Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Insights into the unprecedented epoxidation mechanism of Fumitremorgin B endoperoxidase (FtmOx1) from *Aspergillus fumigatus* by QM/MM calculations

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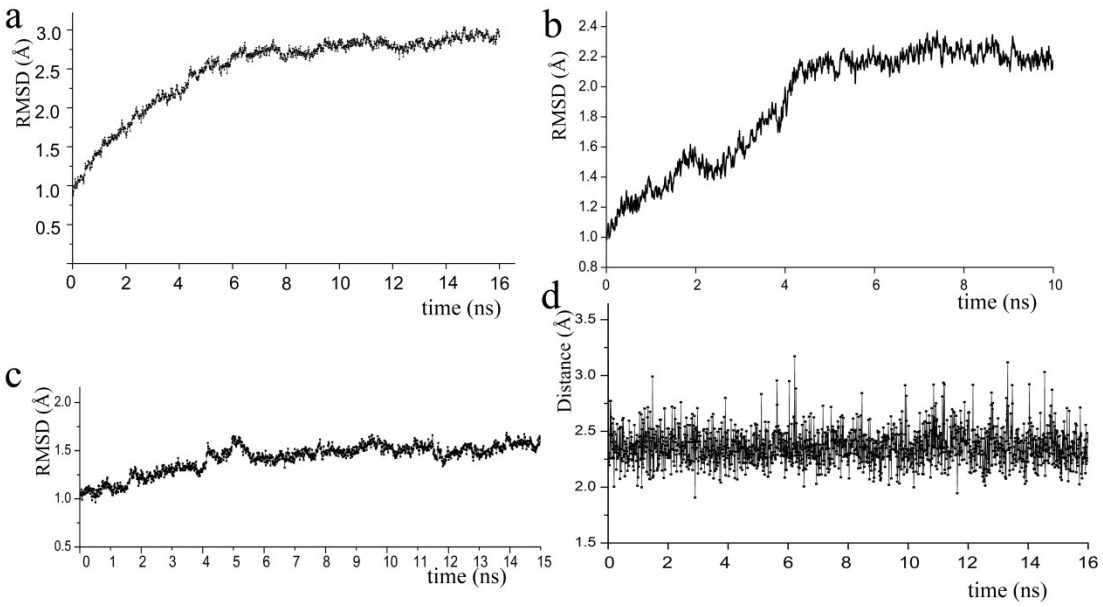


Figure S1. a) RMSDs of FtmOx1 from 16 ns MD (I) simulations. b) RMSDs of mutant FtmOx1 from10 ns MD (II) simulations. c) RMSDs of FtmOx1 (IM3) with the second dioxygen bound to the substrate radical from 10 ns MD (III) simulations. d) The time course of r6 derived from 16 ns MD (I) simulations.

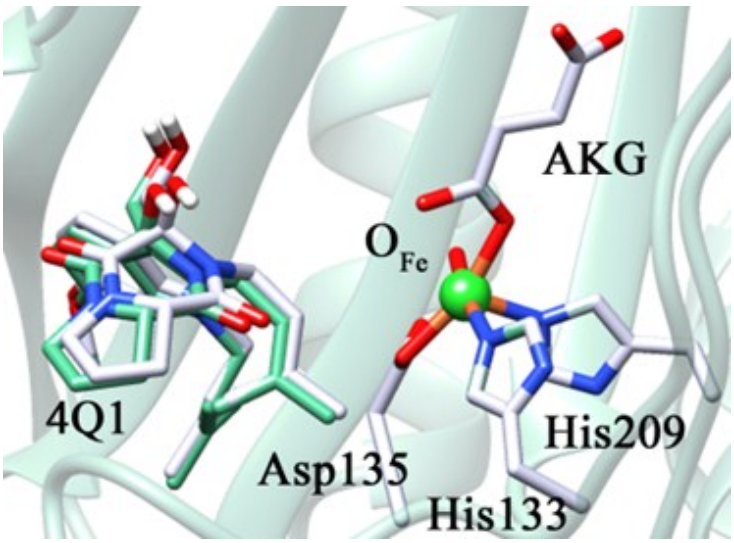


Figure S2. The comparison of the docked structure of the substrate (shown in purple) with the created computational model (shown in green) by superimposing the two crystal structures (4ZON and 4Y5S).

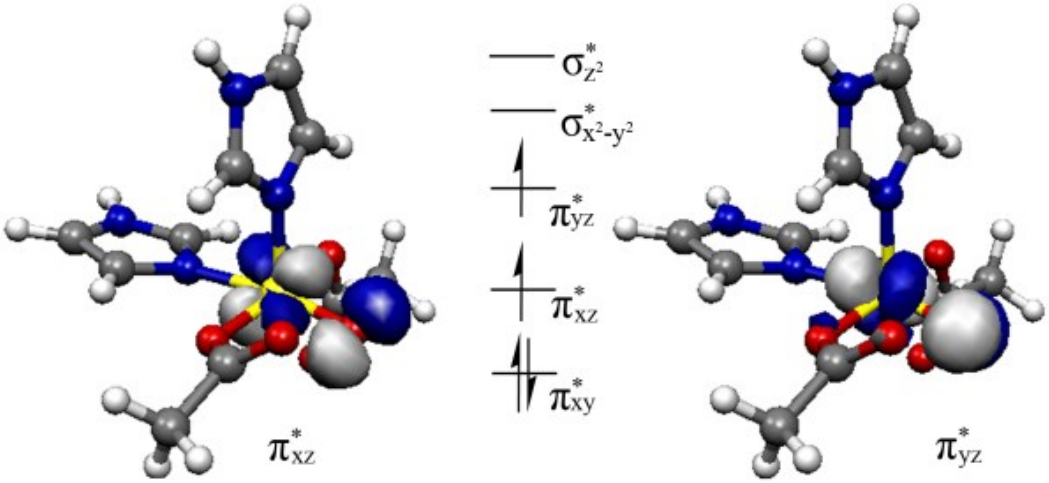


Figure S3. Orbital occupation of ^{3}R.

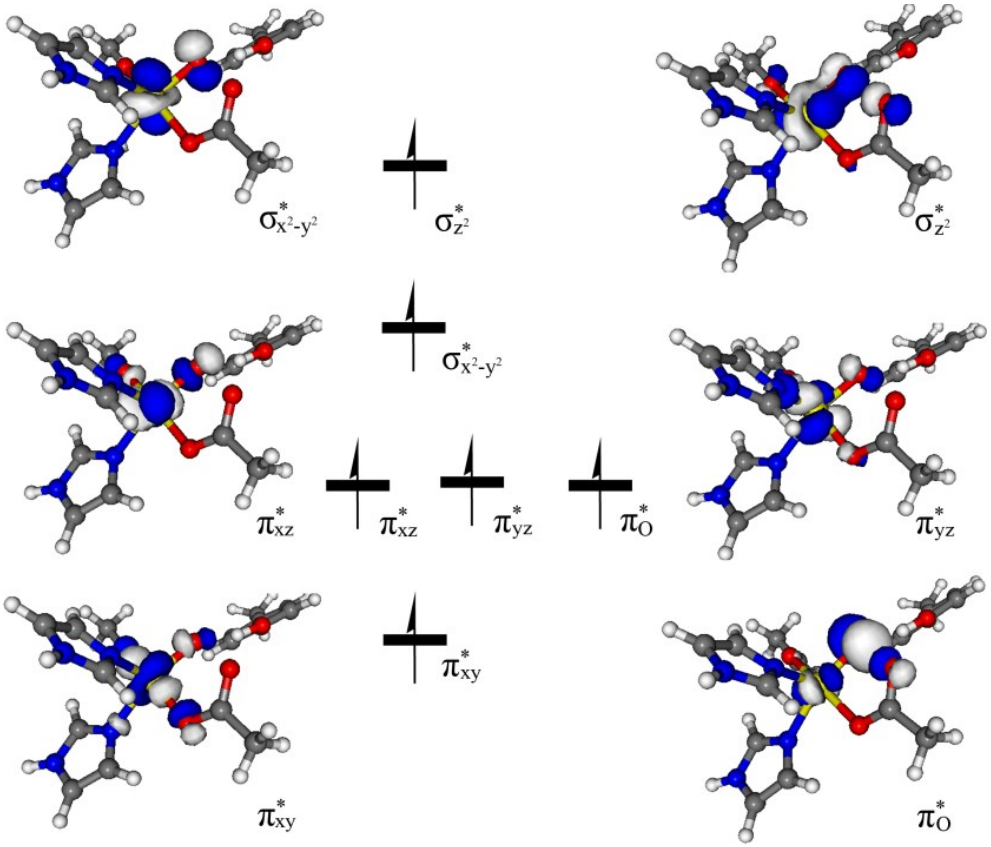


Figure S4. Orbital occupation of ^{7}R.

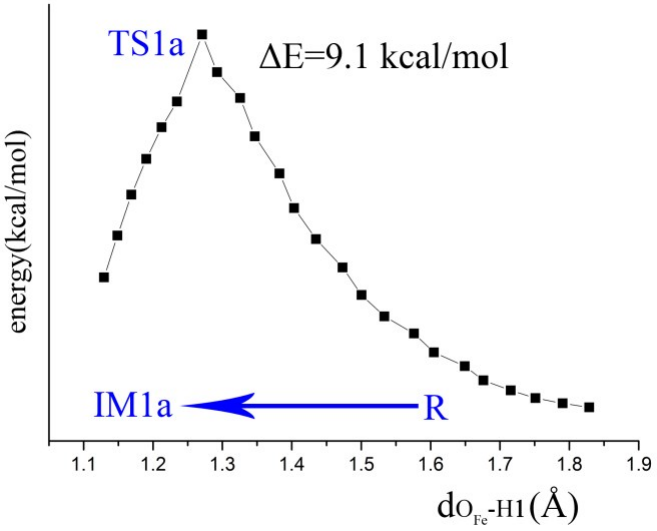
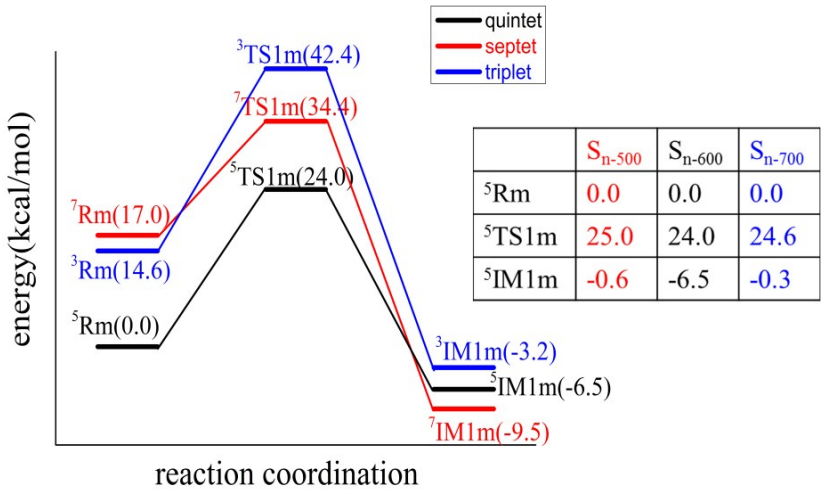


Figure S5. Calculated scan potential energy profile. All the energies (in kcal/mol) are relative to the R in the quintet spin state. ΔE represents the potential energy difference between TS1 and R. Note that the energy data have not included the dispersion correction.



	S_{n-500}	S_{n-600}	S_{n-700}
^{5}Rm	0.0	0.0	0.0
^{5}TS1m	25.0	24.0	24.6
^{5}IM1m	-0.6	-6.5	-0.3

Figure S6. Potential energy profiles for the hydrogen abstraction of mutant FtmOx1 (Y228A) were calculated by QM/MM. All the energies are relative to the ^{5}Rm. Note that the energy data have not included the dispersion correction.

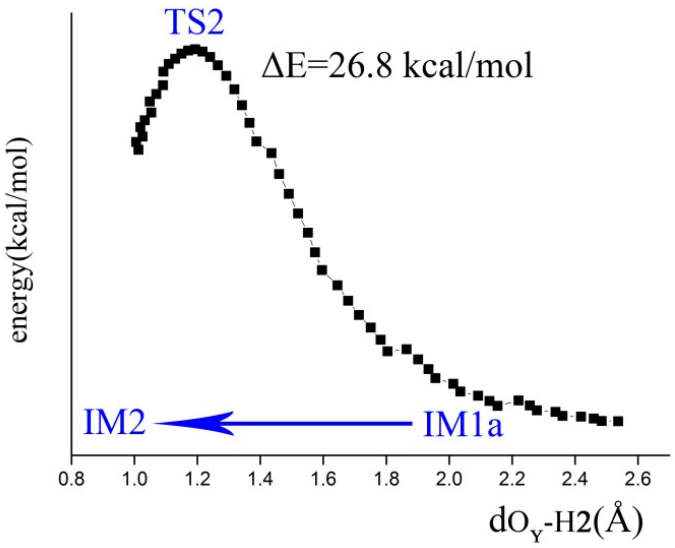


Figure S7. Scanned potential energy profile. All the energies (in kcal/mol) are relative to the IM1a. ΔE represents the potential energy difference between TS2 and IM1a. Note that the energy data have not included the dispersion correction.

