- 9 1.0816 3- 12 1.4106 3- 15 1.5386 4- 6 1.0822
13) 4- 10 1.0858 11- 12 1.4068 13- 14 1.0749 13- 15 1.9498
17) 13- 17 1.2912 15- 16 1.0903 15- 18 1.2474 17- 19 1.2828
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21) 18- 19 1.9664
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 109.165 1- 4- 10 110.586 1- 11- 12 111.721
4) 1- 13- 14 120.276 1- 13- 15 104.710 1- 13- 17 115.630
7) 2- 3- 9 111.831 2- 3- 12 110.444 2- 3- 15 110.535
10) 2- 4- 6 110.674 2- 4- 10 112.048 3- 2- 4 108.956
13) 3- 2- 5 110.125 3- 2- 8 108.230 3- 15- 16 114.484
16) 3- 15- 18 120.971 4- 1- 7 112.225 4- 1- 11 108.561
19) 4- 1- 13 110.051 4- 2- 3 108.956 4- 2- 5 111.537
22) 4- 2- 8 110.380 5- 2- 3 110.125 5- 2- 4 111.537
25) 5- 2- 8 107.553 6- 4- 10 107.193 7- 1- 4 112.225
28) 7- 1- 11 104.712 7- 1- 13 111.245 8- 2- 3 108.230
31) 8- 2- 4 110.380 8- 2- 5 107.553 9- 3- 12 103.636
34) 9- 3- 15 109.259 10- 4- 6 107.193 11- 1- 4 108.561
37) 11- 1- 7 104.712 11- 1- 13 109.876 12- 3- 9 103.636
40) 12- 3- 15 110.952 13- 1- 4 110.051 13- 1- 7 111.245
43) 13- 1- 11 109.876 13- 15- 16 99.063 13- 15- 18 102.705
46) 13- 17- 19 112.343 14- 13- 15 96.883 14- 13- 17 116.186
49) 15- 3- 9 109.259 15- 3- 12 110.952 15- 13- 14 96.883
52) 15- 13- 17 96.545 15- 18- 19 103.383 16- 15- 18 116.792
55) 17- 13- 14 116.186 17- 13- 15 96.545 18- 15- 16 116.792
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -19.921 1- 11- 12- 3 -28.079
1- 13- 15- 3 -18.195 1- 4- 2- 5 -141.700
1- 4- 2- 8 98.795 1- 13- 15- 16 97.858
1- 13- 15- 18 -141.886 1- 13- 17- 19 165.244
2- 4- 1- 7 -157.970 2- 3- 12- 11 -39.176
2- 4- 1- 11 -42.718 2- 3- 15- 13 74.827
2- 4- 1- 13 77.570 2- 3- 15- 16 -28.053
2- 3- 15- 18 -176.368 3- 2- 4- 6 -138.858
3- 2- 4- 10 101.559 3- 15- 13- 14 -142.024
3- 15- 13- 17 100.508 3- 15- 18- 19 -110.409
4- 2- 3- 9 178.766 4- 1- 11- 12 73.049
4- 2- 3- 12 63.908 4- 1- 13- 14 55.675
4- 1- 13- 15 -51.586 4- 2- 3- 15 -59.263
4- 1- 13- 17 -156.458 5- 2- 4- 6 99.362
5- 2- 3- 9 -58.601 5- 2- 4- 10 -20.221
5- 2- 3- 12 -173.460 5- 2- 3- 15 63.369
6- 4- 1- 7 -38.063 6- 4- 2- 8 -20.143
6- 4- 1- 11 77.189 6- 4- 1- 13 -162.523
7- 1- 4- 10 79.635 7- 1- 11- 12 -166.905
7- 1- 13- 14 -69.349 7- 1- 13- 15 -176.610
7- 1- 13- 17 78.519 8- 2- 3- 9 58.713
8- 2- 4- 10 -139.726 8- 2- 3- 12 -56.145
8- 2- 3- 15 -179.317 9- 3- 12- 11 -159.098
9- 3- 15- 13 -161.701 9- 3- 15- 16 95.418
9- 3- 15- 18 -52.897 10- 4- 1- 11 -165.113
10- 4- 1- 13 -44.825 11- 1- 13- 14 175.165
11- 1- 13- 15 67.904 11- 12- 3- 15 83.752
11- 1- 13- 17 -36.967 12- 3- 15- 13 -48.048
12- 11- 1- 13 -47.347 12- 3- 15- 16 -150.929
12- 3- 15- 18 60.756 13- 17- 19- 18 -57.467
13- 15- 18- 19 -5.173 14- 13- 15- 16 -25.972
14- 13- 15- 18 94.285 14- 13- 17- 19 -45.544
15- 18- 19- 17 33.749 15- 13- 17- 19 55.458
16- 15- 13- 17 -143.440 16- 15- 18- 19 101.969
17- 13- 15- 18 -23.183

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5295 1- 7 1.0820 1- 11 1.4123 1- 13 1.5074
5) 2- 3 1.5236 2- 4 1.5427 2- 5 1.0832 2- 8 1.0821
9) 3- 9 1.0813 3- 12 1.4159 3- 15 1.5383 4- 6 1.0814
13) 4- 10 1.0844 11- 12 1.4081 13- 14 1.0752 13- 15 1.9202
17) 13- 17 1.2986 15- 16 1.0882 15- 18 1.2562 17- 19 1.2878
21) 18- 19 1.9596
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 109.022 1- 4- 10 110.383 1- 11- 12 111.559
4) 1- 13- 14 119.950 1- 13- 15 105.008 1- 13- 17 115.194
7) 2- 3- 9 112.032 2- 3- 12 110.599 2- 3- 15 110.439
10) 2- 4- 6 110.768 2- 4- 10 112.112 3- 2- 4 108.941
13) 3- 2- 5 109.848 3- 2- 8 108.132 3- 15- 16 114.608
16) 3- 15- 18 120.820 4- 1- 7 112.491 4- 1- 11 108.680
19) 4- 1- 13 110.287 4- 2- 3 108.941 4- 2- 5 111.678
22) 4- 2- 8 110.681 5- 2- 3 109.848 5- 2- 4 111.678
25) 5- 2- 8 107.491 6- 4- 10 107.270 7- 1- 4 112.491
28) 7- 1- 11 104.748 7- 1- 13 110.852 8- 2- 3 108.132
31) 8- 2- 4 110.681 8- 2- 5 107.491 9- 3- 12 103.597
34) 9- 3- 15 109.257 10- 4- 6 107.270 11- 1- 4 108.680
37) 11- 1- 7 104.748 11- 1- 13 109.596 12- 3- 9 103.597
40) 12- 3- 15 110.734 13- 1- 4 110.287 13- 1- 7 110.852
43) 13- 1- 11 109.596 13- 15- 16 99.312 13- 15- 18 103.318
46) 13- 17- 19 112.152 14- 13- 15 97.656 14- 13- 17 116.084
49) 15- 3- 9 109.257 15- 3- 12 110.734 15- 13- 14 97.656
52) 15- 13- 17 97.026 15- 18- 19 103.024 16- 15- 18 115.968
55) 17- 13- 14 116.084 17- 13- 15 97.026 18- 15- 16 115.968
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -19.097 1- 11- 12- 3 -27.027
1- 13- 15- 3 -18.073 1- 4- 2- 5 -140.611
1- 4- 2- 8 99.668 1- 13- 15- 16 98.320
1- 13- 15- 18 -142.023 1- 13- 17- 19 165.325
2- 4- 1- 7 -159.011 2- 3- 12- 11 -39.922
2- 4- 1- 11 -43.490 2- 3- 15- 13 74.615
2- 4- 1- 13 76.671 2- 3- 15- 16 -28.911
2- 3- 15- 18 -175.427 3- 2- 4- 6 -137.976
3- 2- 4- 10 102.237 3- 15- 13- 14 -141.960
3- 15- 13- 17 100.423 3- 15- 18- 19 -111.135
4- 2- 3- 9 178.861 4- 1- 11- 12 72.750
4- 2- 3- 12 63.835 4- 1- 13- 14 56.824
4- 1- 13- 15 -51.456 4- 2- 3- 15 -59.100
4- 1- 13- 17 -156.887 5- 2- 4- 6 100.511
5- 2- 3- 9 -58.518 5- 2- 4- 10 -19.277
5- 2- 3- 12 -173.544 5- 2- 3- 15 63.521
6- 4- 1- 7 -39.013 6- 4- 2- 8 -19.210
6- 4- 1- 11 76.507 6- 4- 1- 13 -163.331
7- 1- 4- 10 78.574 7- 1- 11- 12 -166.814
7- 1- 13- 14 -68.432 7- 1- 13- 15 -176.712
7- 1- 13- 17 77.857 8- 2- 3- 9 58.511
8- 2- 4- 10 -138.997 8- 2- 3- 12 -56.515
8- 2- 3- 15 -179.450 9- 3- 12- 11 -160.135
9- 3- 15- 13 -161.726 9- 3- 15- 16 94.748
9- 3- 15- 18 -51.769 10- 4- 1- 11 -165.906
10- 4- 1- 13 -45.744 11- 1- 13- 14 176.432
11- 1- 13- 15 68.152 11- 12- 3- 15 82.841
11- 1- 13- 17 -37.279 12- 3- 15- 13 -48.241

12- 11- 1- 13 -47.838 12- 3- 15- 16 -151.767
12- 3- 15- 18 61.716 13- 17- 19- 18 -56.563
13- 15- 18- 19 -4.696 14- 13- 15- 16 -25.567
14- 13- 15- 18 94.090 14- 13- 17- 19 -47.047
15- 18- 19- 17 33.065 15- 13- 17- 19 55.063
16- 15- 13- 17 -143.184 16- 15- 18- 19 102.777
17- 13- 15- 18 -23.527