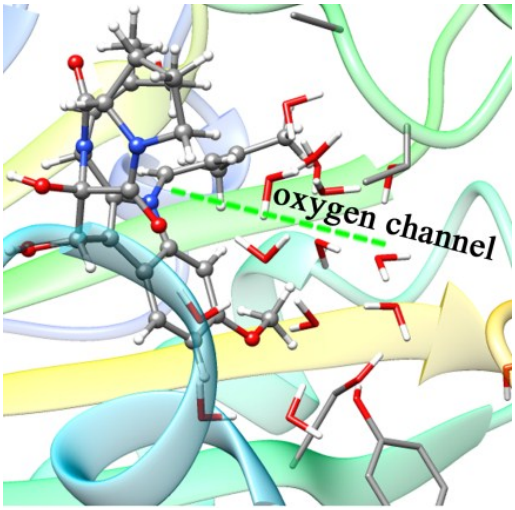


Figure S8. The channel for oxygen entrance.

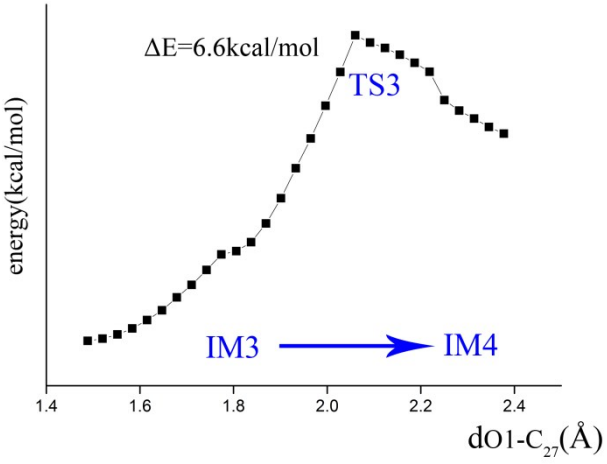


Figure S9. Scanned potential energy profile. All the energies (in kcal/mol) are relative to the IM3. ΔE represents the energy difference between the highest point (supposed as TS3) and IM3. Note that the energy data have not included the dispersion correction.

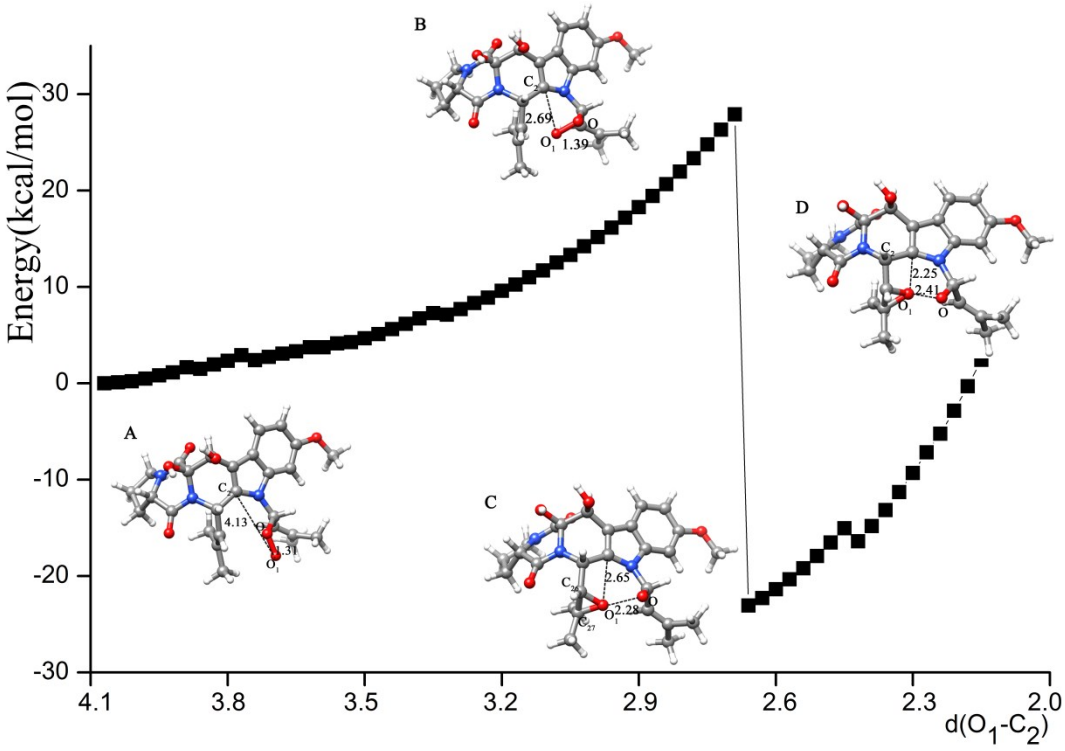


Figure S10. The scanned energy profile along the distance of d(O1-C2) with increment of 0.03 Å. The shown structures represent the starting point (A), two inflection point (B, C), and the ending point (D). All the energies (in kcal/mol) are relative to the IM3.

The force field parameters for substrate 4Q1:

* Built parameters for 4Q1.mol2

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*       by user vzoete         Tue Dec    1 03:52:03 CET 2015


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DEFA FIRS NONE LAST NONE

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BOND C1    C2
BOND H18   C12
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BOND C5    C4
BOND H10   C2
BOND C2    C3
BOND C12   H17
BOND C12   H16
BOND C12   C11
BOND C13   H20
BOND C13   C11
BOND C13   H19
BOND C4    C3
BOND C4    C8
BOND C3    N
BOND C11   C10
BOND H14   C9
BOND H22   C14
BOND C10   C9
BOND C10   H15
BOND N     C9
BOND N     C7
BOND C8    C14
BOND C8    C7
BOND O2    C21
BOND C9    H13
BOND C14   O1
BOND C14   C15
BOND O1    H31
BOND C7    C16
BOND C21   C15
BOND C21   N2
BOND H5    C24
BOND H30   C20
BOND C15   O4
BOND C15   N1
BOND H4    C24
BOND C24   N2
BOND C24   C25
BOND N2    C22
BOND C16   H23
BOND C16   N1
BOND C16   C17
BOND O4    H32
BOND N1    C23
BOND C20   H29
BOND C20   H28
BOND C20   C18
BOND C17   C18
BOND C17   H24
BOND H3    C25
BOND C18   C19
BOND C25   H2
BOND C25   C26
BOND C22   C23
BOND C22   H6
BOND C22   C26
BOND C23   O3
BOND H27   C19
BOND H1    C26
BOND C26   H
BOND C19   H25
BOND C19   H26
IMPH C1    C6    C2    O
IMPH C2    C3    C1    H10
IMPH C3    N     C2    C4
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IMPH C6 C5 C1 H12 0.40 116.88 1.38
IMPH N C7 C3 C9
IMPH C4 C5 C3 C8
IMPH C9 C10 N H14
IMPH C9 H14 N H13
IMPH C10 C11 C9 H15
IMPH C11 C12 C10 C13
IMPH C8 C7 C4 C14
IMPH C14 C15 C8 O1
IMPH C14 O1 C8 H22
IMPH C15 N1 C14 C21
IMPH C15 C21 C14 O4
IMPH C7 C8 N C16
IMPH C16 N1 C7 C17
IMPH C16 N1 C7 H23
IMPH C17 C18 C16 H24
IMPH C18 C20 C17 C19
IMPH C21 N2 C15 O2
IMPH N2 C22 C21 C24
IMPH N1 C16 C15 C23
IMPH C23 C22 N1 O3
IMPH C24 C25 N2 H5
IMPH C24 H5 N2 H4
IMPH C25 C26 C24 H3
IMPH C25 H3 C24 H2
IMPH C26 C22 C25 H1
IMPH C26 C22 C25 H
IMPH C22 C23 N2 H6
IMPH C H9 O H8
IMPH C H9 O H7
IMPH C5 C4 C6 H11
IMPH C12 H18 C11 H17
IMPH C12 H18 C11 H16
IMPH C13 H21 C11 H20
IMPH C13 H21 C11 H19
IMPH C19 H27 C18 H25
IMPH C19 H27 C18 H26
IMPH C20 H30 C18 H29
IMPH C20 H30 C18 H28
IC C1 C2 C3 C4 1.37 120.77 0.13 116.23 1.38
IC C1 C2 C3 N 1.37 120.77 179.60 130.90 1.36
IC C1 C6 C5 C4 1.38 119.38 -0.34 119.38 1.38
IC C1 C6 C5 H11 1.38 119.38 -179.61 121.54 1.07
IC C1 O C H7 1.35 112.31 -0.01 109.45 1.07
IC C1 O C H8 1.35 112.31 -119.99 109.46 1.07
IC C1 O C H9 1.35 112.31 120.01 109.48 1.07
IC C2 C1 C6 C5 1.37 121.72 -0.34 119.38 1.38
IC C2 C1 C6 H12 1.37 121.72 179.66 120.31 1.07
IC C2 C1 O C 1.37 115.11 33.35 112.31 1.42
IC C2 C3 C4 C5 1.37 116.23 -0.05 125.01 1.38
IC C2 C3 C4 C8 1.37 116.23 -179.84 103.27 1.45
IC C2 C3 N C7 1.37 130.90 -179.89 109.26 1.36
IC C2 C3 N C9 1.37 130.90 0.57 120.91 1.48
IC C3 C2 C1 C6 1.37 120.77 0.06 121.72 1.38
IC C3 C2 C1 O 1.37 120.77 -178.92 115.11 1.35
IC C3 C4 C5 C6 1.38 125.01 -0.22 116.88 1.38
IC C3 C4 C5 H11 1.38 125.01 179.78 121.58 1.07
IC C3 C4 C8 C7 1.38 103.27 -0.56 108.34 1.45
IC C3 C4 C8 C14 1.38 103.27 -179.94 121.93 1.45
IC C3 N C7 C8 1.36 109.26 0.01 106.26 1.45
IC C3 N C7 C16 1.36 109.26 179.28 139.32 1.48
IC C3 N C9 C10 1.36 120.91 -59.67 109.80 1.52
IC C3 N C9 H13 1.36 120.91 -174.96 106.69 1.07
IC C3 N C9 H14 1.36 120.91

55.59 106.69 1.07
IC C4 C3 C2 H10 1.38 116.23 -179.89 119.60 1.07
IC C4 C3 N C7 1.38 112.87 -0.40 109.26 1.36
IC C4 C3 N C9 1.38 112.87 -179.94 120.91 1.48
IC C4 C5 C6 H12 1.38 116.88 -179.59 120.31 1.07
IC C4 C8 C7 N 1.45 108.34 0.36 106.26 1.36
IC C4 C8 C7 C16 1.45 108.34 -179.12 114.41 1.48
IC C4 C8 C14 C15 1.45 121.93 142.57 104.06 1.52
IC C4 C8 C14 O1 1.45 121.93 -100.80 110.56 1.43
IC C4 C8 C14 H22 1.45 121.93 19.27 112.04 1.07
IC C5 C4 C3 N 1.38 125.01 -179.61 112.87 1.36
IC C5 C4 C8 C7 1.38 131.72 179.66 108.34 1.45
IC C5 C4 C8 C14 1.38 131.72 0.29 121.93 1.45
IC C5 C6 C1 O 1.38 119.38 178.56 123.16 1.35
IC C6 C1 C2 H10 1.38 121.72 -179.93 119.63 1.07
IC C6 C1 O C 1.38 123.16 -145.61 112.31 1.42
IC C6 C5 C4 C8 1.38 116.88 179.51 131.72 1.45
IC N C3 C2 H10 1.36 130.90 -0.41 119.60 1.07
IC N C3 C4 C8 1.36 112.87 0.59 103.27 1.45
IC N C7 C8 C14 1.36 106.26 179.67 129.73 1.45
IC N C7 C16 N1 1.36 139.32 -139.05 105.84 1.50
IC N C7 C16 C17 1.36 139.32 -7.39 115.04 1.53
IC N C7 C16 H23 1.36 139.32 102.94 111.62 1.07
IC N C9 C10 C11 1.48 109.80 118.90 122.68 1.34
IC N C9 C10 H15 1.48 109.80 -61.06 118.65 1.07
IC C7 N C9 C10 1.36 129.82 120.89 109.80 1.52
IC C7 N C9 H13 1.36 129.82 5.60 106.69 1.07
IC C7 N C9 H14 1.36 129.82 -123.85 106.69 1.07
IC C7 C8 C14 C15 1.45 129.73 -36.66 104.06 1.52
IC C7 C8 C14 O1 1.45 129.73 79.97 110.56 1.43
IC C7 C8 C14 H22 1.45 129.73 -159.96 112.04 1.07
IC C7 C16 N1 C15 1.48 105.84 -46.12 121.64 1.49
IC C7 C16 N1 C23 1.48 105.84 134.49 123.86 1.35
IC C7 C16 C17 C18 1.48 115.04 -63.55 126.80 1.35
IC C7 C16 C17 H24 1.48 115.04 116.45 116.57 1.07
IC C8 C4 C5 H11 1.45 131.72 -0.49 121.58 1.07
IC C8 C7 N C9 1.45 106.26 179.50 129.82 1.48
IC C8 C7 C16 N1 1.45 114.41 40.18 105.84 1.50
IC C8 C7 C16 C17 1.45 114.41 171.84 115.04 1.53
IC C8 C7 C16 H23 1.45 114.41 -77.83 111.62 1.07
IC C8 C14 C15 N1 1.45 104.06 29.39 118.30 1.49
IC C8 C14 C15 C21 1.45 104.06 -92.13 102.15 1.50
IC C8 C14 C15 O4 1.45 104.06 152.10 106.66 1.43
IC C8 C14 O1 H31 1.45 110.56 178.62 109.48 0.96
IC O C1 C2 H10 1.35 115.11