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5412 1- 7 1.0994 1- 11 1.4379 1- 13 1.4901
5) 2- 3 1.5215 2- 4 1.5335 2- 5 1.0955 2- 8 1.0927
9) 3- 9 1.1012 3- 12 1.4405 3- 15 1.5319 4- 6 1.0938
13) 4- 10 1.0958 11- 12 1.4819 13- 14 1.0874 13- 15 2.7993
17) 13- 17 1.3196 15- 16 1.1135 15- 18 1.2239 17- 19 1.2798
21) 18- 19 2.8841
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 110.074 1- 4- 10 110.530 1- 11- 12 109.692
4) 1- 13- 14 126.507 1- 13- 15 91.815 1- 13- 17 117.511
7) 2- 3- 9 109.741 2- 3- 12 112.482 2- 3- 15 113.856
10) 2- 4- 6 109.847 2- 4- 10 111.505 3- 2- 4 111.239
13) 3- 2- 5 109.344 3- 2- 8 107.751 3- 15- 16 115.314
16) 3- 15- 18 123.265 4- 1- 7 111.119 4- 1- 11 109.204
19) 4- 1- 13 110.314 4- 2- 3 111.239 4- 2- 5 111.151
22) 4- 2- 8 109.893 5- 2- 3 109.344 5- 2- 4 111.151
25) 5- 2- 8 107.325 6- 4- 10 106.915 7- 1- 4 111.119
28) 7- 1- 11 101.001 7- 1- 13 112.312 8- 2- 3 107.751
31) 8- 2- 4 109.893 8- 2- 5 107.325 9- 3- 12 104.452
34) 9- 3- 15 106.060 10- 4- 6 106.915 11- 1- 4 109.204
37) 11- 1- 7 101.001 11- 1- 13 112.561 12- 3- 9 104.452
40) 12- 3- 15 109.634 13- 1- 4 110.314 13- 1- 7 112.312
43) 13- 1- 11 112.561 13- 15- 16 104.253 13- 15- 18 88.213
46) 13- 17- 19 119.506 14- 13- 15 84.616 14- 13- 17 115.970
49) 15- 3- 9 106.060 15- 3- 12 109.634 15- 13- 14 84.616
52) 15- 13- 17 92.695 15- 18- 19 112.385 16- 15- 18 121.190
55) 17- 13- 14 115.970 17- 13- 15 92.695 18- 15- 16 121.190
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -34.509 1- 11- 12- 3 -47.409
1- 13- 15- 3 -18.858 1- 4- 2- 5 -156.610
1- 4- 2- 8 84.733 1- 13- 15- 16 95.507
1- 13- 15- 18 -142.713 1- 13- 17- 19 175.262
2- 4- 1- 7 -138.462 2- 3- 12- 11 -18.238
2- 4- 1- 11 -27.903 2- 3- 15- 13 75.484
2- 4- 1- 13 96.302 2- 3- 15- 16 -26.916
2- 3- 15- 18 158.561 3- 2- 4- 6 -154.559
3- 2- 4- 10 87.101 3- 15- 13- 14 -145.361
3- 15- 13- 17 98.797 3- 15- 18- 19 -83.848
4- 2- 3- 9 176.985 4- 1- 11- 12 73.502
4- 2- 3- 12 61.170 4- 1- 13- 14 31.429
4- 1- 13- 15 -53.215 4- 2- 3- 15 -64.325
4- 1- 13- 17 -147.203 5- 2- 4- 6 83.339
5- 2- 3- 9 -59.872 5- 2- 4- 10 -35.000
5- 2- 3- 12 -175.688 5- 2- 3- 15 58.818
6- 4- 1- 7 -18.554 6- 4- 2- 8 -35.318
6- 4- 1- 11 92.005 6- 4- 1- 13 -143.790
7- 1- 4- 10 99.327 7- 1- 11- 12 -169.343
7- 1- 13- 14 -93.126 7- 1- 13- 15 -177.771

7- 1- 13- 17 88.242 8- 2- 3- 9 56.473
8- 2- 4- 10 -153.657 8- 2- 3- 12 -59.343
8- 2- 3- 15 175.163 9- 3- 12- 11 -137.196
9- 3- 15- 13 -163.744 9- 3- 15- 16 93.857
9- 3- 15- 18 -80.667 10- 4- 1- 11 -150.115
10- 4- 1- 13 -25.910 11- 1- 13- 14 153.679
11- 1- 13- 15 69.034 11- 12- 3- 15 109.522
11- 1- 13- 17 -24.953 12- 3- 15- 13 -51.506
12- 11- 1- 13 -49.372 12- 3- 15- 16 -153.906
12- 3- 15- 18 31.571 13- 17- 19- 18 -74.560
13- 15- 18- 19 -3.668 14- 13- 15- 16 -30.996
14- 13- 15- 18 90.784 14- 13- 17- 19 -3.515
15- 18- 19- 17 36.286 15- 13- 17- 19 81.807
16- 15- 13- 17 -146.837 16- 15- 18- 19 101.940
17- 13- 15- 18 -25.058

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5380 1- 7 1.0982 1- 11 1.4312 1- 13 1.4891
5) 2- 3 1.5232 2- 4 1.5390 2- 5 1.0945 2- 8 1.0923
9) 3- 9 1.0993 3- 12 1.4317 3- 15 1.5398 4- 6 1.0932
13) 4- 10 1.0950 11- 12 1.4689 13- 14 1.0857 13- 15 2.4398
17) 13- 17 1.3364 15- 16 1.1132 15- 18 1.2242 17- 19 1.2577
21) 18- 19 2.5560
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 109.812 1- 4- 10 110.461 1- 11- 12 110.257
4) 1- 13- 14 127.081 1- 13- 15 99.607 1- 13- 17 116.788
7) 2- 3- 9 110.314 2- 3- 12 111.989 2- 3- 15 113.544
10) 2- 4- 6 110.209 2- 4- 10 111.841 3- 2- 4 110.827
13) 3- 2- 5 109.691 3- 2- 8 107.562 3- 15- 16 115.349
16) 3- 15- 18 123.032 4- 1- 7 111.914 4- 1- 11 109.057
19) 4- 1- 13 108.819 4- 2- 3 110.827 4- 2- 5 111.370
22) 4- 2- 8 109.877 5- 2- 3 109.691 5- 2- 4 111.370
25) 5- 2- 8 107.380 6- 4- 10 107.185 7- 1- 4 111.914
28) 7- 1- 11 101.539 7- 1- 13 113.435 8- 2- 3 107.562
31) 8- 2- 4 109.877 8- 2- 5 107.380 9- 3- 12 103.127
34) 9- 3- 15 106.277 10- 4- 6 107.185 11- 1- 4 109.057
37) 11- 1- 7 101.539 11- 1- 13 111.891 12- 3- 9 103.127
40) 12- 3- 15 110.925 13- 1- 4 108.819 13- 1- 7 113.435
43) 13- 1- 11 111.891 13- 15- 16 94.978 13- 15- 18 97.800
46) 13- 17- 19 118.721 14- 13- 15 86.932 14- 13- 17 115.332
49) 15- 3- 9 106.277 15- 3- 12 110.925 15- 13- 14 86.932
52) 15- 13- 17 92.140 15- 18- 19 105.076 16- 15- 18 120.695
55) 17- 13- 14 115.332 17- 13- 15 92.140 18- 15- 16 120.695
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -28.163 1- 11- 12- 3 -39.466
1- 13- 15- 3 -17.128 1- 4- 2- 5 -150.573
1- 4- 2- 8 90.575 1- 13- 15- 16 98.042
1- 13- 15- 18 -140.013 1- 13- 17- 19 174.252
2- 4- 1- 7 -146.592 2- 3- 12- 11 -27.104
2- 4- 1- 11 -35.056 2- 3- 15- 13 74.601
2- 4- 1- 13 87.252 2- 3- 15- 16 -19.284
2- 3- 15- 18 171.673 3- 2- 4- 6 -147.724
3- 2- 4- 10 93.151 3- 15- 13- 14 -144.236
3- 15- 13- 17 100.501 3- 15- 18- 19 -96.283

4- 2- 3- 9 177.428 4- 1- 11- 12 74.458
4- 2- 3- 12 63.182 4- 1- 13- 14 40.015
4- 1- 13- 15 -53.419 4- 2- 3- 15 -63.408
4- 1- 13- 17 -150.765 5- 2- 4- 6 89.866
5- 2- 3- 9 -59.190 5- 2- 4- 10 -29.259
5- 2- 3- 12 -173.436 5- 2- 3- 15 59.974
6- 4- 1- 7 -26.778 6- 4- 2- 8 -28.986
6- 4- 1- 11 84.758 6- 4- 1- 13 -152.934
7- 1- 4- 10 91.231 7- 1- 11- 12 -167.279
7- 1- 13- 14 -85.258 7- 1- 13- 15 -178.691
7- 1- 13- 17 83.962 8- 2- 3- 9 57.299
8- 2- 4- 10 -148.111 8- 2- 3- 12 -56.947
8- 2- 3- 15 176.463 9- 3- 12- 11 -145.700
9- 3- 15- 13 -163.951 9- 3- 15- 16 102.164
9- 3- 15- 18 -66.879 10- 4- 1- 11 -157.233
10- 4- 1- 13 -34.925 11- 1- 13- 14 160.591
11- 1- 13- 15 67.158 11- 12- 3- 15 100.892
11- 1- 13- 17 -30.188 12- 3- 15- 13 -52.547
12- 11- 1- 13 -45.981 12- 3- 15- 16 -146.431
12- 3- 15- 18 44.525 13- 17- 19- 18 -69.910
13- 15- 18- 19 -5.315 14- 13- 15- 16 -29.067
14- 13- 15- 18 92.879 14- 13- 17- 19 -15.251
15- 18- 19- 17 36.967 15- 13- 17- 19 72.367
16- 15- 13- 17 -144.330 16- 15- 18- 19 95.239
17- 13- 15- 18 -22.384

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5415 1- 7 1.0971 1- 11 1.4279 1- 13 1.5085
5) 2- 3 1.5318 2- 4 1.5497 2- 5 1.0946 2- 8 1.0935
9) 3- 9 1.0960 3- 12 1.4265 3- 15 1.5620 4- 6 1.0932
13) 4- 10 1.0967 11- 12 1.4812 13- 14 1.0874 13- 15 1.9664
17) 13- 17 1.3253 15- 16 1.1108 15- 18 1.2607 17- 19 1.3244
21) 18- 19 2.1230
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.903 1- 4- 10 110.398 1- 11- 12 110.094
4) 1- 13- 14 120.876 1- 13- 15 105.648 1- 13- 17 115.186
7) 2- 3- 9 112.074 2- 3- 12 111.428 2- 3- 15 110.654
10) 2- 4- 6 110.824 2- 4- 10 112.023 3- 2- 4 109.131
13) 3- 2- 5 109.945 3- 2- 8 108.179 3- 15- 16 113.247
16) 3- 15- 18 120.794 4- 1- 7 112.064 4- 1- 11 108.933
19) 4- 1- 13 110.103 4- 2- 3 109.131 4- 2- 5 111.432
22) 4- 2- 8 110.612 5- 2- 3 109.945 5- 2- 4 111.432
25) 5- 2- 8 107.478 6- 4- 10 107.287 7- 1- 4 112.064
28) 7- 1- 11 103.491 7- 1- 13 111.564 8- 2- 3 108.179
31) 8- 2- 4 110.612 8- 2- 5 107.478 9- 3- 12 102.630
34) 9- 3- 15 108.229 10- 4- 6 107.287 11- 1- 4 108.933
37) 11- 1- 7 103.491 11- 1- 13 110.486 12- 3- 9 102.630
40) 12- 3- 15 111.552 13- 1- 4 110.103 13- 1- 7 111.564
43) 13- 1- 11 110.486 13- 15- 16 98.488 13- 15- 18 104.024
46) 13- 17- 19 111.880 14- 13- 15 95.486 14- 13- 17 115.547
49) 15- 3- 9 108.229 15- 3- 12 111.552 15- 13- 14 95.486
52) 15- 13- 17 97.868 15- 18- 19 101.935 16- 15- 18 118.205
55) 17- 13- 14 115.547 17- 13- 15 97.868 18- 15- 16 118.205
Dihedrals
I J K L Theta I J K L Theta