1.10 119.63 1.07
IC O C1 C6 H12 1.35 123.16 -1.45 120.31 1.07
IC C9 N C7 C16 1.48 129.82 -1.23 139.32 1.48
IC C9 C10 C11 C12 1.52 122.68 1.44 121.76 1.50
IC C9 C10 C11 C13 1.52 122.68 -178.96 118.31 1.50
IC C10 C11 C12 H16 1.34 121.76 0.00 109.46 1.07
IC C10 C11 C12 H17 1.34 121.76 120.01 109.45 1.07
IC C10 C11 C12 H18 1.34 121.76 -120.00 109.51 1.07
IC C10 C11 C13 H19 1.34 118.31 -0.00 109.48 1.07
IC C10 C11 C13 H20 1.34 118.31 -119.98 109.45 1.07
IC C10 C11 C13 H21 1.34 118.31 119.99 109.45 1.07
IC C11 C10 C9 H13 1.34 122.68 -125.83 106.72 1.07
IC C11 C10 C9 H14 1.34 122.68 3.64 106.70 1.07
IC C12 C11 C10 H15 1.50 121.76 -178.60 118.67 1.07
IC C12 C11 C13 H19 1.50 119.93 179.60 109.48 1.07
IC C12 C11 C13 H20 1.50 119.93 59.62 109.45 1.07
IC C12 C11 C13 H21 1.50 119.93 -60.41 109.45 1.07
IC C13 C11 C10 H15 1.50 118.31 1.00 118.67 1.07
IC C13 C11 C12 H16 1.50 119.93 -179.59 109.46 1.07
IC C13 C11 C12 H17 1.50 119.93 -59.58 109.45 1.07
IC C13 C11 C12 H18 1.50 119.93 60.41 109.51 1.07
IC C14 C8 C7 C16 1.45 129.73 0.19 114.41 1.48
IC C14 C15 N1 C16 1.52 118.30 9.54 121.64 1.50
IC C14 C15 N1 C23 1.52 118.30 -171.02 114.50 1.35
IC C14 C15 C21 N2 1.52 102.15 163.80 116.33 1.32
IC C14 C15 C21 O2 1.52 102.15 -15.86 120.85 1.22
IC C14 C15 O4 H32 1.52 106.66 -172.27 109.47 0.96
IC C15 C14 O1 H31 1.52 108.77 -67.71 109.48 0.96
IC C15 N1 C16 C17 1.49 121.64 -176.30 117.63 1.53
IC C15 N1 C16 H23 1.49 121.64 73.87 108.63 1.07
IC C15 N1 C23 C22 1.49 114.50 23.76 117.28 1.51
IC C15 N1 C23 O3 1.49 114.50 -154.79 125.70 1.22
IC C15 C21 N2 C22 1.50 116.33 8.95 119.75 1.46
IC C15 C21 N2 C24 1.50 116.33 -171.06 126.80 1.46
IC N1 C15 C14 O1 1.49 118.30 -88.47 108.77 1.43
IC N1 C15 C14 H22 1.49 118.30 151.58 113.73 1.07
IC N1 C15 C21 N2 1.49 110.50 37.05 116.33 1.32
IC N1 C15 C21 O2 1.49 110.50 -142.61 120.85 1.22
IC N1 C15 O4 H32 1.49 108.65 -43.70 109.47 0.96
IC N1 C16 C17 C18 1.50 117.63 62.23 126.80 1.35
IC N1 C16 C17 H24 1.50 117.63 -117.78 116.57 1.07
IC N1 C23 C22 N2 1.35 117.28 21.63 113.02 1.46
IC N1 C23 C22 C26 1.35 117.28 137.08 111.98 1.52
IC N1 C23 C22 H6 1.35 117.28 -100.27 103.38 1.07
IC C16 N1 C15 C21 1.50 121.64

126.70 110.50 1.50
IC C16 N1 C15 O4 1.50 121.64 -112.17 108.65 1.43
IC C16 N1 C23 C22 1.50 123.86 -156.81 117.28 1.51
IC C16 N1 C23 O3 1.50 123.86 24.64 125.70 1.22
IC C16 C17 C18 C19 1.53 126.80 -179.21 118.96 1.50
IC C16 C17 C18 C20 1.53 126.80 0.79 122.21 1.50
IC C17 C16 N1 C23 1.53 117.63 4.31 123.86 1.35
IC C17 C18 C19 H25 1.35 118.96 0.01 109.45 1.07
IC C17 C18 C19 H26 1.35 118.96 120.01 109.45 1.07
IC C17 C18 C19 H27 1.35 118.96 -119.97 109.47 1.07
IC C17 C18 C20 H28 1.35 122.21 179.98 109.48 1.07
IC C17 C18 C20 H29 1.35 122.21 -60.01 109.50 1.07
IC C17 C18 C20 H30 1.35 122.21 60.00 109.45 1.07
IC C18 C17 C16 H23 1.35 126.80 178.09 97.85 1.07
IC C19 C18 C17 H24 1.50 118.96 0.79 116.63 1.07
IC C19 C18 C20 H28 1.50 118.82 -0.01 109.48 1.07
IC C19 C18 C20 H29 1.50 118.82 119.99 109.50 1.07
IC C19 C18 C20 H30 1.50 118.82 -119.99 109.45 1.07
IC C20 C18 C17 H24 1.50 122.21 -179.21 116.63 1.07
IC C20 C18 C19 H25 1.50 118.82 -179.99 109.45 1.07
IC C20 C18 C19 H26 1.50 118.82 -60.00 109.45 1.07
IC C20 C18 C19 H27 1.50 118.82 60.03 109.47 1.07
IC O1 C14 C15 C21 1.43 108.77 150.00 102.15 1.50
IC O1 C14 C15 O4 1.43 108.77 34.23 106.66 1.43
IC C21 C15 C14 H22 1.50 102.15 30.05 113.73 1.07
IC C21 C15 N1 C23 1.50 110.50 -53.85 114.50 1.35
IC C21 C15 O4 H32 1.50 110.29 77.56 109.47 0.96
IC C21 N2 C22 C23 1.32 119.75 -39.69 113.02 1.51
IC C21 N2 C22 C26 1.32 119.75 -160.56 102.73 1.52
IC C21 N2 C22 H6 1.32 119.75 76.94 112.50 1.07
IC C21 N2 C24 C25 1.32 126.80 -179.59 103.07 1.52
IC C21 N2 C24 H4 1.32 126.80 -65.27 108.14 1.07
IC C21 N2 C24 H5 1.32 126.80 66.07 108.13 1.07
IC N2 C21 C15 O4 1.32 116.33 -83.10 110.29 1.43
IC N2 C22 C23 O3 1.46 113.02 -159.70 117.01 1.22
IC N2 C22 C26 C25 1.46 102.73 -30.91 103.69 1.52
IC N2 C22 C26 H 1.46 102.73 -145.30 107.97 1.07
IC N2 C22 C26 H1 1.46 102.73 83.52 107.99 1.07
IC N2 C24 C25 C26 1.46 103.07 -20.46 106.13 1.52
IC N2 C24 C25 H2 1.46 103.07 94.33 107.49 1.07
IC N2 C24 C25 H3 1.46 103.07 -135.24 107.49 1.07
IC C22 N2 C21 O2 1.46 119.75 -171.40 122.82 1.22
IC C22 N2 C24 C25 1.46 113.45 0.40 103.07 1.52
IC C22 N2 C24 H4 1.46 113.45 114.72 108.14 1.07
IC C22 N2 C24 H5 1.46 113.45 -

113.94 108.13 1.07
IC C22 C26 C25 C24 1.52 103.69
32.41 106.13 1.52
IC C22 C26 C25 H2 1.52 103.69 -
82.37 107.50 1.07
IC C22 C26 C25 H3 1.52 103.69
147.19 107.49 1.07
IC C23 N1 C15 O4 1.35 114.50
67.28 108.65 1.43
IC C23 N1 C16 H23 1.35 123.86 -
105.52 108.63 1.07
IC C23 C22 N2 C24 1.51 113.02
140.32 113.45 1.46
IC C23 C22 C26 C25 1.51 111.98 -
152.48 103.69 1.52
IC C23 C22 C26 H 1.51 111.98
93.13 107.97 1.07
IC C23 C22 C26 H1 1.51 111.98 -
38.06 107.99 1.07
IC O2 C21 C15 O4 1.22 120.85
97.24 110.29 1.43
IC O2 C21 N2 C24 1.22 122.82
8.59 126.80 1.46
IC O3 C23 C22 C26 1.22 117.01 -
44.24 111.98 1.52
IC O3 C23 C22 H6 1.22 117.01
78.40 103.38 1.07
IC O4 C15 C14 H22 1.43 106.66 -
85.72 113.73 1.07
IC C24 N2 C22 C26 1.46 113.45
19.45 102.73 1.52
IC C24 N2 C22 H6 1.46 113.45 -
103.06 112.50 1.07
IC C24 C25 C26 H 1.52 106.13
146.80 107.98 1.07
IC C24 C25 C26 H1 1.52 106.13 -
82.01 108.00 1.07
IC C25 C26 C22 H6 1.52 103.69
90.87 113.58 1.07
IC C26 C25 C24 H4 1.52 106.13 -
134.80 108.11 1.07
IC C26 C25 C24 H5 1.52 106.13
93.88 108.12 1.07
IC H C26 C22 H6 1.07 107.97 -
23.52 113.58 1.07
IC H C26 C25 H2 1.07 107.98
32.02 107.50 1.07
IC H C26 C25 H3 1.07 107.98 -
98.41 107.49 1.07
IC H1 C26 C22 H6 1.07 107.99 -
154.71 113.58 1.07
IC H1 C26 C25 H2 1.07 108.00
163.21 107.50 1.07
IC H1 C26 C25 H3 1.07 108.00
32.78 107.49 1.07
IC H2 C25 C24 H4 1.07 107.49 -
20.02 108.11 1.07
IC H2 C25 C24 H5 1.07 107.49 -
151.34 108.12 1.07
IC H3 C25 C24 H4 1.07 107.49
110.41 108.11 1.07
IC H3 C25 C24 H5 1.07 107.49 -
20.91 108.12 1.07
IC H11 C5 C6 H12 1.07 121.54
0.40 120.31 1.07
IC H13 C9 C10 H15 1.07 106.72
54.21 118.65 1.07
IC H14 C9 C10 H15 1.07 106.70 -
176.32 118.65 1.07
IC H22 C14 O1 H31 1.07 107.65
55.95 109.48 0.96
IC H23 C16 C17 H24 1.07 97.85
-1.91 116.57 1.07
IC C6 C2 *C1 O 0.00 0.00
180.00 0.00 0.00
IC C3 C1 *C2 H10 0.00 0.00
180.00 0.00 0.00
IC N C2 *C3 C4 0.00 0.00
180.00 0.00 0.00
IC C5 C1 *C6 H12 0.00 0.00
180.00 0.00 0.00
IC C7 C3 *N C9 0.00 0.00
180.00 0.00 0.00
IC C5 C3 *C4 C8 0.00 0.00
180.00 0.00 0.00
IC C10 N *C9 H14 0.00 0.00
120.00 0.00 0.00
IC H14 N *C9 H13 0.00 0.00 -