1- 4- 2- 3 -19.570 1- 11- 12- 3 -27.300
1- 13- 15- 3 -18.226 1- 4- 2- 5 -141.175
1- 4- 2- 8 99.329 1- 13- 15- 16 96.244
1- 13- 15- 18 -141.763 1- 13- 17- 19 170.534
2- 4- 1- 7 -158.317 2- 3- 12- 11 -39.858
2- 4- 1- 11 -44.416 2- 3- 15- 13 74.739
2- 4- 1- 13 76.886 2- 3- 15- 16 -26.812
2- 3- 15- 18 -175.551 3- 2- 4- 6 -138.407
3- 2- 4- 10 101.805 3- 15- 13- 14 -142.440
3- 15- 13- 17 100.776 3- 15- 18- 19 -111.581
4- 2- 3- 9 179.392 4- 1- 11- 12 73.135
4- 2- 3- 12 65.022 4- 1- 13- 14 55.406
4- 1- 13- 15 -51.042 4- 2- 3- 15 -59.704
4- 1- 13- 17 -157.829 5- 2- 4- 6 99.989
5- 2- 3- 9 -58.108 5- 2- 4- 10 -19.799
5- 2- 3- 12 -172.477 5- 2- 3- 15 62.797
6- 4- 1- 7 -38.252 6- 4- 2- 8 -19.507
6- 4- 1- 11 75.650 6- 4- 1- 13 -163.049
7- 1- 4- 10 79.293 7- 1- 11- 12 -167.479
7- 1- 13- 14 -69.677 7- 1- 13- 15 -176.126
7- 1- 13- 17 77.087 8- 2- 3- 9 58.987
8- 2- 4- 10 -139.295 8- 2- 3- 12 -55.382
8- 2- 3- 15 179.891 9- 3- 12- 11 -159.967
9- 3- 15- 13 -162.102 9- 3- 15- 16 96.348
9- 3- 15- 18 -52.392 10- 4- 1- 11 -166.806
10- 4- 1- 13 -45.504 11- 1- 13- 14 175.776
11- 1- 13- 15 69.327 11- 12- 3- 15 84.364
11- 1- 13- 17 -37.460 12- 3- 15- 13 -49.917
12- 11- 1- 13 -47.933 12- 3- 15- 16 -151.468
12- 3- 15- 18 59.793 13- 17- 19- 18 -58.997
13- 15- 18- 19 -6.680 14- 13- 15- 16 -27.969
14- 13- 15- 18 94.023 14- 13- 17- 19 -40.891
15- 18- 19- 17 36.136 15- 13- 17- 19 59.073
16- 15- 13- 17 -144.754 16- 15- 18- 19 101.173
17- 13- 15- 18 -22.761

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 4 1.5375 1- 7 1.0959 1- 11 1.4381 1- 13 1.5091
5) 2- 3 1.5295 2- 4 1.5476 2- 5 1.0935 2- 8 1.0933
9) 3- 9 1.0954 3- 12 1.4321 3- 15 1.5633 4- 6 1.0923
13) 4- 10 1.0950 11- 12 1.4830 13- 14 1.0878 13- 15 1.9148
17) 13- 17 1.3355 15- 16 1.1070 15- 18 1.2735 17- 19 1.3298
21) 18- 19 2.1160
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 4- 6 108.785 1- 4- 10 110.094 1- 11- 12 109.768
4) 1- 13- 14 120.082 1- 13- 15 106.404 1- 13- 17 114.417
7) 2- 3- 9 112.329 2- 3- 12 111.748 2- 3- 15 110.573
10) 2- 4- 6 111.028 2- 4- 10 112.118 3- 2- 4 109.080
13) 3- 2- 5 109.567 3- 2- 8 108.064 3- 15- 16 113.357
16) 3- 15- 18 120.277 4- 1- 7 112.375 4- 1- 11 109.105
19) 4- 1- 13 110.314 4- 2- 3 109.080 4- 2- 5 111.642
22) 4- 2- 8 111.017 5- 2- 3 109.567 5- 2- 4 111.642
25) 5- 2- 8 107.392 6- 4- 10 107.377 7- 1- 4 112.375
28) 7- 1- 11 103.672 7- 1- 13 111.056 8- 2- 3 108.064
31) 8- 2- 4 111.017 8- 2- 5 107.392 9- 3- 12 102.637
34) 9- 3- 15 108.111 10- 4- 6 107.377 11- 1- 4 109.105
37) 11- 1- 7 103.672 11- 1- 13 110.111 12- 3- 9 102.637

40) 12- 3- 15 111.159 13- 1- 4 110.314 13- 1- 7 111.056
43) 13- 1- 11 110.111 13- 15- 16 99.230 13- 15- 18 105.174
46) 13- 17- 19 111.775 14- 13- 15 96.860 14- 13- 17 115.416
49) 15- 3- 9 108.111 15- 3- 12 111.159 15- 13- 14 96.860
52) 15- 13- 17 98.648 15- 18- 19 101.162 16- 15- 18 117.088
55) 17- 13- 14 115.416 17- 13- 15 98.648 18- 15- 16 117.088
Dihedrals
I J K L Theta I J K L Theta
1- 4- 2- 3 -18.397 1- 11- 12- 3 -26.153
1- 13- 15- 3 -17.988 1- 4- 2- 5 -139.628
1- 4- 2- 8 100.574 1- 13- 15- 16 96.910
1- 13- 15- 18 -141.619 1- 13- 17- 19 170.947
2- 4- 1- 7 -159.990 2- 3- 12- 11 -40.709
2- 4- 1- 11 -45.590 2- 3- 15- 13 74.431
2- 4- 1- 13 75.490 2- 3- 15- 16 -28.346
2- 3- 15- 18 -174.084 3- 2- 4- 6 -137.219
3- 2- 4- 10 102.673 3- 15- 13- 14 -142.161
3- 15- 13- 17 100.740 3- 15- 18- 19 -112.811
4- 2- 3- 9 179.646 4- 1- 11- 12 73.031
4- 2- 3- 12 64.907 4- 1- 13- 14 57.418
4- 1- 13- 15 -50.908 4- 2- 3- 15 -59.483
4- 1- 13- 17 -158.713 5- 2- 4- 6 101.550
5- 2- 3- 9 -57.868 5- 2- 4- 10 -18.558
5- 2- 3- 12 -172.607 5- 2- 3- 15 63.004
6- 4- 1- 7 -39.734 6- 4- 2- 8 -18.248
6- 4- 1- 11 74.666 6- 4- 1- 13 -164.254
7- 1- 4- 10 77.674 7- 1- 11- 12 -167.043
7- 1- 13- 14 -67.855 7- 1- 13- 15 -176.181
7- 1- 13- 17 76.014 8- 2- 3- 9 58.850
8- 2- 4- 10 -138.355 8- 2- 3- 12 -55.889
8- 2- 3- 15 179.722 9- 3- 12- 11 -161.282
9- 3- 15- 13 -162.220 9- 3- 15- 16 95.002
9- 3- 15- 18 -50.736 10- 4- 1- 11 -167.926
10- 4- 1- 13 -46.845 11- 1- 13- 14 177.896
11- 1- 13- 15 69.571 11- 12- 3- 15 83.352
11- 1- 13- 17 -38.235 12- 3- 15- 13 -50.294
12- 11- 1- 13 -48.172 12- 3- 15- 16 -153.072
12- 3- 15- 18 61.190 13- 17- 19- 18 -57.711
13- 15- 18- 19 -6.313 14- 13- 15- 16 -27.263
14- 13- 15- 18 94.208 14- 13- 17- 19 -43.448
15- 18- 19- 17 35.385 15- 13- 17- 19 58.442
16- 15- 13- 17 -144.363 16- 15- 18- 19 102.676
17- 13- 15- 18 -22.892

Optimised structures for the transition state for primary ozonide 18a formation at all levels reported.

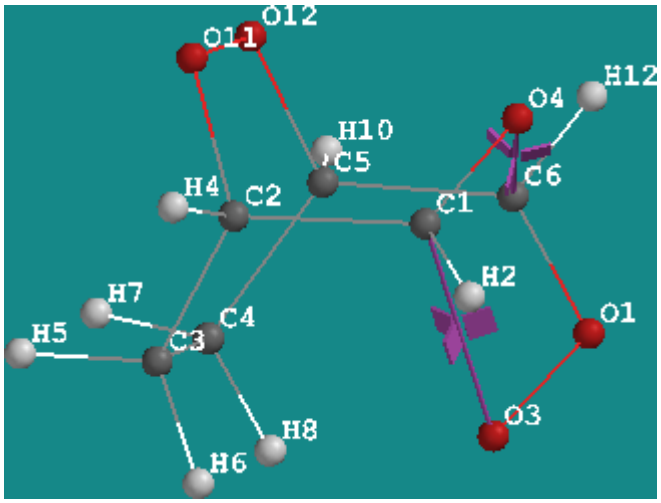

Figure S17: Optimised geometry for primary ozonide TS formation **18a**.