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120.00      0.00    0.00
IC C11    C9     *C10    H15      0.00       0.00
180.00      0.00    0.00
IC C12    C10    *C11    C13      0.00       0.00
180.00      0.00    0.00
IC C7     C4     *C8     C14      0.00       0.00
180.00      0.00    0.00
IC C15    C8     *C14    O1       0.00       0.00
120.00      0.00    0.00
IC O1     C8     *C14    H22      0.00       0.00 -
120.00      0.00    0.00
IC N1     C14    *C15    C21      0.00       0.00
120.00      0.00    0.00
IC C21    C14    *C15    O4       0.00       0.00 -
120.00      0.00    0.00
IC C8     N      *C7     C16      0.00       0.00
180.00      0.00    0.00
IC N1     C7     *C16    C17      0.00       0.00
120.00      0.00    0.00
IC N1     C7     *C16    H23      0.00       0.00 -
120.00      0.00    0.00
IC C18    C16    *C17    H24      0.00       0.00
180.00      0.00    0.00
IC C20    C17    *C18    C19      0.00       0.00
180.00      0.00    0.00
IC N2     C15    *C21    O2       0.00       0.00
180.00      0.00    0.00
IC C22    C21    *N2     C24      0.00       0.00
180.00      0.00    0.00
IC C16    C15    *N1     C23      0.00       0.00
180.00      0.00    0.00
IC C22    N1     *C23    O3       0.00       0.00
180.00      0.00    0.00
IC C25    N2     *C24    H5       0.00       0.00
120.00      0.00    0.00
IC H5     N2     *C24    H4       0.00       0.00 -
120.00      0.00    0.00
IC C26    C24    *C25    H3       0.00       0.00
120.00      0.00    0.00
IC H3     C24    *C25    H2       0.00       0.00 -
120.00      0.00    0.00
IC C22    C25    *C26    H1       0.00       0.00
120.00      0.00    0.00
IC C22    C25    *C26    H        0.00       0.00 -
120.00      0.00    0.00
IC C23    N2     *C22    H6       0.00       0.00 -
120.00      0.00    0.00
IC H9     O      *C      H8       0.00       0.00
120.00      0.00    0.00
IC H9     O      *C      H7       0.00       0.00 -
120.00      0.00    0.00
IC C4     C6     *C5     H11      0.00       0.00
180.00      0.00    0.00
IC H18    C11    *C12    H17      0.00       0.00
120.00      0.00    0.00
IC H18    C11    *C12    H16      0.00       0.00 -
120.00      0.00    0.00
IC H21    C11    *C13    H20      0.00       0.00
120.00      0.00    0.00
IC H21    C11    *C13    H19      0.00       0.00 -
120.00      0.00    0.00
IC H27    C18    *C19    H25      0.00       0.00
120.00      0.00    0.00
IC H27    C18    *C19    H26      0.00       0.00 -
120.00      0.00    0.00
IC H30    C18    *C20    H29      0.00       0.00
120.00      0.00    0.00
IC H30    C18    *C20    H28      0.00       0.00 -
120.00      0.00    0.00
END
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Absolute QM/MM single-point energies (E, a.u.) and the dispersion correction (ΔE, a.u.), as well as Cartesian coordinates of QM regions:

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[1]R
E=-3110.347924    ΔE=-0.281961
N     -10.760      -1.808      -8.306
H     -11.723      -1.592      -8.539
C      -9.924      -2.659      -9.002
C     -10.086      -1.319      -7.243
```

H	-10.504	-0.627	-6.529	H	0.498	3.716	-8.862
N	-8.856	-1.828	-7.226	C	1.597	1.996	-8.181
C	-8.741	-2.663	-8.319	H	2.544	2.514	-8.077
H	-7.831	-3.206	-8.508	N	-2.025	0.044	-8.704
C	-4.547	-4.538	-6.659	C	-2.387	-1.322	-8.263
H	-4.430	-5.408	-6.005	H	-3.462	-1.426	-8.409
H	-3.571	-4.044	-6.700	H	-2.193	-1.379	-7.189
C	-5.496	-3.549	-5.968	C	-1.639	-2.387	-9.031
O	-6.549	-3.145	-6.621	H	-1.732	-2.312	-10.112
O	-5.227	-3.151	-4.827	C	-0.874	-3.378	-8.540
N	-9.451	-5.303	-4.527	C	-0.601	-3.645	-7.080
H	-9.532	-6.318	-4.569	H	-1.013	-2.893	-6.405
C	-10.318	-4.400	-3.938	H	-1.007	-4.622	-6.794
C	-8.454	-4.603	-5.105	H	0.481	-3.714	-6.906
H	-7.657	-5.074	-5.652	C	-0.195	-4.353	-9.470
N	-8.620	-3.303	-4.912	H	-0.419	-4.146	-10.520
C	-9.783	-3.164	-4.183	H	-0.500	-5.378	-9.234
H	-10.143	-2.188	-3.899	H	0.894	-4.322	-9.331
C	0.994	-1.174	-3.937	C	-2.805	1.081	-9.219
H	1.759	-0.501	-4.335	C	-2.047	2.226	-9.287
H	1.092	-2.142	-4.444	C	-2.616	3.501	-9.764
C	-0.396	-0.607	-4.190	H	-1.821	4.159	-10.127
C	-1.530	-1.433	-4.186	O	-3.353	4.137	-8.715
H	-1.432	-2.480	-3.912	H	-3.852	4.848	-9.154
C	-2.792	-0.956	-4.552	C	-3.551	3.267	-10.970
H	-3.645	-1.629	-4.560	O	-4.329	4.460	-11.102
C	-2.941	0.380	-4.941	H	-5.292	4.302	-10.992
O	-4.122	0.891	-5.415	C	-2.748	3.164	-12.294
H	-4.821	0.214	-5.493	O	-1.547	3.430	-12.382
C	-0.586	0.746	-4.508	C	-4.269	1.094	-9.639
H	0.263	1.425	-4.494	H	-4.844	1.537	-8.819
C	-1.839	1.239	-4.871	C	-4.899	-0.260	-9.927
H	-1.966	2.283	-5.134	H	-5.731	-0.494	-9.269
C	1.558	0.614	-7.864	C	-4.583	-1.145	-10.885
O	2.739	0.049	-7.475	C	-3.489	-0.963	-11.901
C	2.783	-1.376	-7.432	H	-2.790	-1.807	-11.877
H	2.335	-1.817	-8.327	H	-3.908	-0.953	-12.916
H	2.269	-1.759	-6.543	H	-2.908	-0.051	-11.759
H	3.834	-1.664	-7.413	C	-5.384	-2.414	-11.038
C	0.376	-0.113	-7.980	H	-6.156	-2.513	-10.271
H	0.331	-1.159	-7.726	H	-5.883	-2.440	-12.015
C	-0.758	0.554	-8.464	H	-4.733	-3.298	-10.993
C	-0.734	1.927	-8.812	N	-4.383	2.055	-10.821
C	0.462	2.651	-8.641	C	-5.311	1.873	-11.816

O	-6.361	1.245	-11.708
C	-4.952	2.491	-13.169
H	-5.524	3.423	-13.283
C	-5.250	1.532	-14.336
H	-6.295	1.577	-14.647
H	-5.053	0.501	-14.033
C	-4.258	1.978	-15.421
H	-4.671	2.812	-15.993
H	-4.026	1.173	-16.120
C	-3.004	2.445	-14.659
H	-2.529	3.320	-15.110
H	-2.245	1.658	-14.580
N	-3.518	2.761	-13.318
C	-8.600	0.587	-4.555
O	-8.422	-0.711	-4.504
O	-8.411	1.274	-5.568
C	-9.042	1.243	-3.251
H	-8.584	0.742	-2.394
H	-8.666	2.270	-3.302
Fe	-7.517	-1.703	-5.832
O	-6.613	-0.487	-6.385

^{3}R

E=-3110.383269 ΔE=-0.282447

N	-10.705	-1.783	-8.305
H	-11.665	-1.548	-8.536
C	-9.885	-2.651	-9.001
C	-10.025	-1.301	-7.246
H	-10.427	-0.599	-6.534
N	-8.802	-1.832	-7.233
C	-8.700	-2.675	-8.324
H	-7.799	-3.232	-8.510
C	-4.511	-4.573	-6.686
H	-4.377	-5.435	-6.026
H	-3.546	-4.059	-6.733
C	-5.495	-3.601	-6.020
O	-6.506	-3.176	-6.710
O	-5.290	-3.233	-4.849
N	-9.416	-5.312	-4.500
H	-9.503	-6.327	-4.546
C	-10.284	-4.403	-3.914
C	-8.411	-4.621	-5.069
H	-7.614	-5.094	-5.615
N	-8.574	-3.318	-4.874
C	-9.742	-3.170	-4.150
H	-10.093	-2.191	-3.871
C	0.996	-1.212	-3.926
H	1.762	-0.545	-4.334
H	1.090	-2.186	-4.422
C	-0.392	-0.643	-4.180
C	-1.527	-1.468	-4.190
H	-1.431	-2.519	-3.929
C	-2.787	-0.985	-4.554
H	-3.642	-1.657	-4.576
C	-2.933	0.357	-4.924
O	-4.112	0.877	-5.392
H	-4.802	0.193	-5.493
C	-0.579	0.714	-4.482
H	0.272	1.391	-4.458
C	-1.830	1.214	-4.841
H	-1.955	2.261	-5.090
C	1.556	0.596	-7.859
O	2.737	0.028	-7.473
C	2.779	-1.397	-7.434
H	2.333	-1.835	-8.332
H	2.260	-1.782	-6.549
H	3.829	-1.686	-7.412
C	0.372	-0.129	-7.973
H	0.326	-1.175	-7.720
C	-0.762	0.542	-8.452
C	-0.736	1.915	-8.799
C	0.463	2.636	-8.632
H	0.502	3.702	-8.851
C	1.597	1.977	-8.176
H	2.547	2.493	-8.076
N	-2.031	0.036	-8.688
C	-2.393	-1.332	-8.251
H	-3.469	-1.434	-8.386
H	-2.190	-1.393	-7.178
C	-1.651	-2.393	-9.030
H	-1.749	-2.312	-10.110
C	-0.881	-3.386	-8.550
C	-0.600	-3.662	-7.093
H	-1.012	-2.917	-6.410
H	-1.000	-4.643	-6.811
H	0.484	-3.726	-6.924
C	-0.203	-4.352	-9.489
H	-0.430	-4.139	-10.537

H	-0.502	-5.381	-9.259
H	0.886	-4.318	-9.353
C	-2.811	1.076	-9.198
C	-2.049	2.218	-9.268
C	-2.618	3.496	-9.738
H	-1.824	4.154	-10.104
O	-3.346	4.130	-8.683
H	-3.852	4.839	-9.119
C	-3.561	3.268	-10.939
O	-4.335	4.466	-11.056
H	-5.300	4.307	-10.987
C	-2.765	3.168	-12.269
O	-1.564	3.432	-12.363
C	-4.277	1.092	-9.610
H	-4.849	1.532	-8.786
C	-4.907	-0.261	-9.901
H	-5.729	-0.503	-9.232
C	-4.595	-1.140	-10.865
C	-3.510	-0.949	-11.890
H	-2.806	-1.790	-11.872
H	-3.937	-0.938	-12.901
H	-2.932	-0.034	-11.749
C	-5.390	-2.412	-11.016
H	-6.144	-2.525	-10.234
H	-5.908	-2.432	-11.984
H	-4.733	-3.292	-10.993
N	-4.395	2.057	-10.789
C	-5.328	1.879	-11.780
O	-6.379	1.255	-11.668
C	-4.975	2.501	-13.135
H	-5.547	3.434	-13.243
C	-5.281	1.548	-14.305
H	-6.328	1.598	-14.610
H	-5.086	0.516	-14.006
C	-4.292	1.995	-15.392
H	-4.703	2.834	-15.959
H	-4.066	1.193	-16.096
C	-3.033	2.453	-14.633
H	-2.554	3.328	-15.083
H	-2.278	1.662	-14.559
N	-3.541	2.769	-13.290
C	-8.642	0.627	-4.675
O	-8.489	-0.661	-4.582
O	-8.475	1.276	-5.724
C	-9.048	1.347	-3.393
H	-8.527	0.918	-2.531
H	-8.726	2.385	-3.517
Fe	-7.512	-1.788	-5.798
O	-6.447	-0.650	-6.224

^{5}R

E=-3110.394543 ΔE=-0.281286

N	-10.705	-1.783	-8.305
H	-11.665	-1.548	-8.536
C	-9.885	-2.651	-9.001
C	-10.025	-1.301	-7.246
H	-10.427	-0.599	-6.534
N	-8.802	-1.832	-7.233
C	-8.700	-2.675	-8.324
H	-7.799	-3.232	-8.510
C	-4.511	-4.573	-6.686
H	-4.377	-5.435	-6.026
H	-3.546	-4.059	-6.733
C	-5.495	-3.601	-6.020
O	-6.506	-3.176	-6.710
O	-5.290	-3.233	-4.849
N	-9.416	-5.312	-4.500
H	-9.503	-6.327	-4.546
C	-10.284	-4.403	-3.914
C	-8.411	-4.621	-5.069
H	-7.614	-5.094	-5.615
N	-8.574	-3.318	-4.874
C	-9.742	-3.170	-4.150
H	-10.093	-2.191	-3.871
C	0.996	-1.212	-3.926
H	1.762	-0.545	-4.334
H	1.090	-2.186	-4.422
C	-0.392	-0.643	-4.180
C	-1.527	-1.468	-4.190
H	-1.431	-2.519	-3.929
C	-2.787	-0.985	-4.554
H	-3.642	-1.657	-4.576
C	-2.933	0.357	-4.924
O	-4.112	0.877	-5.392
H	-4.802	0.193	-5.493
C	-0.579	0.714	-4.482
H	0.272	1.391	-4.458
C	-1.830	1.214	-4.841

H	-1.955	2.261	-5.090
C	1.556	0.596	-7.859
O	2.737	0.028	-7.473
C	2.779	-1.397	-7.434
H	2.333	-1.835	-8.332
H	2.260	-1.782	-6.549
H	3.829	-1.686	-7.412
C	0.372	-0.129	-7.973
H	0.326	-1.175	-7.720
C	-0.762	0.542	-8.452
C	-0.736	1.915	-8.799
C	0.463	2.636	-8.632
H	0.502	3.702	-8.851
C	1.597	1.977	-8.176
H	2.547	2.493	-8.076
N	-2.031	0.036	-8.688
C	-2.393	-1.332	-8.251
H	-3.469	-1.434	-8.386
H	-2.190	-1.393	-7.178
C	-1.651	-2.393	-9.030
H	-1.749	-2.312	-10.110
C	-0.881	-3.386	-8.550
C	-0.600	-3.662	-7.093
H	-1.012	-2.917	-6.410
H	-1.000	-4.643	-6.811
H	0.484	-3.726	-6.924
C	-0.203	-4.352	-9.489
H	-0.430	-4.139	-10.537
H	-0.502	-5.381	-9.259
H	0.886	-4.318	-9.353
C	-2.811	1.076	-9.198
C	-2.049	2.218	-9.268
C	-2.618	3.496	-9.738
H	-1.824	4.154	-10.104
O	-3.346	4.130	-8.683
H	-3.852	4.839	-9.119
C	-3.561	3.268	-10.939
O	-4.335	4.466	-11.056
H	-5.300	4.307	-10.987
C	-2.765	3.168	-12.269
O	-1.564	3.432	-12.363
C	-4.277	1.092	-9.610
H	-4.849	1.532	-8.786
C	-4.907	-0.261	-9.901
H	-5.729	-0.503	-9.232
C	-4.595	-1.140	-10.865
C	-3.510	-0.949	-11.890
H	-2.806	-1.790	-11.872
H	-3.937	-0.938	-12.901
H	-2.932	-0.034	-11.749
C	-5.390	-2.412	-11.016
H	-6.144	-2.525	-10.234
H	-5.908	-2.432	-11.984
H	-4.733	-3.292	-10.993
N	-4.395	2.057	-10.789
C	-5.328	1.879	-11.780
O	-6.379	1.255	-11.668
C	-4.975	2.501	-13.135
H	-5.547	3.434	-13.243
C	-5.281	1.548	-14.305
H	-6.328	1.598	-14.610
H	-5.086	0.516	-14.006
C	-4.292	1.995	-15.392
H	-4.703	2.834	-15.959
H	-4.066	1.193	-16.096
C	-3.033	2.453	-14.633
H	-2.554	3.328	-15.083
H	-2.278	1.662	-14.559
N	-3.541	2.769	-13.290
C	-8.642	0.627	-4.675
O	-8.489	-0.661	-4.582
O	-8.475	1.276	-5.724
C	-9.048	1.347	-3.393
H	-8.527	0.918	-2.531
H	-8.726	2.385	-3.517
Fe	-7.512	-1.788	-5.798
O	-6.447	-0.650	-6.224

^{7}R

E=-3110.376035 ΔE=-0.279098

N	-11.015	-1.943	-8.606
H	-11.983	-1.773	-8.874
C	-10.117	-2.769	-9.259
C	-10.393	-1.406	-7.537
H	-10.864	-0.728	-6.840
N	-9.138	-1.846	-7.471
C	-8.957	-2.701	-8.542
H	-8.015	-3.203	-8.695

C	-4.520	-4.543	-6.814	C	-2.393	-1.289	-8.251
H	-4.331	-5.415	-6.181	H	-3.469	-1.392	-8.389
H	-3.568	-4.010	-6.905	H	-2.194	-1.354	-7.178
C	-5.470	-3.606	-6.050	C	-1.647	-2.346	-9.032
O	-6.456	-3.041	-6.696	H	-1.717	-2.241	-10.113
O	-5.245	-3.392	-4.854	C	-0.903	-3.360	-8.554
N	-9.465	-5.358	-4.439	C	-0.663	-3.670	-7.097
H	-9.535	-6.375	-4.495	H	-1.079	-2.930	-6.411
C	-10.361	-4.465	-3.872	H	-1.087	-4.649	-6.845
C	-8.455	-4.648	-4.977	H	0.415	-3.758	-6.903
H	-7.627	-5.105	-5.493	C	-0.219	-4.318	-9.497
N	-8.646	-3.348	-4.786	H	-0.417	-4.074	-10.545
C	-9.834	-3.223	-4.091	H	-0.546	-5.345	-9.302
H	-10.213	-2.250	-3.822	H	0.867	-4.309	-9.336
C	0.909	-1.213	-3.958	C	-2.804	1.118	-9.201
H	1.677	-0.559	-4.383	C	-2.040	2.259	-9.276
H	0.982	-2.191	-4.449	C	-2.610	3.533	-9.754
C	-0.474	-0.622	-4.198	H	-1.815	4.191	-10.118
C	-1.623	-1.427	-4.223	O	-3.347	4.170	-8.705
H	-1.544	-2.483	-3.976	H	-3.847	4.879	-9.146
C	-2.877	-0.920	-4.582	C	-3.547	3.300	-10.959
H	-3.741	-1.579	-4.609	O	-4.325	4.495	-11.085
C	-3.004	0.431	-4.934	H	-5.289	4.334	-11.005
O	-4.165	0.982	-5.397	C	-2.746	3.198	-12.285
H	-4.884	0.325	-5.542	O	-1.546	3.468	-12.375
C	-0.641	0.743	-4.477	C	-4.269	1.142	-9.614
H	0.219	1.407	-4.440	H	-4.831	1.602	-8.795
C	-1.884	1.267	-4.829	C	-4.912	-0.207	-9.881
H	-1.993	2.320	-5.058	H	-5.730	-0.434	-9.203
C	1.557	0.627	-7.855	C	-4.620	-1.097	-10.842
O	2.734	0.051	-7.470	C	-3.532	-0.929	-11.867
C	2.764	-1.375	-7.435	H	-2.860	-1.795	-11.865
H	2.304	-1.807	-8.329	H	-3.957	-0.884	-12.878
H	2.252	-1.758	-6.544	H	-2.921	-0.039	-11.712
H	3.812	-1.674	-7.426	C	-5.447	-2.348	-10.984
C	0.368	-0.090	-7.962	H	-6.192	-2.445	-10.193
H	0.315	-1.135	-7.703	H	-5.980	-2.353	-11.944
C	-0.761	0.583	-8.446	H	-4.811	-3.245	-10.971
C	-0.729	1.955	-8.801	N	-4.380	2.089	-10.808
C	0.474	2.669	-8.639	C	-5.307	1.904	-11.802
H	0.519	3.733	-8.865	O	-6.358	1.277	-11.696
C	1.606	2.006	-8.180	C	-4.950	2.523	-13.156
H	2.558	2.517	-8.085	H	-5.522	3.456	-13.266
N	-2.031	0.080	-8.683	C	-5.252	1.570	-14.327

H	-6.299	1.612	-14.632
H	-5.049	0.538	-14.033
C	-4.267	2.027	-15.413
H	-4.683	2.866	-15.976
H	-4.040	1.230	-16.122
C	-3.009	2.486	-14.654
H	-2.535	3.365	-15.099
H	-2.251	1.697	-14.585
N	-3.517	2.792	-13.307
C	-8.734	0.683	-4.809
O	-8.744	-0.581	-4.586
O	-8.136	1.186	-5.795
C	-9.411	1.675	-3.874
H	-8.598	2.136	-3.299
H	-9.797	2.452	-4.540
Fe	-7.740	-1.746	-5.902
O	-6.393	-0.479	-6.233

^{3}TS1a

E=-3110.359781 ΔE=-0.294832

N	-10.483	-1.737	-8.495
H	-11.455	-1.513	-8.667
C	-9.729	-2.677	-9.167
C	-9.693	-1.151	-7.565
H	-10.041	-0.374	-6.901
N	-8.472	-1.675	-7.592
C	-8.489	-2.633	-8.588
H	-7.616	-3.231	-8.795
C	-4.390	-4.909	-6.728
H	-4.506	-5.760	-6.051
H	-3.341	-4.620	-6.692
C	-5.165	-3.722	-6.165
O	-6.030	-3.131	-6.948
O	-4.952	-3.331	-5.010
N	-9.140	-5.069	-4.803
H	-9.307	-6.070	-4.847
C	-9.924	-4.108	-4.190
C	-8.084	-4.453	-5.367
H	-7.342	-4.992	-5.927
N	-8.123	-3.146	-5.136
C	-9.271	-2.919	-4.398
H	-9.534	-1.923	-4.081
C	1.045	-1.176	-3.757
H	1.825	-0.537	-4.183
H	1.080	-2.148	-4.263
C	-0.322	-0.542	-3.953
C	-1.483	-1.326	-3.990
H	-1.419	-2.391	-3.780
C	-2.726	-0.782	-4.321
H	-3.601	-1.422	-4.384
C	-2.825	0.582	-4.640
O	-3.971	1.135	-5.131
H	-4.578	0.437	-5.488
C	-0.466	0.839	-4.159
H	0.407	1.485	-4.092
C	-1.699	1.399	-4.486
H	-1.791	2.463	-4.673
C	1.038	0.550	-7.600
O	2.203	-0.064	-7.226
C	2.260	-1.484	-7.311
H	1.822	-1.842	-8.251
H	1.743	-1.959	-6.470
H	3.316	-1.760	-7.298
C	-0.209	-0.082	-7.590
H	-0.310	-1.090	-7.221
C	-1.314	0.639	-8.070
C	-1.169	1.954	-8.575
C	0.082	2.590	-8.517
H	0.192	3.617	-8.860
C	1.178	1.888	-8.036
H	2.172	2.325	-8.022
N	-2.639	0.226	-8.270
C	-3.093	-1.059	-7.704
H	-4.372	-0.955	-7.313
H	-2.658	-1.136	-6.706
C	-2.687	-2.171	-8.596
H	-3.012	-2.060	-9.622
C	-1.749	-3.127	-8.356
C	-1.140	-3.480	-7.026
H	-1.543	-2.919	-6.182
H	-1.277	-4.551	-6.828
H	-0.052	-3.341	-7.058
C	-1.144	-3.872	-9.521
H	-1.709	-3.733	-10.446
H	-1.043	-4.940	-9.309
H	-0.129	-3.493	-9.703
C	-3.286	1.241	-8.985
C	-2.431	2.303	-9.136

C	-2.860	3.578	-9.740
H	-1.994	4.141	-10.106
O	-3.576	4.335	-8.764
H	-4.021	5.047	-9.256
C	-3.754	3.334	-10.970
O	-4.473	4.550	-11.192
H	-5.443	4.437	-11.086
C	-2.896	3.148	-12.253
O	-1.677	3.346	-12.291
C	-4.676	1.245	-9.589
H	-5.370	1.687	-8.869
C	-5.206	-0.138	-9.938
H	-6.079	-0.424	-9.360
C	-4.756	-0.987	-10.876
C	-3.576	-0.736	-11.780
H	-2.854	-1.562	-11.720
H	-3.898	-0.700	-12.828
H	-3.038	0.185	-11.552
C	-5.479	-2.288	-11.127
H	-6.309	-2.439	-10.437
H	-5.883	-2.310	-12.147
H	-4.797	-3.146	-11.039
N	-4.643	2.165	-10.811
C	-5.518	1.970	-11.850
O	-6.578	1.356	-11.776
C	-5.086	2.542	-13.203
H	-5.621	3.489	-13.360
C	-5.371	1.568	-14.360
H	-6.402	1.643	-14.712
H	-5.227	0.537	-14.028
C	-4.324	1.958	-15.414
H	-4.686	2.795	-16.014
H	-4.094	1.134	-16.091
C	-3.084	2.394	-14.612
H	-2.559	3.242	-15.062
H	-2.360	1.582	-14.486
N	-3.638	2.761	-13.300
C	-8.177	0.688	-4.848
O	-7.594	-0.465	-4.745
O	-8.326	1.300	-5.926
C	-8.655	1.336	-3.543
H	-8.087	0.954	-2.691
H	-8.430	2.402	-3.658
Fe	-6.821	-1.654	-6.069
O	-5.462	-0.599	-6.602

^{5}TS1a

E=-3110.379979 ΔE=-0.281900

N	-10.773	-1.793	-8.417
H	-11.743	-1.609	-8.651
C	-9.926	-2.659	-9.081
C	-10.089	-1.241	-7.390
H	-10.518	-0.525	-6.704
N	-8.844	-1.710	-7.358
C	-8.735	-2.598	-8.411
H	-7.817	-3.133	-8.592
C	-4.501	-4.595	-6.670
H	-4.363	-5.472	-6.031
H	-3.536	-4.079	-6.714
C	-5.467	-3.642	-5.961
O	-6.441	-3.117	-6.646
O	-5.298	-3.366	-4.765
N	-9.434	-5.265	-4.576
H	-9.525	-6.279	-4.632
C	-10.292	-4.362	-3.968
C	-8.421	-4.575	-5.128
H	-7.627	-5.046	-5.678
N	-8.569	-3.274	-4.898
C	-9.738	-3.129	-4.174
H	-10.083	-2.154	-3.870
C	0.891	-1.182	-3.956
H	1.641	-0.498	-4.367
H	1.004	-2.150	-4.460
C	-0.513	-0.642	-4.209
C	-1.637	-1.484	-4.195
H	-1.520	-2.525	-3.902
C	-2.909	-1.040	-4.570
H	-3.744	-1.731	-4.556
C	-3.109	0.289	-4.998
O	-4.278	0.760	-5.471
H	-5.179	0.000	-5.622
C	-0.737	0.700	-4.558
H	0.097	1.399	-4.557
C	-1.997	1.159	-4.939
H	-2.137	2.195	-5.225
C	1.556	0.599	-7.868
O	2.736	0.032	-7.480
C	2.775	-1.393	-7.432

H	2.328	-1.836	-8.327
H	2.256	-1.771	-6.543
H	3.824	-1.684	-7.409
C	0.372	-0.125	-7.983
H	0.324	-1.171	-7.728
C	-0.760	0.545	-8.466
C	-0.733	1.918	-8.812
C	0.464	2.639	-8.641
H	0.502	3.705	-8.859
C	1.598	1.981	-8.184
H	2.547	2.497	-8.080
N	-2.029	0.039	-8.705
C	-2.395	-1.326	-8.262
H	-3.471	-1.425	-8.400
H	-2.197	-1.382	-7.188
C	-1.654	-2.391	-9.036
H	-1.749	-2.313	-10.116
C	-0.885	-3.383	-8.553
C	-0.606	-3.656	-7.095
H	-1.021	-2.911	-6.413
H	-1.001	-4.639	-6.813
H	0.478	-3.716	-6.924
C	-0.205	-4.351	-9.490
H	-0.433	-4.139	-10.539
H	-0.504	-5.379	-9.260
H	0.883	-4.317	-9.354
C	-2.807	1.078	-9.217
C	-2.045	2.221	-9.284
C	-2.613	3.499	-9.754
H	-1.818	4.158	-10.115
O	-3.348	4.129	-8.701
H	-3.849	4.841	-9.135
C	-3.550	3.272	-10.960
O	-4.324	4.469	-11.083
H	-5.289	4.311	-11.004
C	-2.748	3.171	-12.285
O	-1.547	3.435	-12.374
C	-4.272	1.096	-9.633
H	-4.842	1.538	-8.808
C	-4.906	-0.254	-9.926
H	-5.739	-0.488	-9.269
C	-4.595	-1.137	-10.887
C	-3.501	-0.957	-11.903
H	-2.805	-1.805	-11.880
H	-3.919	-0.943	-12.918
H	-2.915	-0.049	-11.758
C	-5.401	-2.402	-11.043
H	-6.170	-2.502	-10.274
H	-5.904	-2.423	-12.019
H	-4.754	-3.289	-11.004
N	-4.386	2.062	-10.813
C	-5.315	1.886	-11.807
O	-6.370	1.266	-11.700
C	-4.954	2.504	-13.160
H	-5.525	3.436	-13.276
C	-5.253	1.547	-14.328
H	-6.299	1.593	-14.638
H	-5.057	0.515	-14.027
C	-4.262	1.993	-15.413
H	-4.674	2.831	-15.981
H	-4.034	1.191	-16.115
C	-3.007	2.454	-14.650
H	-2.527	3.328	-15.100
H	-2.251	1.664	-14.572
N	-3.520	2.771	-13.309
C	-8.532	0.630	-4.560
O	-8.349	-0.667	-4.434
O	-8.395	1.228	-5.634
C	-8.945	1.366	-3.295
H	-8.397	0.979	-2.431
H	-8.663	2.411	-3.454
Fe	-7.397	-1.732	-5.680
O	-6.194	-0.603	-5.967

^{7}TS1a

E=-3110.369592 ΔE=-0.280385

N	-10.862	-1.874	-8.546
H	-11.828	-1.691	-8.801
C	-9.996	-2.738	-9.194
C	-10.208	-1.330	-7.498
H	-10.652	-0.622	-6.813
N	-8.966	-1.804	-7.436
C	-8.825	-2.686	-8.491
H	-7.902	-3.223	-8.640
C	-4.464	-4.600	-6.833
H	-4.277	-5.477	-6.206
H	-3.513	-4.065	-6.921
C	-5.425	-3.669	-6.071

O	-6.408	-3.115	-6.711	H	-1.720	-2.250	-10.114
O	-5.196	-3.463	-4.869	C	-0.896	-3.370	-8.563
N	-9.426	-5.303	-4.432	C	-0.651	-3.687	-7.107
H	-9.513	-6.316	-4.503	H	-1.080	-2.960	-6.416
C	-10.317	-4.404	-3.866	H	-1.061	-4.673	-6.862
C	-8.396	-4.601	-4.944	H	0.428	-3.759	-6.914
H	-7.572	-5.064	-5.458	C	-0.207	-4.320	-9.511
N	-8.567	-3.301	-4.734	H	-0.407	-4.071	-10.557
C	-9.766	-3.167	-4.058	H	-0.527	-5.349	-9.320
H	-10.133	-2.190	-3.785	H	0.879	-4.304	-9.350
C	0.835	-1.173	-3.966	C	-2.809	1.105	-9.183
H	1.584	-0.496	-4.389	C	-2.042	2.244	-9.253
H	0.921	-2.142	-4.472	C	-2.610	3.522	-9.725
C	-0.563	-0.613	-4.184	H	-1.815	4.183	-10.082
C	-1.697	-1.455	-4.196	O	-3.349	4.149	-8.673
H	-1.581	-2.504	-3.935	H	-3.854	4.858	-9.110
C	-2.953	-1.000	-4.581	C	-3.544	3.296	-10.934
H	-3.796	-1.684	-4.634	O	-4.319	4.493	-11.051