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5265 1- 10 1.0808 1- 17 2.1541 1- 18 1.2216
5) 2- 4 1.5380 2- 6 1.5223 2- 7 1.0797 2- 11 1.0837
9) 3- 4 1.5276 3- 5 1.5361 3- 8 1.0865 3- 16 1.3966
13) 4- 9 1.0844 4- 12 1.0784 5- 13 1.0756 5- 18 1.9396
17) 5- 19 1.2509 6- 14 1.0845 6- 15 1.4089 15- 16 1.4093
21) 17- 19 1.4153
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 106.685 1- 6- 15 109.442 1- 17- 19 93.652
4) 2- 4- 9 109.955 2- 4- 12 111.494 2- 6- 14 110.717
7) 2- 6- 15 110.009 3- 4- 9 105.425 3- 4- 12 110.090
10) 3- 5- 13 115.219 3- 5- 18 102.079 3- 5- 19 124.355
13) 4- 2- 6 108.770 4- 2- 7 111.459 4- 2- 11 110.271
16) 4- 3- 5 119.242 4- 3- 8 108.389 4- 3- 16 111.615
19) 5- 3- 4 119.242 5- 3- 8 101.923 5- 3- 16 111.088
22) 6- 1- 10 117.822 6- 1- 17 100.195 6- 1- 18 119.022
25) 6- 2- 4 108.770 6- 2- 7 110.739 6- 2- 11 107.243
28) 6- 15- 16 114.838 7- 2- 4 111.459 7- 2- 6 110.739
31) 7- 2- 11 108.274 8- 3- 4 108.389 8- 3- 5 101.923
34) 8- 3- 16 102.762 9- 4- 12 108.348 10- 1- 6 117.822
37) 10- 1- 17 88.456 10- 1- 18 120.859 11- 2- 4 110.271
40) 11- 2- 6 107.243 11- 2- 7 108.274 12- 4- 9 108.348
43) 13- 5- 18 96.593 13- 5- 19 114.741 14- 6- 15 102.349
46) 15- 6- 14 102.349 16- 3- 4 111.615 16- 3- 5 111.088
49) 16- 3- 8 102.762 17- 1- 6 100.195 17- 1- 10 88.456
52) 17- 1- 18 96.512 18- 1- 6 119.022 18- 1- 10 120.859
55) 18- 1- 17 96.512 18- 5- 13 96.593 18- 5- 19 95.017
58) 19- 5- 13 114.741 19- 5- 18 95.017
Dihedrals
I J K L Theta I J K L Theta
1- 18- 5- 3 60.514 1- 6- 2- 4 -73.678
1- 17- 19- 5 -41.747 1- 6- 2- 7 49.131
1- 6- 2- 11 167.073 1- 18- 5- 13 178.117
1- 6- 15- 16 69.241 1- 18- 5- 19 -66.220
2- 4- 3- 5 79.580 2- 4- 3- 8 -164.594
2- 6- 1- 10 -85.818 2- 4- 3- 16 -52.129
2- 6- 15- 16 -60.151 2- 6- 1- 17 7.848
2- 6- 1- 18 111.236 3- 4- 2- 6 1.712
```

3- 16- 15- 6 7.440 3- 4- 2- 7 -120.662
3- 4- 2- 11 119.051 3- 5- 19- 17 -46.620
4- 3- 5- 13 163.734 4- 2- 6- 14 164.103
4- 2- 6- 15 51.703 4- 3- 16- 15 48.957
4- 3- 5- 18 -92.936 4- 3- 5- 19 11.814
5- 18- 1- 6 -72.339 5- 3- 4- 9 -161.232
5- 18- 1- 10 125.248 5- 3- 4- 12 -44.577
5- 3- 16- 15 -86.764 5- 18- 1- 17 33.150
6- 2- 4- 9 -114.737 6- 2- 4- 12 125.072
6- 1- 17- 19 113.050 7- 2- 4- 9 122.889
7- 2- 4- 12 2.697 7- 2- 6- 14 -73.089
7- 2- 6- 15 174.512 8- 3- 4- 9 -45.407
8- 3- 4- 12 71.248 8- 3- 5- 13 44.543
8- 3- 16- 15 164.912 8- 3- 5- 18 147.873
8- 3- 5- 19 -107.377 9- 4- 2- 11 2.602
9- 4- 3- 16 67.058 10- 1- 6- 14 38.484
10- 1- 6- 15 148.517 10- 1- 17- 19 -128.946
11- 2- 4- 12 -117.590 11- 2- 6- 14 44.853
11- 2- 6- 15 -67.546 12- 4- 3- 16 -176.286
13- 5- 3- 16 -64.326 13- 5- 19- 17 161.342
14- 6- 15- 16 -177.869 14- 6- 1- 17 132.150
14- 6- 1- 18 -124.462 15- 6- 1- 17 -117.817
15- 6- 1- 18 -14.429 16- 3- 5- 18 39.004
16- 3- 5- 19 143.754 17- 19- 5- 18 61.708
18- 1- 17- 19 -8.058

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5234 1- 10 1.0805 1- 17 2.1775 1- 18 1.2251
5) 2- 4 1.5368 2- 6 1.5217 2- 7 1.0797 2- 11 1.0828
9) 3- 4 1.5260 3- 5 1.5347 3- 8 1.0856 3- 16 1.4022
13) 4- 9 1.0835 4- 12 1.0784 5- 13 1.0758 5- 18 1.9038
17) 5- 19 1.2606 6- 14 1.0839 6- 15 1.4124 15- 16 1.4100
21) 17- 19 1.4177
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 106.434 1- 6- 15 109.166 1- 17- 19 93.285
4) 2- 4- 9 109.984 2- 4- 12 111.643 2- 6- 14 110.827
7) 2- 6- 15 110.176 3- 4- 9 105.447 3- 4- 12 109.998
10) 3- 5- 13 114.965 3- 5- 18 102.985 3- 5- 19 124.132
13) 4- 2- 6 108.814 4- 2- 7 111.652 4- 2- 11 110.423
16) 4- 3- 5 119.564 4- 3- 8 108.524 4- 3- 16 111.436
19) 5- 3- 4 119.564 5- 3- 8 101.936 5- 3- 16 110.734
22) 6- 1- 10 117.882 6- 1- 17 101.010 6- 1- 18 119.335
25) 6- 2- 4 108.814 6- 2- 7 110.536 6- 2- 11 107.146
28) 6- 15- 16 114.815 7- 2- 4 111.652 7- 2- 6 110.536
31) 7- 2- 11 108.173 8- 3- 4 108.524 8- 3- 5 101.936
34) 8- 3- 16 102.844 9- 4- 12 108.208 10- 1- 6 117.882
37) 10- 1- 17 89.013 10- 1- 18 120.470 11- 2- 4 110.423
40) 11- 2- 6 107.146 11- 2- 7 108.173 12- 4- 9 108.208
43) 13- 5- 18 96.983 13- 5- 19 114.186 14- 6- 15 102.529
46) 15- 6- 14 102.529 16- 3- 4 111.436 16- 3- 5 110.734
49) 16- 3- 8 102.844 17- 1- 6 101.010 17- 1- 10 89.013
52) 17- 1- 18 95.187 18- 1- 6 119.335 18- 1- 10 120.470
55) 18- 1- 17 95.187 18- 5- 13 96.983 18- 5- 19 95.778
58) 19- 5- 13 114.186 19- 5- 18 95.778
Dihedrals

I J K L Theta I J K L Theta
1- 18- 5- 3 59.661 1- 6- 2- 4 -73.529
1- 17- 19- 5 -39.914 1- 6- 2- 7 49.419
1- 6- 2- 11 167.071 1- 18- 5- 13 177.347
1- 6- 15- 16 69.821 1- 18- 5- 19 -67.360
2- 4- 3- 5 78.840 2- 4- 3- 8 -165.004
2- 6- 1- 10 -87.195 2- 4- 3- 16 -52.458
2- 6- 15- 16 -59.580 2- 6- 1- 17 7.570
2- 6- 1- 18 109.985 3- 4- 2- 6 1.772
3- 16- 15- 6 6.570 3- 4- 2- 7 -120.503
3- 4- 2- 11 119.107 3- 5- 19- 17 -48.812
4- 3- 5- 13 163.528 4- 2- 6- 14 164.447
4- 2- 6- 15 51.675 4- 3- 16- 15 49.663
4- 3- 5- 18 -92.291 4- 3- 5- 19 14.036
5- 18- 1- 6 -71.291 5- 3- 4- 9 -161.915
5- 18- 1- 10 126.342 5- 3- 4- 12 -45.456
5- 3- 16- 15 -86.012 5- 18- 1- 17 34.432
6- 2- 4- 9 -114.733 6- 2- 4- 12 125.134
6- 1- 17- 19 112.094 7- 2- 4- 9 122.992
7- 2- 4- 12 2.859 7- 2- 6- 14 -72.606
7- 2- 6- 15 174.623 8- 3- 4- 9 -45.758
8- 3- 4- 12 70.701 8- 3- 5- 13 43.975
8- 3- 16- 15 165.740 8- 3- 5- 18 148.156
8- 3- 5- 19 -105.517 9- 4- 2- 11 2.602
9- 4- 3- 16 66.788 10- 1- 6- 14 37.097
10- 1- 6- 15 147.094 10- 1- 17- 19 -129.668
11- 2- 4- 12 -117.531 11- 2- 6- 14 45.047
11- 2- 6- 15 -67.725 12- 4- 3- 16 -176.754
13- 5- 3- 16 -64.868 13- 5- 19- 17 161.487
14- 6- 15- 16 -177.593 14- 6- 1- 17 131.862
14- 6- 1- 18 -125.723 15- 6- 1- 17 -118.141
15- 6- 1- 18 -15.726 16- 3- 5- 18 39.313
16- 3- 5- 19 145.640 17- 19- 5- 18 61.152
18- 1- 17- 19 -9.158

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5252 1- 10 1.1002 1- 17 2.2354 1- 18 1.2405
5) 2- 4 1.5364 2- 6 1.5224 2- 7 1.0919 2- 11 1.0944
9) 3- 4 1.5261 3- 5 1.5203 3- 8 1.1019 3- 16 1.4253
13) 4- 9 1.0951 4- 12 1.0918 5- 13 1.0884 5- 18 2.2103
17) 5- 19 1.2757 6- 14 1.1005 6- 15 1.4288 15- 16 1.5007
21) 17- 19 1.3685
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 106.884 1- 6- 15 110.663 1- 17- 19 91.287
4) 2- 4- 9 109.933 2- 4- 12 111.284 2- 6- 14 110.146
7) 2- 6- 15 110.787 3- 4- 9 105.028 3- 4- 12 109.575
10) 3- 5- 13 118.856 3- 5- 18 99.170 3- 5- 19 126.704
13) 4- 2- 6 109.636 4- 2- 7 111.183 4- 2- 11 109.971
16) 4- 3- 5 119.035 4- 3- 8 108.129 4- 3- 16 112.578
19) 5- 3- 4 119.035 5- 3- 8 102.226 5- 3- 16 112.117
22) 6- 1- 10 117.224 6- 1- 17 99.209 6- 1- 18 119.834
25) 6- 2- 4 109.636 6- 2- 7 110.106 6- 2- 11 107.589
28) 6- 15- 16 113.147 7- 2- 4 111.183 7- 2- 6 110.106
31) 7- 2- 11 108.277 8- 3- 4 108.129 8- 3- 5 102.226
34) 8- 3- 16 100.334 9- 4- 12 108.221 10- 1- 6 117.224
37) 10- 1- 17 84.766 10- 1- 18 121.230 11- 2- 4 109.971
40) 11- 2- 6 107.589 11- 2- 7 108.277 12- 4- 9 108.221

43) 13- 5- 18 101.203 13- 5- 19 111.842 14- 6- 15 100.647
46) 15- 6- 14 100.647 16- 3- 4 112.578 16- 3- 5 112.117
49) 16- 3- 8 100.334 17- 1- 6 99.209 17- 1- 10 84.766
52) 17- 1- 18 98.909 18- 1- 6 119.834 18- 1- 10 121.230
55) 18- 1- 17 98.909 18- 5- 13 101.203 18- 5- 19 85.778
58) 19- 5- 13 111.842 19- 5- 18 85.778
Dihedrals
I J K L Theta I J K L Theta
1- 18- 5- 3 59.847 1- 6- 2- 4 -75.803
1- 17- 19- 5 -53.415 1- 6- 2- 7 46.824
1- 6- 2- 11 164.624 1- 18- 5- 13 -178.126
1- 6- 15- 16 70.100 1- 18- 5- 19 -66.676
2- 4- 3- 5 81.827 2- 4- 3- 8 -162.286
2- 6- 1- 10 -78.951 2- 4- 3- 16 -52.375
2- 6- 15- 16 -60.647 2- 6- 1- 17 9.874
2- 6- 1- 18 115.767 3- 4- 2- 6 2.880
3- 16- 15- 6 9.772 3- 4- 2- 7 -119.105
3- 4- 2- 11 120.981 3- 5- 19- 17 -28.038
4- 3- 5- 13 158.811 4- 2- 6- 14 162.307
4- 2- 6- 15 51.834 4- 3- 16- 15 46.129
4- 3- 5- 18 -92.909 4- 3- 5- 19 -1.344
5- 18- 1- 6 -73.106 5- 3- 4- 9 -158.597
5- 18- 1- 10 122.213 5- 3- 4- 12 -42.552
5- 3- 16- 15 -91.294 5- 18- 1- 17 32.954
6- 2- 4- 9 -113.806 6- 2- 4- 12 126.311
6- 1- 17- 19 114.187 7- 2- 4- 9 124.209
7- 2- 4- 12 4.326 7- 2- 6- 14 -75.066
7- 2- 6- 15 174.461 8- 3- 4- 9 -42.710
8- 3- 4- 12 73.335 8- 3- 5- 13 39.837
8- 3- 16- 15 160.860 8- 3- 5- 18 148.116
8- 3- 5- 19 -120.318 9- 4- 2- 11 4.295
9- 4- 3- 16 67.202 10- 1- 6- 14 44.637
10- 1- 6- 15 153.350 10- 1- 17- 19 -129.035
11- 2- 4- 12 -115.587 11- 2- 6- 14 42.735
11- 2- 6- 15 -67.738 12- 4- 3- 16 -176.754
13- 5- 3- 16 -66.793 13- 5- 19- 17 170.645
14- 6- 15- 16 -177.148 14- 6- 1- 17 133.462
14- 6- 1- 18 -120.645 15- 6- 1- 17 -117.825
15- 6- 1- 18 -11.932 16- 3- 5- 18 41.486
16- 3- 5- 19 133.052 17- 19- 5- 18 70.259
18- 1- 17- 19 -8.195

MP2/6-311G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5293 1- 10 1.0998 1- 17 2.1924 1- 18 1.2343
5) 2- 4 1.5378 2- 6 1.5226 2- 7 1.0907 2- 11 1.0938
9) 3- 4 1.5275 3- 5 1.5250 3- 8 1.1006 3- 16 1.4171
13) 4- 9 1.0946 4- 12 1.0910 5- 13 1.0883 5- 18 2.1695
17) 5- 19 1.2699 6- 14 1.0992 6- 15 1.4233 15- 16 1.4820
21) 17- 19 1.3556
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 106.817 1- 6- 15 111.033 1- 17- 19 92.310
4) 2- 4- 9 109.935 2- 4- 12 111.388 2- 6- 14 110.419
7) 2- 6- 15 110.528 3- 4- 9 104.909 3- 4- 12 109.881
10) 3- 5- 13 118.659 3- 5- 18 99.020 3- 5- 19 126.433
13) 4- 2- 6 109.074 4- 2- 7 111.209 4- 2- 11 110.060

16) 4- 3- 5 118.622 4- 3- 8 108.038 4- 3- 16 112.485
19) 5- 3- 4 118.622 5- 3- 8 102.139 5- 3- 16 112.682
22) 6- 1- 10 117.173 6- 1- 17 99.244 6- 1- 18 119.925
25) 6- 2- 4 109.074 6- 2- 7 110.321 6- 2- 11 107.693
28) 6- 15- 16 113.188 7- 2- 4 111.209 7- 2- 6 110.321
31) 7- 2- 11 108.417 8- 3- 4 108.038 8- 3- 5 102.139
34) 8- 3- 16 100.508 9- 4- 12 108.173 10- 1- 6 117.173
37) 10- 1- 17 85.881 10- 1- 18 120.797 11- 2- 4 110.060
40) 11- 2- 6 107.693 11- 2- 7 108.417 12- 4- 9 108.173
43) 13- 5- 18 102.108 13- 5- 19 111.698 14- 6- 15 100.719
46) 15- 6- 14 100.719 16- 3- 4 112.485 16- 3- 5 112.682
49) 16- 3- 8 100.508 17- 1- 6 99.244 17- 1- 10 85.881
52) 17- 1- 18 99.169 18- 1- 6 119.925 18- 1- 10 120.797
55) 18- 1- 17 99.169 18- 5- 13 102.108 18- 5- 19 86.899
58) 19- 5- 13 111.698 19- 5- 18 86.899
Dihedrals
I J K L Theta I J K L Theta
1- 18- 5- 3 60.673 1- 6- 2- 4 -75.844
1- 17- 19- 5 -51.834 1- 6- 2- 7 46.585
1- 6- 2- 11 164.733 1- 18- 5- 13 -177.274
1- 6- 15- 16 68.339 1- 18- 5- 19 -65.740
2- 4- 3- 5 81.684 2- 4- 3- 8 -162.869
2- 6- 1- 10 -80.688 2- 4- 3- 16 -52.848
2- 6- 15- 16 -62.069 2- 6- 1- 17 9.412
2- 6- 1- 18 115.670 3- 4- 2- 6 3.444
3- 16- 15- 6 11.036 3- 4- 2- 7 -118.449
3- 4- 2- 11 121.388 3- 5- 19- 17 -30.264
4- 3- 5- 13 156.814 4- 2- 6- 14 162.372
4- 2- 6- 15 51.804 4- 3- 16- 15 45.771
4- 3- 5- 18 -93.992 4- 3- 5- 19 -1.177
5- 18- 1- 6 -73.664 5- 3- 4- 9 -158.948
5- 18- 1- 10 123.295 5- 3- 4- 12 -42.876
5- 3- 16- 15 -91.527 5- 18- 1- 17 32.636
6- 2- 4- 9 -112.940 6- 2- 4- 12 127.168
6- 1- 17- 19 114.725 7- 2- 4- 9 125.166
7- 2- 4- 12 5.274 7- 2- 6- 14 -75.199
7- 2- 6- 15 174.233 8- 3- 4- 9 -43.502
8- 3- 4- 12 72.570 8- 3- 5- 13 38.245
8- 3- 16- 15 160.455 8- 3- 5- 18 147.440
8- 3- 5- 19 -119.746 9- 4- 2- 11 5.003
9- 4- 3- 16 66.519 10- 1- 6- 14 42.985
10- 1- 6- 15 151.913 10- 1- 17- 19 -128.393
11- 2- 4- 12 -114.889 11- 2- 6- 14 42.949
11- 2- 6- 15 -67.618 12- 4- 3- 16 -177.409
13- 5- 3- 16 -68.737 13- 5- 19- 17 170.463
14- 6- 15- 16 -178.815 14- 6- 1- 17 133.085
14- 6- 1- 18 -120.657 15- 6- 1- 17 -117.987
15- 6- 1- 18 -11.729 16- 3- 5- 18 40.458
16- 3- 5- 19 133.272 17- 19- 5- 18 68.662
18- 1- 17- 19 -7.839

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5350 1- 10 1.1014 1- 17 2.2838 1- 18 1.2315
5) 2- 4 1.5445 2- 6 1.5320 2- 7 1.0922 2- 11 1.0947
9) 3- 4 1.5345 3- 5 1.5309 3- 8 1.1017 3- 16 1.4191
13) 4- 9 1.0956 4- 12 1.0914 5- 13 1.0883 5- 18 2.2096

17) 5- 19 1.2751 6- 14 1.1001 6- 15 1.4242 15- 16 1.4880
21) 17- 19 1.3871
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 106.598 1- 6- 15 110.594 1- 17- 19 91.242
4) 2- 4- 9 109.833 2- 4- 12 111.225 2- 6- 14 109.838
7) 2- 6- 15 111.121 3- 4- 9 105.474 3- 4- 12 109.775
10) 3- 5- 13 117.717 3- 5- 18 100.399 3- 5- 19 126.890
13) 4- 2- 6 109.790 4- 2- 7 111.026 4- 2- 11 110.084
16) 4- 3- 5 118.624 4- 3- 8 108.401 4- 3- 16 112.270
19) 5- 3- 4 118.624 5- 3- 8 102.126 5- 3- 16 112.470
22) 6- 1- 10 117.201 6- 1- 17 100.113 6- 1- 18 120.080
25) 6- 2- 4 109.790 6- 2- 7 109.960 6- 2- 11 107.730
28) 6- 15- 16 113.725 7- 2- 4 111.026 7- 2- 6 109.960
31) 7- 2- 11 108.178 8- 3- 4 108.401 8- 3- 5 102.126
34) 8- 3- 16 100.699 9- 4- 12 108.275 10- 1- 6 117.201
37) 10- 1- 17 84.091 10- 1- 18 121.321 11- 2- 4 110.084
40) 11- 2- 6 107.730 11- 2- 7 108.178 12- 4- 9 108.275
43) 13- 5- 18 100.131 13- 5- 19 112.351 14- 6- 15 101.213
46) 15- 6- 14 101.213 16- 3- 4 112.270 16- 3- 5 112.470
49) 16- 3- 8 100.699 17- 1- 6 100.113 17- 1- 10 84.091
52) 17- 1- 18 97.443 18- 1- 6 120.080 18- 1- 10 121.321
55) 18- 1- 17 97.443 18- 5- 13 100.131 18- 5- 19 86.915
58) 19- 5- 13 112.351 19- 5- 18 86.915
Dihedrals
I J K L Theta I J K L Theta
1- 18- 5- 3 58.070 1- 6- 2- 4 -75.721
1- 17- 19- 5 -50.750 1- 6- 2- 7 46.715
1- 6- 2- 11 164.398 1- 18- 5- 13 178.944
1- 6- 15- 16 72.782 1- 18- 5- 19 -68.894
2- 4- 3- 5 82.513 2- 4- 3- 8 -161.780
2- 6- 1- 10 -77.353 2- 4- 3- 16 -51.436
2- 6- 15- 16 -57.957 2- 6- 1- 17 11.163
2- 6- 1- 18 115.958 3- 4- 2- 6 1.186
3- 16- 15- 6 5.975 3- 4- 2- 7 -120.616
3- 4- 2- 11 119.621 3- 5- 19- 17 -31.945
4- 3- 5- 13 160.990 4- 2- 6- 14 163.142
4- 2- 6- 15 51.982 4- 3- 16- 15 48.694
4- 3- 5- 18 -91.646 4- 3- 5- 19 2.329
5- 18- 1- 6 -71.721 5- 3- 4- 9 -158.024
5- 18- 1- 10 122.149 5- 3- 4- 12 -41.582
5- 3- 16- 15 -88.157 5- 18- 1- 17 34.558
6- 2- 4- 9 -115.685 6- 2- 4- 12 124.468
6- 1- 17- 19 111.677 7- 2- 4- 9 122.513
7- 2- 4- 12 2.666 7- 2- 6- 14 -74.422
7- 2- 6- 15 174.418 8- 3- 4- 9 -42.318
8- 3- 4- 12 74.124 8- 3- 5- 13 41.973
8- 3- 16- 15 163.814 8- 3- 5- 18 149.337
8- 3- 5- 19 -116.688 9- 4- 2- 11 2.750
9- 4- 3- 16 68.027 10- 1- 6- 14 45.491
10- 1- 6- 15 154.685 10- 1- 17- 19 -131.685
11- 2- 4- 12 -117.096 11- 2- 6- 14 43.261
11- 2- 6- 15 -67.899 12- 4- 3- 16 -175.531
13- 5- 3- 16 -65.146 13- 5- 19- 17 168.438
14- 6- 15- 16 -174.538 14- 6- 1- 17 134.007
14- 6- 1- 18 -121.197 15- 6- 1- 17 -116.799
15- 6- 1- 18 -12.003 16- 3- 5- 18 42.218
16- 3- 5- 19 136.193 17- 19- 5- 18 68.749
18- 1- 17- 19 -10.786

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5341 1- 10 1.1008 1- 17 2.2126 1- 18 1.2388
5) 2- 4 1.5434 2- 6 1.5304 2- 7 1.0922 2- 11 1.0941
9) 3- 4 1.5329 3- 5 1.5302 3- 8 1.1008 3- 16 1.4245
13) 4- 9 1.0946 4- 12 1.0914 5- 13 1.0888 5- 18 2.1915
17) 5- 19 1.2789 6- 14 1.0994 6- 15 1.4293 15- 16 1.4900
21) 17- 19 1.3952
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 106.406 1- 6- 15 110.195 1- 17- 19 92.522
4) 2- 4- 9 109.977 2- 4- 12 111.460 2- 6- 14 109.998
7) 2- 6- 15 111.025 3- 4- 9 105.550 3- 4- 12 109.647
10) 3- 5- 13 117.565 3- 5- 18 100.748 3- 5- 19 126.902
13) 4- 2- 6 109.788 4- 2- 7 111.305 4- 2- 11 110.284
16) 4- 3- 5 118.766 4- 3- 8 108.521 4- 3- 16 112.229
19) 5- 3- 4 118.766 5- 3- 8 101.890 5- 3- 16 112.365
22) 6- 1- 10 116.978 6- 1- 17 101.007 6- 1- 18 119.937
25) 6- 2- 4 109.788 6- 2- 7 109.807 6- 2- 11 107.567
28) 6- 15- 16 113.499 7- 2- 4 111.305 7- 2- 6 109.807
31) 7- 2- 11 108.002 8- 3- 4 108.521 8- 3- 5 101.890
34) 8- 3- 16 100.813 9- 4- 12 107.984 10- 1- 6 116.978
37) 10- 1- 17 85.321 10- 1- 18 120.825 11- 2- 4 110.284
40) 11- 2- 6 107.567 11- 2- 7 108.002 12- 4- 9 107.984
43) 13- 5- 18 101.226 13- 5- 19 111.997 14- 6- 15 101.335
46) 15- 6- 14 101.335 16- 3- 4 112.229 16- 3- 5 112.365
49) 16- 3- 8 100.813 17- 1- 6 101.007 17- 1- 10 85.321
52) 17- 1- 18 98.495 18- 1- 6 119.937 18- 1- 10 120.825
55) 18- 1- 17 98.495 18- 5- 13 101.226 18- 5- 19 86.883
58) 19- 5- 13 111.997 19- 5- 18 86.883
Dihedrals
I J K L Theta I J K L Theta
1- 18- 5- 3 58.685 1- 6- 2- 4 -74.420
1- 17- 19- 5 -49.342 1- 6- 2- 7 48.263
1- 6- 2- 11 165.557 1- 18- 5- 13 179.875
1- 6- 15- 16 73.054 1- 18- 5- 19 -68.310
2- 4- 3- 5 82.650 2- 4- 3- 8 -161.768
2- 6- 1- 10 -80.539 2- 4- 3- 16 -51.242
2- 6- 15- 16 -57.782 2- 6- 1- 17 9.792
2- 6- 1- 18 116.390 3- 4- 2- 6 0.219
3- 16- 15- 6 5.057 3- 4- 2- 7 -121.573
3- 4- 2- 11 118.574 3- 5- 19- 17 -34.093
4- 3- 5- 13 159.234 4- 2- 6- 14 164.299
4- 2- 6- 15 52.955 4- 3- 16- 15 49.463
4- 3- 5- 18 -91.944 4- 3- 5- 19 2.260
5- 18- 1- 6 -72.769 5- 3- 4- 9 -157.697
5- 18- 1- 10 124.820 5- 3- 4- 12 -41.616
5- 3- 16- 15 -87.450 5- 18- 1- 17 35.217
6- 2- 4- 9 -116.804 6- 2- 4- 12 123.468
6- 1- 17- 19 111.408 7- 2- 4- 9 121.404
7- 2- 4- 12 1.676 7- 2- 6- 14 -73.018
7- 2- 6- 15 175.638 8- 3- 4- 9 -42.115
8- 3- 4- 12 73.966 8- 3- 5- 13 40.162
8- 3- 16- 15 164.767 8- 3- 5- 18 148.983
8- 3- 5- 19 -116.813 9- 4- 2- 11 1.552
9- 4- 3- 16 68.412 10- 1- 6- 14 42.617
10- 1- 6- 15 151.680 10- 1- 17- 19 -131.990
11- 2- 4- 12 -118.177 11- 2- 6- 14 44.276
11- 2- 6- 15 -67.068 12- 4- 3- 16 -175.508