C	-3.115	0.353	-4.979	H	-5.285	4.333	-10.997
O	-4.237	0.828	-5.505	C	-2.738	3.200	-12.258
H	-5.072	0.140	-5.642	O	-1.537	3.466	-12.340
C	-0.763	0.751	-4.479	C	-4.272	1.131	-9.602
H	0.082	1.433	-4.444	H	-4.840	1.586	-8.785
C	-2.007	1.230	-4.857	C	-4.911	-0.219	-9.878
H	-2.148	2.276	-5.102	H	-5.736	-0.449	-9.209
C	1.554	0.604	-7.840	C	-4.607	-1.105	-10.837
O	2.731	0.025	-7.458	C	-3.517	-0.928	-11.859
C	2.764	-1.400	-7.442	H	-2.843	-1.793	-11.864
H	2.305	-1.821	-8.341	H	-3.942	-0.876	-12.870
H	2.251	-1.795	-6.556	H	-2.908	-0.037	-11.698
H	3.812	-1.698	-7.435	C	-5.425	-2.363	-10.984
C	0.363	-0.112	-7.946	H	-6.165	-2.471	-10.189
H	0.311	-1.159	-7.697	H	-5.962	-2.368	-11.940
C	-0.766	0.564	-8.428	H	-4.780	-3.254	-10.978
C	-0.732	1.936	-8.779	N	-4.376	2.083	-10.792
C	0.473	2.648	-8.618	C	-5.299	1.901	-11.791
H	0.519	3.712	-8.845	O	-6.348	1.272	-11.692
C	1.605	1.983	-8.163	C	-4.939	2.528	-13.141
H	2.559	2.492	-8.073	H	-5.513	3.459	-13.250
N	-2.036	0.063	-8.665	C	-5.234	1.580	-14.318
C	-2.398	-1.310	-8.247	H	-6.280	1.623	-14.627
H	-3.474	-1.414	-8.385	H	-5.033	0.547	-14.027
H	-2.198	-1.387	-7.175	C	-4.244	2.042	-15.397
C	-1.647	-2.359	-9.034	H	-4.657	2.886	-15.955

H	-4.015	1.250	-16.110
C	-2.990	2.495	-14.629
H	-2.509	3.373	-15.070
H	-2.236	1.704	-14.556
N	-3.505	2.802	-13.286
C	-8.788	0.748	-4.847
O	-8.682	-0.512	-4.596
O	-8.340	1.278	-5.891
C	-9.425	1.702	-3.845
H	-8.598	2.103	-3.243
H	-9.789	2.522	-4.467
Fe	-7.584	-1.712	-5.815
O	-6.177	-0.548	-5.960

^{3}IM1a

E=-3110.393429 ΔE=-0.0.280711

N	-10.745	-1.840	-8.340
H	-11.704	-1.615	-8.580
C	-9.910	-2.696	-9.030
C	-10.066	-1.354	-7.276
H	-10.467	-0.637	-6.576
N	-8.841	-1.865	-7.252
C	-8.730	-2.703	-8.342
H	-7.823	-3.253	-8.522
C	-4.501	-4.562	-6.685
H	-4.389	-5.422	-6.016
H	-3.525	-4.069	-6.729
C	-5.474	-3.564	-6.038
O	-6.538	-3.228	-6.681
O	-5.205	-3.102	-4.908
N	-9.450	-5.312	-4.513
H	-9.545	-6.325	-4.562
C	-10.297	-4.401	-3.905
C	-8.446	-4.626	-5.092
H	-7.661	-5.098	-5.656
N	-8.589	-3.325	-4.878
C	-9.742	-3.171	-4.135
H	-10.074	-2.189	-3.836
C	1.037	-1.188	-3.899
H	1.811	-0.531	-4.306
H	1.096	-2.160	-4.402
C	-0.337	-0.588	-4.115
C	-1.486	-1.420	-4.167
H	-1.378	-2.483	-3.968
C	-2.728	-0.917	-4.489
H	-3.599	-1.562	-4.569
C	-2.891	0.493	-4.793
O	-3.989	0.957	-5.213
H	-5.880	-0.157	-5.877
C	-0.498	0.808	-4.313
H	0.371	1.457	-4.229
C	-1.726	1.343	-4.624
H	-1.857	2.407	-4.777
C	1.540	0.553	-7.812
O	2.720	-0.016	-7.419
C	2.778	-1.440	-7.432
H	2.347	-1.850	-8.350
H	2.250	-1.865	-6.569
H	3.830	-1.721	-7.402
C	0.358	-0.173	-7.933
H	0.316	-1.224	-7.700
C	-0.776	0.496	-8.416
C	-0.751	1.872	-8.756
C	0.446	2.593	-8.583
H	0.486	3.658	-8.804
C	1.581	1.934	-8.126
H	2.530	2.451	-8.029
N	-2.041	-0.012	-8.666
C	-2.403	-1.386	-8.249
H	-3.479	-1.488	-8.385
H	-2.202	-1.464	-7.177
C	-1.654	-2.434	-9.037
H	-1.759	-2.348	-10.116
C	-0.871	-3.422	-8.566
C	-0.583	-3.703	-7.111
H	-1.007	-2.966	-6.425
H	-0.974	-4.689	-6.833
H	0.501	-3.756	-6.943
C	-0.188	-4.378	-9.512
H	-0.421	-4.161	-10.558
H	-0.481	-5.409	-9.286
H	0.901	-4.338	-9.380
C	-2.818	1.026	-9.183
C	-2.061	2.173	-9.237
C	-2.639	3.450	-9.702
H	-1.849	4.123	-10.049
O	-3.390	4.061	-8.650
H	-3.903	4.766	-9.083

C	-3.562	3.223	-10.919
O	-4.341	4.415	-11.044
H	-5.305	4.259	-10.936
C	-2.748	3.138	-12.238
O	-1.546	3.406	-12.314
C	-4.278	1.035	-9.615
H	-4.859	1.469	-8.795
C	-4.894	-0.324	-9.907
H	-5.691	-0.584	-9.215
C	-4.588	-1.194	-10.882
C	-3.519	-0.990	-11.921
H	-2.800	-1.818	-11.905
H	-3.956	-0.995	-12.928
H	-2.956	-0.064	-11.793
C	-5.375	-2.473	-11.025
H	-6.116	-2.594	-10.233
H	-5.907	-2.494	-11.985
H	-4.710	-3.348	-11.016
N	-4.388	2.004	-10.789
C	-5.309	1.828	-11.792
O	-6.354	1.191	-11.702
C	-4.946	2.470	-13.134
H	-5.518	3.404	-13.232
C	-5.236	1.533	-14.320
H	-6.280	1.580	-14.636
H	-5.039	0.497	-14.035
C	-4.239	1.999	-15.392
H	-4.649	2.844	-15.951
H	-4.005	1.208	-16.105
C	-2.989	2.451	-14.615
H	-2.509	3.333	-15.048
H	-2.233	1.661	-14.545
N	-3.511	2.746	-13.272
C	-8.621	0.582	-4.566
O	-8.296	-0.680	-4.463
O	-8.631	1.211	-5.634
C	-9.006	1.286	-3.268
H	-8.484	0.857	-2.409
H	-8.690	2.327	-3.392
Fe	-7.508	-1.806	-5.773
O	-6.455	-0.578	-6.541

[5]IM1a

E=-3110.421317 ΔE=-0.278585

N	-10.902	-1.908	-8.454
H	-11.870	-1.732	-8.705
C	-10.021	-2.739	-9.121
C	-10.249	-1.387	-7.387
H	-10.695	-0.684	-6.699
N	-9.003	-1.836	-7.332
C	-8.853	-2.685	-8.410
H	-7.922	-3.203	-8.575
C	-4.500	-4.555	-6.724
H	-4.376	-5.418	-6.063
H	-3.524	-4.063	-6.784
C	-5.445	-3.559	-6.035
O	-6.495	-3.151	-6.670
O	-5.153	-3.172	-4.887
N	-9.416	-5.266	-4.503
H	-9.520	-6.278	-4.572
C	-10.271	-4.358	-3.899
C	-8.389	-4.582	-5.038
H	-7.597	-5.051	-5.595
N	-8.524	-3.283	-4.799
C	-9.697	-3.130	-4.086
H	-10.027	-2.151	-3.779
C	1.040	-1.198	-3.901
H	1.812	-0.540	-4.311
H	1.100	-2.171	-4.402
C	-0.337	-0.603	-4.113
C	-1.483	-1.439	-4.159
H	-1.368	-2.503	-3.968
C	-2.730	-0.938	-4.462
H	-3.599	-1.587	-4.535
C	-2.902	0.473	-4.751
O	-4.010	0.940	-5.145
H	-5.693	-0.132	-5.687
C	-0.504	0.794	-4.306
H	0.364	1.444	-4.228
C	-1.738	1.326	-4.598
H	-1.874	2.391	-4.744
C	1.527	0.540	-7.808
O	2.705	-0.029	-7.410
C	2.766	-1.454	-7.433
H	2.347	-1.857	-8.360
H	2.228	-1.887	-6.581
H	3.818	-1.733	-7.393
C	0.346	-0.188	-7.939

H	0.305	-1.241	-7.712
C	-0.787	0.483	-8.423
C	-0.763	1.861	-8.754
C	0.433	2.582	-8.573
H	0.472	3.648	-8.788
C	1.567	1.923	-8.115
H	2.515	2.440	-8.012
N	-2.051	-0.025	-8.680
C	-2.415	-1.401	-8.271
H	-3.490	-1.504	-8.421
H	-2.228	-1.482	-7.196
C	-1.656	-2.446	-9.052
H	-1.754	-2.360	-10.132
C	-0.875	-3.432	-8.577
C	-0.597	-3.715	-7.120
H	-1.024	-2.979	-6.437
H	-0.988	-4.701	-6.845
H	0.487	-3.767	-6.945
C	-0.185	-4.387	-9.519
H	-0.410	-4.167	-10.566
H	-0.482	-5.418	-9.299
H	0.903	-4.349	-9.379
C	-2.828	1.016	-9.192
C	-2.072	2.164	-9.237
C	-2.652	3.445	-9.689
H	-1.863	4.124	-10.027
O	-3.406	4.042	-8.631
H	-3.922	4.750	-9.056
C	-3.574	3.228	-10.908
O	-4.355	4.420	-11.020
H	-5.321	4.259	-10.942
C	-2.758	3.153	-12.227
O	-1.556	3.425	-12.298
C	-4.290	1.032	-9.619
H	-4.863	1.467	-8.795
C	-4.921	-0.318	-9.920
H	-5.737	-0.565	-9.247
C	-4.620	-1.189	-10.896
C	-3.533	-0.999	-11.918
H	-2.829	-1.841	-11.897
H	-3.955	-0.990	-12.931
H	-2.954	-0.085	-11.777
C	-5.430	-2.450	-11.059
H	-6.181	-2.567	-10.275
H	-5.952	-2.451	-12.025
H	-4.783	-3.339	-11.052
N	-4.397	2.007	-10.789
C	-5.322	1.844	-11.791
O	-6.377	1.224	-11.698
C	-4.951	2.483	-13.133
H	-5.526	3.413	-13.239
C	-5.231	1.540	-14.317
H	-6.274	1.581	-14.637
H	-5.030	0.506	-14.028
C	-4.232	2.008	-15.386
H	-4.644	2.849	-15.948
H	-3.991	1.216	-16.096
C	-2.988	2.468	-14.605
H	-2.511	3.352	-15.038
H	-2.227	1.683	-14.530
N	-3.516	2.763	-13.264
C	-8.624	0.626	-4.542
O	-8.290	-0.629	-4.388
O	-8.599	1.225	-5.626
C	-9.038	1.360	-3.269
H	-8.500	0.973	-2.399
H	-8.752	2.405	-3.428
Fe	-7.457	-1.743	-5.707
O	-6.330	-0.518	-6.319

^{7}IM1a

E=-3110.411203 ΔE=-0.278862

N	-10.903	-1.889	-8.579
H	-11.869	-1.704	-8.839
C	-10.033	-2.751	-9.225
C	-10.254	-1.347	-7.528
H	-10.689	-0.630	-6.847
N	-9.013	-1.818	-7.465
C	-8.865	-2.700	-8.518
H	-7.941	-3.238	-8.659
C	-4.465	-4.606	-6.814
H	-4.354	-5.483	-6.167
H	-3.480	-4.135	-6.875
C	-5.391	-3.597	-6.105
O	-6.474	-3.221	-6.691
O	-5.038	-3.178	-4.985
N	-9.433	-5.310	-4.513
H	-9.524	-6.323	-4.574

C	-10.295	-4.408	-3.910	H	-1.040	-4.736	-6.901
C	-8.421	-4.611	-5.065	H	0.438	-3.804	-6.952
H	-7.621	-5.074	-5.618	C	-0.213	-4.358	-9.550
N	-8.573	-3.312	-4.845	H	-0.422	-4.105	-10.593
C	-9.742	-3.174	-4.121	H	-0.527	-5.390	-9.361
H	-10.086	-2.197	-3.821	H	0.874	-4.338	-9.398
C	1.054	-1.182	-3.902	C	-2.798	1.060	-9.161
H	1.829	-0.521	-4.302	C	-2.027	2.197	-9.217
H	1.119	-2.151	-4.409	C	-2.592	3.481	-9.684
C	-0.321	-0.589	-4.126	H	-1.794	4.144	-10.033
C	-1.462	-1.430	-4.202	O	-3.334	4.102	-8.632
H	-1.349	-2.493	-4.006	H	-3.842	4.811	-9.066
C	-2.700	-0.937	-4.551	C	-3.521	3.264	-10.899
H	-3.563	-1.592	-4.651	O	-4.298	4.459	-11.015
C	-2.865	0.472	-4.857	H	-5.262	4.301	-10.921
O	-3.949	0.928	-5.324	C	-2.708	3.179	-12.220
H	-5.587	-0.094	-6.002	O	-1.504	3.444	-12.292
C	-0.490	0.808	-4.312	C	-4.259	1.093	-9.589
H	0.371	1.464	-4.204	H	-4.828	1.547	-8.772
C	-1.717	1.334	-4.644	C	-4.902	-0.254	-9.867
H	-1.856	2.398	-4.793	H	-5.705	-0.493	-9.175
C	1.553	0.528	-7.793	C	-4.614	-1.134	-10.838
O	2.724	-0.060	-7.401	C	-3.536	-0.954	-11.872
C	2.764	-1.485	-7.440	H	-2.863	-1.820	-11.884
H	2.337	-1.872	-8.370	H	-3.969	-0.901	-12.879
H	2.222	-1.920	-6.591	H	-2.924	-0.065	-11.714
H	3.813	-1.780	-7.406	C	-5.438	-2.388	-10.980
C	0.360	-0.181	-7.912	H	-6.167	-2.497	-10.175
H	0.304	-1.232	-7.680	H	-5.988	-2.385	-11.929