```
13- 5- 3- 16 -66.932 13- 5- 19- 17 167.868
14- 6- 15- 16 -174.572 14- 6- 1- 17 132.948
14- 6- 1- 18 -120.454 15- 6- 1- 17 -117.989
15- 6- 1- 18 -11.391 16- 3- 5- 18 41.889
16- 3- 5- 19 136.094 17- 19- 5- 18 67.016
18- 1- 17- 19 -11.486
```

Optimised structures for the transition state for primary ozonide 18b formation at all levels reported.

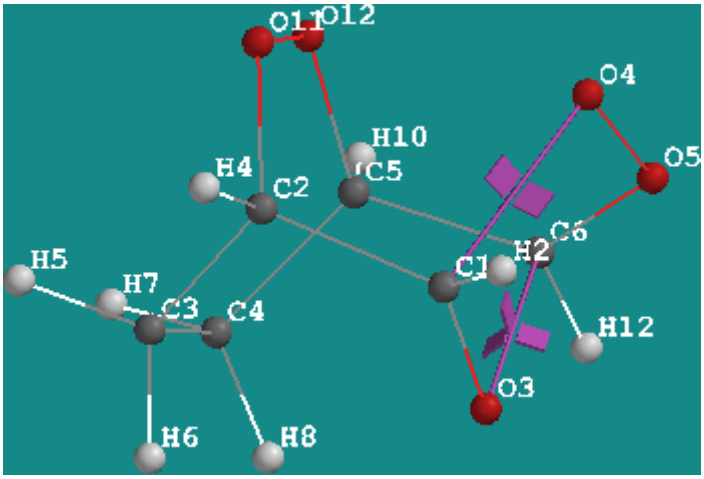

Figure S18: Optimised geometry for primary ozonide TS formation **18b**.

HF/6-31G* (GAS)

```
Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5468 1- 10 1.0816 1- 17 1.2292 1- 18 1.9712
5) 2- 4 1.5427 2- 6 1.5244 2- 7 1.0811 2- 11 1.0832
9) 3- 4 1.5319 3- 5 1.5215 3- 8 1.0881 3- 16 1.3903
13) 4- 9 1.0827 4- 12 1.0816 5- 13 1.0780 5- 17 2.1531
17) 5- 19 1.2347 6- 14 1.0833 6- 15 1.4026 15- 16 1.4048
21) 18- 19 1.4049
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 108.081 1- 6- 15 115.512 1- 18- 19 97.517
4) 2- 4- 9 110.063 2- 4- 12 111.359 2- 6- 14 110.808
7) 2- 6- 15 109.394 3- 4- 9 107.274 3- 4- 12 110.082
10) 3- 5- 13 115.177 3- 5- 17 97.302 3- 5- 19 127.832
13) 4- 2- 6 109.903 4- 2- 7 110.952 4- 2- 11 109.863
16) 4- 3- 5 114.525 4- 3- 8 109.186 4- 3- 16 112.483
19) 5- 3- 4 114.525 5- 3- 8 101.247 5- 3- 16 115.693
22) 6- 1- 10 116.845 6- 1- 17 117.491 6- 1- 18 99.942
25) 6- 2- 4 109.903 6- 2- 7 110.490 6- 2- 11 107.473
28) 6- 15- 16 114.143 7- 2- 4 110.952 7- 2- 6 110.490
31) 7- 2- 11 108.077 8- 3- 4 109.186 8- 3- 5 101.247
34) 8- 3- 16 102.034 9- 4- 12 107.814 10- 1- 6 116.845
37) 10- 1- 17 120.575 10- 1- 18 89.211 11- 2- 4 109.863
40) 11- 2- 6 107.473 11- 2- 7 108.077 12- 4- 9 107.814
43) 13- 5- 17 101.222 13- 5- 19 114.246 14- 6- 15 102.248
46) 15- 6- 14 102.248 16- 3- 4 112.483 16- 3- 5 115.693
```

49) 16- 3- 8 102.034 17- 1- 6 117.491 17- 1- 10 120.575
52) 17- 1- 18 103.369 17- 5- 13 101.222 17- 5- 19 88.617
55) 18- 1- 6 99.942 18- 1- 10 89.211 18- 1- 17 103.369
58) 19- 5- 13 114.246 19- 5- 17 88.617
Dihedrals
I J K L Theta I J K L Theta
1- 17- 5- 3 -66.332 1- 6- 2- 4 -70.171
1- 18- 19- 5 46.605 1- 6- 2- 7 52.600
1- 6- 2- 11 170.304 1- 17- 5- 13 176.108
1- 6- 15- 16 69.902 1- 17- 5- 19 61.652
2- 4- 3- 5 91.104 2- 4- 3- 8 -156.206
2- 6- 1- 10 -140.290 2- 4- 3- 16 -43.692
2- 6- 15- 16 -55.498 2- 6- 1- 17 14.676
2- 6- 1- 18 125.521 3- 4- 2- 6 -8.980
3- 16- 15- 6 -0.129 3- 4- 2- 7 -131.478
3- 4- 2- 11 109.075 3- 5- 19- 18 37.905
4- 3- 5- 13 65.661 4- 2- 6- 14 170.061
4- 2- 6- 15 58.074 4- 3- 16- 15 51.686
4- 3- 5- 17 -40.423 4- 3- 5- 19 -134.362
5- 17- 1- 6 76.970 5- 3- 4- 9 -149.116
5- 17- 1- 10 -129.040 5- 3- 4- 12 -32.064
5- 3- 16- 15 -82.552 5- 17- 1- 18 -31.918
6- 2- 4- 9 -127.055 6- 2- 4- 12 113.438
6- 1- 18- 19 -112.300 7- 2- 4- 9 110.447
7- 2- 4- 12 -9.060 7- 2- 6- 14 -67.168
7- 2- 6- 15 -179.155 8- 3- 4- 9 -36.426
8- 3- 4- 12 80.626 8- 3- 5- 13 -51.663
8- 3- 16- 15 168.551 8- 3- 5- 17 -157.747
8- 3- 5- 19 108.314 9- 4- 2- 11 -9.000
9- 4- 3- 16 76.089 10- 1- 6- 14 -18.892
10- 1- 6- 15 94.878 10- 1- 18- 19 130.564
11- 2- 4- 12 -128.507 11- 2- 6- 14 50.536
11- 2- 6- 15 -61.451 12- 4- 3- 16 -166.859
13- 5- 3- 16 -161.028 13- 5- 19- 18 -161.962
14- 6- 15- 16 -173.002 14- 6- 1- 17 136.074
14- 6- 1- 18 -113.081 15- 6- 1- 17 -110.156
15- 6- 1- 18 0.689 16- 3- 5- 17 92.889
16- 3- 5- 19 -1.051 17- 5- 19- 18 -60.271
17- 1- 18- 19 9.258

HF/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5467 1- 10 1.0830 1- 17 1.2325 1- 18 1.9374
5) 2- 4 1.5415 2- 6 1.5232 2- 7 1.0809 2- 11 1.0828
9) 3- 4 1.5298 3- 5 1.5164 3- 8 1.0877 3- 16 1.3989
13) 4- 9 1.0816 4- 12 1.0812 5- 13 1.0781 5- 17 2.1438
17) 5- 19 1.2450 6- 14 1.0829 6- 15 1.4071 15- 16 1.4055
21) 18- 19 1.4029
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 107.844 1- 6- 15 115.237 1- 18- 19 98.136
4) 2- 4- 9 110.136 2- 4- 12 111.475 2- 6- 14 110.916
7) 2- 6- 15 109.466 3- 4- 9 107.214 3- 4- 12 109.924
10) 3- 5- 13 115.527 3- 5- 17 98.248 3- 5- 19 127.539
13) 4- 2- 6 110.022 4- 2- 7 111.212 4- 2- 11 110.019
16) 4- 3- 5 114.808 4- 3- 8 109.321 4- 3- 16 112.504
19) 5- 3- 4 114.808 5- 3- 8 101.141 5- 3- 16 115.296

22) 6- 1- 10 116.226 6- 1- 17 117.718 6- 1- 18 100.789
25) 6- 2- 4 110.022 6- 2- 7 110.231 6- 2- 11 107.329
28) 6- 15- 16 114.044 7- 2- 4 111.212 7- 2- 6 110.231
31) 7- 2- 11 107.929 8- 3- 4 109.321 8- 3- 5 101.141
34) 8- 3- 16 102.097 9- 4- 12 107.790 10- 1- 6 116.226
37) 10- 1- 17 120.011 10- 1- 18 90.196 11- 2- 4 110.019
40) 11- 2- 6 107.329 11- 2- 7 107.929 12- 4- 9 107.790
43) 13- 5- 17 101.701 13- 5- 19 113.852 14- 6- 15 102.259
46) 15- 6- 14 102.259 16- 3- 4 112.504 16- 3- 5 115.296
49) 16- 3- 8 102.097 17- 1- 6 117.718 17- 1- 10 120.011
52) 17- 1- 18 103.544 17- 5- 13 101.701 17- 5- 19 88.129
55) 18- 1- 6 100.789 18- 1- 10 90.196 18- 1- 17 103.544
58) 19- 5- 13 113.852 19- 5- 17 88.129
Dihedrals
I J K L Theta I J K L Theta
1- 17- 5- 3 -65.684 1- 6- 2- 4 -70.711
1- 18- 19- 5 45.594 1- 6- 2- 7 52.294
1- 6- 2- 11 169.596 1- 17- 5- 13 175.976
1- 6- 15- 16 69.380 1- 17- 5- 19 61.997
2- 4- 3- 5 89.816 2- 4- 3- 8 -157.377
2- 6- 1- 10 -138.783 2- 4- 3- 16 -44.694
2- 6- 15- 16 -56.272 2- 6- 1- 17 13.925
2- 6- 1- 18 125.606 3- 4- 2- 6 -7.603
3- 16- 15- 6 1.231 3- 4- 2- 7 -130.030
3- 4- 2- 11 110.442 3- 5- 19- 18 39.433
4- 3- 5- 13 66.561 4- 2- 6- 14 169.552
4- 2- 6- 15 57.454 4- 3- 16- 15 51.100
4- 3- 5- 17 -40.676 4- 3- 5- 19 -134.677
5- 17- 1- 6 76.947 5- 3- 4- 9 -150.327
5- 17- 1- 10 -131.412 5- 3- 4- 12 -33.421
5- 3- 16- 15 -83.177 5- 17- 1- 18 -33.178
6- 2- 4- 9 -125.675 6- 2- 4- 12 114.724
6- 1- 18- 19 -111.658 7- 2- 4- 9 111.898
7- 2- 4- 12 -7.702 7- 2- 6- 14 -67.444
7- 2- 6- 15 -179.541 8- 3- 4- 9 -37.519
8- 3- 4- 12 79.386 8- 3- 5- 13 -50.990
8- 3- 16- 15 168.168 8- 3- 5- 17 -158.227
8- 3- 5- 19 107.772 9- 4- 2- 11 -7.631
9- 4- 3- 16 75.164 10- 1- 6- 14 -17.222
10- 1- 6- 15 96.252 10- 1- 18- 19 131.564
11- 2- 4- 12 -127.231 11- 2- 6- 14 49.858
11- 2- 6- 15 -62.239 12- 4- 3- 16 -167.931
13- 5- 3- 16 -160.217 13- 5- 19- 18 -161.508
14- 6- 15- 16 -173.936 14- 6- 1- 17 135.487
14- 6- 1- 18 -112.832 15- 6- 1- 17 -111.039
15- 6- 1- 18 0.642 16- 3- 5- 17 92.546
16- 3- 5- 19 -1.455 17- 5- 19- 18 -59.537
17- 1- 18- 19 10.546

MP2/6-31G*

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5302 1- 10 1.1013 1- 17 1.2266 1- 18 2.5618
5) 2- 4 1.5281 2- 6 1.5150 2- 7 1.0937 2- 11 1.0938
9) 3- 4 1.5534 3- 5 1.5025 3- 8 1.0995 3- 16 1.4274
13) 4- 9 1.0937 4- 12 1.0906 5- 13 1.0875 5- 17 3.4022
17) 5- 19 1.2835 6- 14 1.1012 6- 15 1.4357 15- 16 1.4862
21) 18- 19 1.3178
Bond Angles
I J K Theta I J K Theta I J K Theta

1) 1- 6- 14 106.270 1- 6- 15 110.762 1- 18- 19 104.011
4) 2- 4- 9 110.280 2- 4- 12 109.137 2- 6- 14 110.481
7) 2- 6- 15 111.957 3- 4- 9 109.461 3- 4- 12 110.458
10) 3- 5- 13 119.354 3- 5- 17 81.616 3- 5- 19 129.741
13) 4- 2- 6 110.334 4- 2- 7 109.860 4- 2- 11 110.717
16) 4- 3- 5 112.174 4- 3- 8 108.396 4- 3- 16 113.590
19) 5- 3- 4 112.174 5- 3- 8 103.685 5- 3- 16 118.432
22) 6- 1- 10 115.105 6- 1- 17 122.912 6- 1- 18 97.211
25) 6- 2- 4 110.334 6- 2- 7 109.715 6- 2- 11 107.890
28) 6- 15- 16 112.200 7- 2- 4 109.860 7- 2- 6 109.715
31) 7- 2- 11 108.276 8- 3- 4 108.396 8- 3- 5 103.685
34) 8- 3- 16 98.585 9- 4- 12 108.161 10- 1- 6 115.105
37) 10- 1- 17 121.717 10- 1- 18 69.937 11- 2- 4 110.717
40) 11- 2- 6 107.890 11- 2- 7 108.276 12- 4- 9 108.161
43) 13- 5- 17 118.534 13- 5- 19 110.903 14- 6- 15 102.203
46) 15- 6- 14 102.203 16- 3- 4 113.590 16- 3- 5 118.432
49) 16- 3- 8 98.585 17- 1- 6 122.912 17- 1- 10 121.717
52) 17- 1- 18 106.217 17- 5- 13 118.534 17- 5- 19 74.179
55) 18- 1- 6 97.211 18- 1- 10 69.937 18- 1- 17 106.217
58) 19- 5- 13 110.903 19- 5- 17 74.179
Dihedrals
I J K L Theta I J K L Theta
1- 17- 5- 3 -62.521 1- 6- 2- 4 -60.477
1- 18- 19- 5 58.956 1- 6- 2- 7 60.698
1- 6- 2- 11 178.454 1- 17- 5- 13 178.541
1- 6- 15- 16 99.471 1- 17- 5- 19 72.994
2- 4- 3- 5 122.261 2- 4- 3- 8 -123.862
2- 6- 1- 10 -178.620 2- 4- 3- 16 -15.386
2- 6- 15- 16 -29.427 2- 6- 1- 17 -4.460
2- 6- 1- 18 110.198 3- 4- 2- 6 -40.627
3- 16- 15- 6 -30.149 3- 4- 2- 7 -161.716
3- 4- 2- 11 78.741 3- 5- 19- 18 0.471
4- 3- 5- 13 75.772 4- 2- 6- 14 179.713
4- 2- 6- 15 66.519 4- 3- 16- 15 54.271
4- 3- 5- 17 -42.332 4- 3- 5- 19 -103.586
5- 17- 1- 6 75.809 5- 3- 4- 9 -116.839
5- 17- 1- 10 -110.410 5- 3- 4- 12 2.150
5- 3- 16- 15 -80.539 5- 17- 1- 18 -34.310
6- 2- 4- 9 -161.027 6- 2- 4- 12 80.291
6- 1- 18- 19 -95.994 7- 2- 4- 9 77.884
7- 2- 4- 12 -40.798 7- 2- 6- 14 -59.111
7- 2- 6- 15 -172.306 8- 3- 4- 9 -2.962
8- 3- 4- 12 116.027 8- 3- 5- 13 -40.971
8- 3- 16- 15 168.740 8- 3- 5- 17 -159.075
8- 3- 5- 19 139.671 9- 4- 2- 11 -41.659
9- 4- 3- 16 105.514 10- 1- 6- 14 -56.480
10- 1- 6- 15 53.770 10- 1- 18- 19 149.859
11- 2- 4- 12 -160.341 11- 2- 6- 14 58.645
11- 2- 6- 15 -54.549 12- 4- 3- 16 -135.497
13- 5- 3- 16 -148.822 13- 5- 19- 18 -178.929
14- 6- 15- 16 -147.667 14- 6- 1- 17 117.680
14- 6- 1- 18 -127.661 15- 6- 1- 17 -132.070
15- 6- 1- 18 -17.411 16- 3- 5- 17 93.074
16- 3- 5- 19 31.820 17- 5- 19- 18 -63.890
17- 1- 18- 19 31.392

MP2/6-311G*

Geometry information
Bond Lengths

I J R I J R I J R I J R
1) 1- 6 1.5338 1- 10 1.1016 1- 17 1.2171 1- 18 2.5689
5) 2- 4 1.5300 2- 6 1.5158 2- 7 1.0928 2- 11 1.0931
9) 3- 4 1.5545 3- 5 1.5048 3- 8 1.0980 3- 16 1.4208
13) 4- 9 1.0933 4- 12 1.0893 5- 13 1.0866 5- 17 3.4192
17) 5- 19 1.2785 6- 14 1.1002 6- 15 1.4292 15- 16 1.4662
21) 18- 19 1.2997
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 106.081 1- 6- 15 111.139 1- 18- 19 104.439
4) 2- 4- 9 110.301 2- 4- 12 109.269 2- 6- 14 110.439
7) 2- 6- 15 112.113 3- 4- 9 109.378 3- 4- 12 110.611
10) 3- 5- 13 119.308 3- 5- 17 81.428 3- 5- 19 129.879
13) 4- 2- 6 110.104 4- 2- 7 109.890 4- 2- 11 110.659
16) 4- 3- 5 111.923 4- 3- 8 108.261 4- 3- 16 113.344
19) 5- 3- 4 111.923 5- 3- 8 103.533 5- 3- 16 119.183
22) 6- 1- 10 114.989 6- 1- 17 123.135 6- 1- 18 97.153
25) 6- 2- 4 110.104 6- 2- 7 109.740 6- 2- 11 107.981
28) 6- 15- 16 112.433 7- 2- 4 109.890 7- 2- 6 109.740
31) 7- 2- 11 108.424 8- 3- 4 108.261 8- 3- 5 103.533
34) 8- 3- 16 98.570 9- 4- 12 108.167 10- 1- 6 114.989
37) 10- 1- 17 121.635 10- 1- 18 69.721 11- 2- 4 110.659
40) 11- 2- 6 107.981 11- 2- 7 108.424 12- 4- 9 108.167
43) 13- 5- 17 118.718 13- 5- 19 110.805 14- 6- 15 102.267
46) 15- 6- 14 102.267 16- 3- 4 113.344 16- 3- 5 119.183
49) 16- 3- 8 98.570 17- 1- 6 123.135 17- 1- 10 121.635
52) 17- 1- 18 106.170 17- 5- 13 118.718 17- 5- 19 73.984
55) 18- 1- 6 97.153 18- 1- 10 69.721 18- 1- 17 106.170
58) 19- 5- 13 110.805 19- 5- 17 73.984
Dihedrals
I J K L Theta I J K L Theta
1- 17- 5- 3 -62.408 1- 6- 2- 4 -61.519
1- 18- 19- 5 58.774 1- 6- 2- 7 59.563
1- 6- 2- 11 177.565 1- 17- 5- 13 178.784
1- 6- 15- 16 100.217 1- 17- 5- 19 73.471
2- 4- 3- 5 122.444 2- 4- 3- 8 -124.076
2- 6- 1- 10 -178.802 2- 4- 3- 16 -15.816
2- 6- 15- 16 -28.653 2- 6- 1- 17 -4.373
2- 6- 1- 18 110.279 3- 4- 2- 6 -40.037
3- 16- 15- 6 -31.486 3- 4- 2- 7 -161.029
3- 4- 2- 11 79.260 3- 5- 19- 18 0.180
4- 3- 5- 13 75.357 4- 2- 6- 14 179.182
4- 2- 6- 15 65.843 4- 3- 16- 15 55.466
4- 3- 5- 17 -42.848 4- 3- 5- 19 -103.538
5- 17- 1- 6 75.756 5- 3- 4- 9 -116.820
5- 17- 1- 10 -110.177 5- 3- 4- 12 2.218
5- 3- 16- 15 -79.510 5- 17- 1- 18 -34.371
6- 2- 4- 9 -160.206 6- 2- 4- 12 81.011
6- 1- 18- 19 -95.131 7- 2- 4- 9 78.802
7- 2- 4- 12 -39.981 7- 2- 6- 14 -59.736
7- 2- 6- 15 -173.075 8- 3- 4- 9 -3.340
8- 3- 4- 12 115.698 8- 3- 5- 13 -41.021
8- 3- 16- 15 169.682 8- 3- 5- 17 -159.226
8- 3- 5- 19 140.084 9- 4- 2- 11 -40.909
9- 4- 3- 16 104.920 10- 1- 6- 14 -57.063
10- 1- 6- 15 53.335 10- 1- 18- 19 150.821
11- 2- 4- 12 -159.692 11- 2- 6- 14 58.266
11- 2- 6- 15 -55.074 12- 4- 3- 16 -136.043
13- 5- 3- 16 -149.079 13- 5- 19- 18 -178.790
14- 6- 15- 16 -146.953 14- 6- 1- 17 117.366
14- 6- 1- 18 -127.982 15- 6- 1- 17 -132.236
15- 6- 1- 18 -17.584 16- 3- 5- 17 92.715

16- 3- 5- 19 32.025 17- 5- 19- 18 -63.595
17- 1- 18- 19 32.457

DFT/6-31G* (GAS)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5486 1- 10 1.1013 1- 17 1.2275 1- 18 2.2571
5) 2- 4 1.5455 2- 6 1.5291 2- 7 1.0929 2- 11 1.0940
9) 3- 4 1.5496 3- 5 1.5188 3- 8 1.1026 3- 16 1.4104
13) 4- 9 1.0941 4- 12 1.0925 5- 13 1.0895 5- 17 2.5722
17) 5- 19 1.2650 6- 14 1.0997 6- 15 1.4238 15- 16 1.4834
21) 18- 19 1.3723
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 107.040 1- 6- 15 115.198 1- 18- 19 95.278
4) 2- 4- 9 109.932 2- 4- 12 110.773 2- 6- 14 110.425
7) 2- 6- 15 110.688 3- 4- 9 108.013 3- 4- 12 109.261
10) 3- 5- 13 117.437 3- 5- 17 93.851 3- 5- 19 129.470
13) 4- 2- 6 111.010 4- 2- 7 110.442 4- 2- 11 109.869
16) 4- 3- 5 113.800 4- 3- 8 108.038 4- 3- 16 113.787
19) 5- 3- 4 113.800 5- 3- 8 102.007 5- 3- 16 116.601
22) 6- 1- 10 116.691 6- 1- 17 120.088 6- 1- 18 99.343
25) 6- 2- 4 111.010 6- 2- 7 110.073 6- 2- 11 107.304
28) 6- 15- 16 113.414 7- 2- 4 110.442 7- 2- 6 110.073
31) 7- 2- 11 108.045 8- 3- 4 108.038 8- 3- 5 102.007
34) 8- 3- 16 100.502 9- 4- 12 107.966 10- 1- 6 116.691
37) 10- 1- 17 121.798 10- 1- 18 79.963 11- 2- 4 109.869
40) 11- 2- 6 107.304 11- 2- 7 108.045 12- 4- 9 107.966
43) 13- 5- 17 107.679 13- 5- 19 112.019 14- 6- 15 100.668
46) 15- 6- 14 100.668 16- 3- 4 113.787 16- 3- 5 116.601
49) 16- 3- 8 100.502 17- 1- 6 120.088 17- 1- 10 121.798
52) 17- 1- 18 102.130 17- 5- 13 107.679 17- 5- 19 80.381
55) 18- 1- 6 99.343 18- 1- 10 79.963 18- 1- 17 102.130
58) 19- 5- 13 112.019 19- 5- 17 80.381
Dihedrals
I J K L Theta I J K L Theta
1- 17- 5- 3 -61.832 1- 6- 2- 4 -69.542
1- 18- 19- 5 56.080 1- 6- 2- 7 53.051
1- 6- 2- 11 170.392 1- 17- 5- 13 177.760
1- 6- 15- 16 78.477 1- 17- 5- 19 67.572
2- 4- 3- 5 99.155 2- 4- 3- 8 -148.340
2- 6- 1- 10 -157.026 2- 4- 3- 16 -37.667
2- 6- 15- 16 -50.011 2- 6- 1- 17 9.612
2- 6- 1- 18 119.577 3- 4- 2- 6 -15.835
3- 16- 15- 6 -5.833 3- 4- 2- 7 -138.215
3- 4- 2- 11 102.694 3- 5- 19- 18 19.181
4- 3- 5- 13 68.717 4- 2- 6- 14 171.194
4- 2- 6- 15 60.597 4- 3- 16- 15 51.401
4- 3- 5- 17 -43.486 4- 3- 5- 19 -124.191
5- 17- 1- 6 74.327 5- 3- 4- 9 -140.376
5- 17- 1- 10 -119.733 5- 3- 4- 12 -23.170
5- 3- 16- 15 -84.156 5- 17- 1- 18 -34.121
6- 2- 4- 9 -135.156 6- 2- 4- 12 105.604
6- 1- 18- 19 -107.854 7- 2- 4- 9 102.464
7- 2- 4- 12 -16.775 7- 2- 6- 14 -66.213
7- 2- 6- 15 -176.809 8- 3- 4- 9 -27.871
8- 3- 4- 12 89.335 8- 3- 5- 13 -47.375
8- 3- 16- 15 166.607 8- 3- 5- 17 -159.578

8- 3- 5- 19 119.717 9- 4- 2- 11 -16.627
9- 4- 3- 16 82.802 10- 1- 6- 14 -35.793
10- 1- 6- 15 75.197 10- 1- 18- 19 136.477
11- 2- 4- 12 -135.867 11- 2- 6- 14 51.129
11- 2- 6- 15 -59.468 12- 4- 3- 16 -159.992
13- 5- 3- 16 -155.731 13- 5- 19- 18 -173.168
14- 6- 15- 16 -166.802 14- 6- 1- 17 130.845
14- 6- 1- 18 -119.190 15- 6- 1- 17 -118.165
15- 6- 1- 18 -8.200 16- 3- 5- 17 92.066
16- 3- 5- 19 11.361 17- 5- 19- 18 -67.878
17- 1- 18- 19 15.860

DFT/6-31G* (DICHLOROMETHANE)

Geometry information
Bond Lengths
I J R I J R I J R I J R
1) 1- 6 1.5509 1- 10 1.1024 1- 17 1.2386 1- 18 2.1061
5) 2- 4 1.5456 2- 6 1.5292 2- 7 1.0922 2- 11 1.0937
9) 3- 4 1.5422 3- 5 1.5152 3- 8 1.1027 3- 16 1.4171
13) 4- 9 1.0925 4- 12 1.0925 5- 13 1.0903 5- 17 2.4175
17) 5- 19 1.2710 6- 14 1.0986 6- 15 1.4286 15- 16 1.4855
21) 18- 19 1.3937
Bond Angles
I J K Theta I J K Theta I J K Theta
1) 1- 6- 14 107.080 1- 6- 15 115.594 1- 18- 19 96.134
4) 2- 4- 9 110.158 2- 4- 12 111.309 2- 6- 14 110.594
7) 2- 6- 15 110.504 3- 4- 9 107.390 3- 4- 12 109.238
10) 3- 5- 13 117.211 3- 5- 17 96.840 3- 5- 19 128.803
13) 4- 2- 6 110.899 4- 2- 7 111.004 4- 2- 11 109.917
16) 4- 3- 5 114.700 4- 3- 8 108.185 4- 3- 16 113.672
19) 5- 3- 4 114.700 5- 3- 8 101.448 5- 3- 16 115.742
22) 6- 1- 10 116.292 6- 1- 17 119.543 6- 1- 18 100.486
25) 6- 2- 4 110.899 6- 2- 7 109.724 6- 2- 11 107.337
28) 6- 15- 16 113.000 7- 2- 4 111.004 7- 2- 6 109.724
31) 7- 2- 11 107.843 8- 3- 4 108.185 8- 3- 5 101.448
34) 8- 3- 16 100.954 9- 4- 12 107.786 10- 1- 6 116.292
37) 10- 1- 17 120.674 10- 1- 18 84.507 11- 2- 4 109.917
40) 11- 2- 6 107.337 11- 2- 7 107.843 12- 4- 9 107.786
43) 13- 5- 17 106.664 13- 5- 19 111.938 14- 6- 15 100.657
46) 15- 6- 14 100.657 16- 3- 4 113.672 16- 3- 5 115.742
49) 16- 3- 8 100.954 17- 1- 6 119.543 17- 1- 10 120.674
52) 17- 1- 18 103.261 17- 5- 13 106.664 17- 5- 19 81.828
55) 18- 1- 6 100.486 18- 1- 10 84.507 18- 1- 17 103.261
58) 19- 5- 13 111.938 19- 5- 17 81.828
Dihedrals
I J K L Theta I J K L Theta
1- 17- 5- 3 -62.007 1- 6- 2- 4 -71.884
1- 18- 19- 5 52.946 1- 6- 2- 7 51.105
1- 6- 2- 11 168.036 1- 17- 5- 13 176.886
1- 6- 15- 16 73.699 1- 17- 5- 19 66.337
2- 4- 3- 5 93.092 2- 4- 3- 8 -154.509
2- 6- 1- 10 -149.236 2- 4- 3- 16 -43.262
2- 6- 15- 16 -54.468 2- 6- 1- 17 9.842
2- 6- 1- 18 121.746 3- 4- 2- 6 -9.401
3- 16- 15- 6 0.053 3- 4- 2- 7 -131.648
3- 4- 2- 11 109.129 3- 5- 19- 18 26.702
4- 3- 5- 13 69.470 4- 2- 6- 14 168.920
4- 2- 6- 15 58.345 4- 3- 16- 15 50.225
4- 3- 5- 17 -43.263 4- 3- 5- 19 -128.257

5- 17- 1- 6 75.373 5- 3- 4- 9 -146.540
5- 17- 1- 10 -126.480 5- 3- 4- 12 -29.905
5- 3- 16- 15 -85.657 5- 17- 1- 18 -35.022
6- 2- 4- 9 -128.108 6- 2- 4- 12 112.389
6- 1- 18- 19 -109.481 7- 2- 4- 9 109.645
7- 2- 4- 12 -9.857 7- 2- 6- 14 -68.091
7- 2- 6- 15 -178.666 8- 3- 4- 9 -34.142
8- 3- 4- 12 82.494 8- 3- 5- 13 -46.866
8- 3- 16- 15 165.815 8- 3- 5- 17 -159.599
8- 3- 5- 19 115.407 9- 4- 2- 11 -9.577
9- 4- 3- 16 77.106 10- 1- 6- 14 -27.982
10- 1- 6- 15 83.221 10- 1- 18- 19 134.749
11- 2- 4- 12 -129.080 11- 2- 6- 14 48.840
11- 2- 6- 15 -61.735 12- 4- 3- 16 -166.259
13- 5- 3- 16 -155.099 13- 5- 19- 18 -170.271
14- 6- 15- 16 -171.372 14- 6- 1- 17 131.097
14- 6- 1- 18 -117.000 15- 6- 1- 17 -117.700
15- 6- 1- 18 -5.797 16- 3- 5- 17 92.168
16- 3- 5- 19 7.174 17- 5- 19- 18 -65.529
17- 1- 18- 19 14.492