C	-0.764	0.504	-8.395	H	-4.798	-3.281	-10.988
C	-0.721	1.880	-8.735	N	-4.353	2.050	-10.773
C	0.488	2.582	-8.565	C	-5.275	1.883	-11.777
H	0.543	3.647	-8.787	O	-6.329	1.260	-11.686
C	1.614	1.908	-8.110	C	-4.906	2.522	-13.119
H	2.571	2.409	-8.018	H	-5.475	3.457	-13.218
N	-2.035	0.012	-8.644	C	-5.199	1.591	-14.309
C	-2.405	-1.366	-8.249	H	-6.244	1.641	-14.621
H	-3.482	-1.461	-8.388	H	-5.001	0.552	-14.033
H	-2.207	-1.462	-7.178	C	-4.205	2.065	-15.378
C	-1.658	-2.406	-9.050	H	-4.612	2.922	-15.921
H	-1.740	-2.288	-10.128	H	-3.978	1.285	-16.105
C	-0.899	-3.417	-8.592	C	-2.950	2.498	-14.599
C	-0.642	-3.743	-7.140	H	-2.459	3.377	-15.027
H	-1.078	-3.027	-6.442	H	-2.203	1.699	-14.532

N	-3.470	2.792	-13.254
C	-8.663	0.657	-4.551
O	-8.436	-0.626	-4.485
O	-8.601	1.305	-5.609
C	-9.033	1.362	-3.252
H	-8.494	0.933	-2.402
H	-8.731	2.407	-3.374
Fe	-7.565	-1.663	-5.932
O	-6.352	-0.425	-6.507

^{3}TS1b

E=-3110.318718 ΔE=-0.294873

N	-10.483	-1.737	-8.495
H	-11.455	-1.513	-8.667
C	-9.729	-2.677	-9.167
C	-9.693	-1.151	-7.565
H	-10.041	-0.374	-6.901
N	-8.472	-1.675	-7.592
C	-8.489	-2.633	-8.588
H	-7.616	-3.231	-8.795
C	-4.390	-4.909	-6.728
H	-4.506	-5.760	-6.051
H	-3.341	-4.620	-6.692
C	-5.165	-3.722	-6.165
O	-6.030	-3.131	-6.948
O	-4.952	-3.331	-5.010
N	-9.140	-5.069	-4.803
H	-9.307	-6.070	-4.847
C	-9.924	-4.108	-4.190
C	-8.084	-4.453	-5.367
H	-7.342	-4.992	-5.927
N	-8.123	-3.146	-5.136
C	-9.271	-2.919	-4.398
H	-9.534	-1.923	-4.081
C	1.045	-1.176	-3.757
H	1.825	-0.537	-4.183
H	1.080	-2.148	-4.263
C	-0.322	-0.542	-3.953
C	-1.483	-1.326	-3.990
H	-1.419	-2.391	-3.780
C	-2.726	-0.782	-4.321
H	-3.601	-1.422	-4.384
C	-2.825	0.582	-4.640
O	-3.971	1.135	-5.131
H	-4.578	0.437	-5.488
C	-0.466	0.839	-4.159
H	0.407	1.485	-4.092
C	-1.699	1.399	-4.486
H	-1.791	2.463	-4.673
C	1.038	0.550	-7.600
O	2.203	-0.064	-7.226
C	2.260	-1.484	-7.311
H	1.822	-1.842	-8.251
H	1.743	-1.959	-6.470
H	3.316	-1.760	-7.298
C	-0.209	-0.082	-7.590
H	-0.310	-1.090	-7.221
C	-1.314	0.639	-8.070
C	-1.169	1.954	-8.575
C	0.082	2.590	-8.517
H	0.192	3.617	-8.860
C	1.178	1.888	-8.036
H	2.172	2.325	-8.022
N	-2.639	0.226	-8.270
C	-3.093	-1.059	-7.704
H	-4.372	-0.955	-7.313
H	-2.658	-1.136	-6.706
C	-2.687	-2.171	-8.596
H	-3.012	-2.060	-9.622
C	-1.749	-3.127	-8.356
C	-1.140	-3.480	-7.026
H	-1.543	-2.919	-6.182
H	-1.277	-4.551	-6.828
H	-0.052	-3.341	-7.058
C	-1.144	-3.872	-9.521
H	-1.709	-3.733	-10.446
H	-1.043	-4.940	-9.309
H	-0.129	-3.493	-9.703
C	-3.286	1.241	-8.985
C	-2.431	2.303	-9.136
C	-2.860	3.578	-9.740
H	-1.994	4.141	-10.106
O	-3.576	4.335	-8.764
H	-4.021	5.047	-9.256
C	-3.754	3.334	-10.970
O	-4.473	4.550	-11.192
H	-5.443	4.437	-11.086
C	-2.896	3.148	-12.253

O	-1.677	3.346	-12.291
C	-4.676	1.245	-9.589
H	-5.370	1.687	-8.869
C	-5.206	-0.138	-9.938
H	-6.079	-0.424	-9.360
C	-4.756	-0.987	-10.876
C	-3.576	-0.736	-11.780
H	-2.854	-1.562	-11.720
H	-3.898	-0.700	-12.828
H	-3.038	0.185	-11.552
C	-5.479	-2.288	-11.127
H	-6.309	-2.439	-10.437
H	-5.883	-2.310	-12.147
H	-4.797	-3.146	-11.039
N	-4.643	2.165	-10.811
C	-5.518	1.970	-11.850
O	-6.578	1.356	-11.776
C	-5.086	2.542	-13.203
H	-5.621	3.489	-13.360
C	-5.371	1.568	-14.360
H	-6.402	1.643	-14.712
H	-5.227	0.537	-14.028
C	-4.324	1.958	-15.414
H	-4.686	2.795	-16.014
H	-4.094	1.134	-16.091
C	-3.084	2.394	-14.612
H	-2.559	3.242	-15.062
H	-2.360	1.582	-14.486
N	-3.638	2.761	-13.300
C	-8.177	0.688	-4.848
O	-7.594	-0.465	-4.745
O	-8.326	1.300	-5.926
C	-8.655	1.336	-3.543
H	-8.087	0.954	-2.691
H	-8.430	2.402	-3.658
Fe	-6.821	-1.654	-6.069
O	-5.462	-0.599	-6.602

^{5}TS1b

E=-3110.329365 ΔE=-0.292535

N	-10.469	-1.735	-8.472
H	-11.443	-1.515	-8.644
C	-9.708	-2.666	-9.152
C	-9.691	-1.151	-7.537
H	-10.041	-0.384	-6.862
N	-8.464	-1.668	-7.573
C	-8.469	-2.622	-8.575
H	-7.594	-3.220	-8.774
C	-4.382	-4.969	-6.659
H	-4.505	-5.839	-6.006
H	-3.336	-4.675	-6.596
C	-5.195	-3.800	-6.097
O	-6.146	-3.309	-6.822
O	-4.920	-3.335	-4.976
N	-9.240	-5.160	-4.668
H	-9.387	-6.166	-4.696
C	-10.050	-4.203	-4.082
C	-8.196	-4.527	-5.241
H	-7.436	-5.056	-5.788
N	-8.268	-3.217	-5.046
C	-9.425	-3.005	-4.319
H	-9.720	-2.010	-4.024
C	1.025	-1.175	-3.756
H	1.804	-0.537	-4.186
H	1.057	-2.147	-4.262
C	-0.344	-0.541	-3.952
C	-1.501	-1.329	-4.004
H	-1.433	-2.394	-3.798
C	-2.743	-0.792	-4.350
H	-3.612	-1.439	-4.430
C	-2.844	0.570	-4.670
O	-3.987	1.116	-5.185
H	-4.582	0.414	-5.549
C	-0.493	0.840	-4.154
H	0.375	1.491	-4.073
C	-1.725	1.394	-4.498
H	-1.819	2.458	-4.683
C	1.090	0.553	-7.615
O	2.253	-0.060	-7.235
C	2.308	-1.482	-7.302
H	1.866	-1.851	-8.235
H	1.794	-1.944	-6.452
H	3.363	-1.759	-7.291
C	-0.156	-0.081	-7.612
H	-0.256	-1.089	-7.242
C	-1.258	0.640	-8.099
C	-1.114	1.957	-8.598
C	0.137	2.593	-8.534

H	0.247	3.621	-8.875
C	1.232	1.891	-8.051
H	2.226	2.326	-8.030
N	-2.580	0.229	-8.299
C	-3.048	-1.047	-7.727
H	-4.311	-0.956	-7.368
H	-2.621	-1.125	-6.727
C	-2.654	-2.170	-8.608
H	-2.972	-2.064	-9.636
C	-1.732	-3.138	-8.356
C	-1.133	-3.481	-7.020
H	-1.561	-2.934	-6.180
H	-1.243	-4.555	-6.831
H	-0.049	-3.310	-7.040
C	-1.126	-3.893	-9.516
H	-1.716	-3.797	-10.432
H	-0.985	-4.953	-9.281
H	-0.128	-3.485	-9.730
C	-3.232	1.247	-9.000
C	-2.379	2.310	-9.152
C	-2.819	3.585	-9.747
H	-1.960	4.157	-10.113
O	-3.539	4.332	-8.765
H	-3.988	5.044	-9.252
C	-3.719	3.341	-10.974
O	-4.443	4.555	-11.190
H	-5.412	4.436	-11.079
C	-2.866	3.156	-12.260
O	-1.649	3.359	-12.303
C	-4.628	1.249	-9.593
H	-5.319	1.687	-8.867
C	-5.158	-0.133	-9.942
H	-6.027	-0.420	-9.359
C	-4.715	-0.984	-10.882
C	-3.536	-0.743	-11.789
H	-2.814	-1.568	-11.719
H	-3.858	-0.720	-12.838
H	-2.996	0.180	-11.572
C	-5.445	-2.281	-11.127
H	-6.269	-2.430	-10.429
H	-5.860	-2.300	-12.143
H	-4.766	-3.143	-11.045
N	-4.605	2.171	-10.812
C	-5.486	1.976	-11.845
O	-6.549	1.366	-11.762
C	-5.059	2.542	-13.201
H	-5.597	3.488	-13.362
C	-5.344	1.561	-14.352
H	-6.376	1.627	-14.701
H	-5.190	0.533	-14.015
C	-4.303	1.952	-15.411
H	-4.670	2.788	-16.010
H	-4.075	1.128	-16.088
C	-3.061	2.392	-14.616
H	-2.537	3.239	-15.070
H	-2.336	1.581	-14.488
N	-3.612	2.764	-13.303
C	-8.188	0.657	-4.757
O	-7.638	-0.512	-4.650
O	-8.319	1.249	-5.852
C	-8.666	1.337	-3.474
H	-8.098	0.977	-2.612
H	-8.449	2.402	-3.614
Fe	-6.898	-1.630	-6.089
O	-5.447	-0.710	-6.665

^{7}TS1b

E=-3110.323150 ΔE=-0.292984

N	-10.482	-1.746	-8.484
H	-11.457	-1.528	-8.656
C	-9.720	-2.678	-9.162
C	-9.707	-1.161	-7.548
H	-10.058	-0.393	-6.874
N	-8.480	-1.677	-7.582
C	-8.481	-2.632	-8.583
H	-7.603	-3.226	-8.783
C	-4.375	-4.962	-6.663
H	-4.513	-5.824	-6.003
H	-3.324	-4.689	-6.601
C	-5.162	-3.775	-6.104
O	-6.062	-3.224	-6.859
O	-4.922	-3.352	-4.961
N	-9.211	-5.173	-4.694
H	-9.359	-6.179	-4.724
C	-10.019	-4.216	-4.104
C	-8.162	-4.541	-5.260
H	-7.399	-5.071	-5.803
N	-8.230	-3.233	-5.058

C	-9.388	-3.019	-4.334	H	-1.012	-4.962	-9.298
H	-9.675	-2.024	-4.035	H	-0.110	-3.512	-9.714
C	1.038	-1.176	-3.758	C	-3.248	1.246	-9.000
H	1.818	-0.537	-4.183	C	-2.395	2.309	-9.149
H	1.073	-2.147	-4.265	C	-2.832	3.585	-9.746
C	-0.329	-0.540	-3.960	H	-1.971	4.152	-10.113
C	-1.491	-1.322	-4.012	O	-3.549	4.335	-8.765
H	-1.430	-2.388	-3.806	H	-3.995	5.050	-9.251
C	-2.731	-0.776	-4.351	C	-3.732	3.342	-10.973
H	-3.606	-1.415	-4.425	O	-4.453	4.558	-11.191
C	-2.824	0.589	-4.668	H	-5.422	4.442	-11.080
O	-3.965	1.145	-5.169	C	-2.879	3.156	-12.260
H	-4.557	0.452	-5.564	O	-1.662	3.356	-12.304
C	-0.470	0.842	-4.160	C	-4.643	1.249	-9.593
H	0.402	1.487	-4.079	H	-5.332	1.686	-8.865
C	-1.699	1.405	-4.498	C	-5.173	-0.132	-9.945
H	-1.787	2.470	-4.680	H	-6.041	-0.419	-9.360
C	1.073	0.550	-7.613	C	-4.730	-0.982	-10.885
O	2.235	-0.065	-7.234	C	-3.552	-0.734	-11.793
C	2.286	-1.487	-7.309	H	-2.829	-1.558	-11.732
H	1.845	-1.849	-8.245	H	-3.875	-0.700	-12.840
H	1.767	-1.952	-6.463	H	-3.013	0.188	-11.568
H	3.340	-1.767	-7.295	C	-5.456	-2.281	-11.131
C	-0.174	-0.083	-7.610	H	-6.283	-2.430	-10.436
H	-0.276	-1.091	-7.241	H	-5.867	-2.304	-12.148
C	-1.275	0.639	-8.095	H	-4.777	-3.142	-11.044
C	-1.131	1.957	-8.593	N	-4.620	2.173	-10.811
C	0.120	2.593	-8.527	C	-5.500	1.978	-11.845
H	0.232	3.622	-8.864	O	-6.562	1.367	-11.763
C	1.214	1.889	-8.046	C	-5.073	2.545	-13.201
H	2.207	2.327	-8.025	H	-5.609	3.491	-13.363
N	-2.598	0.227	-8.296	C	-5.358	1.565	-14.354
C	-3.062	-1.058	-7.736	H	-6.390	1.634	-14.704
H	-4.320	-0.935	-7.375	H	-5.208	0.536	-14.018
H	-2.637	-1.139	-6.735	C	-4.315	1.954	-15.412
C	-2.655	-2.171	-8.623	H	-4.680	2.790	-16.012
H	-2.966	-2.061	-9.654	H	-4.087	1.129	-16.088
C	-1.732	-3.139	-8.371	C	-3.074	2.393	-14.615
C	-1.142	-3.488	-7.032	H	-2.549	3.240	-15.068
H	-1.569	-2.933	-6.196	H	-2.349	1.582	-14.487
H	-1.267	-4.560	-6.839	N	-3.625	2.764	-13.303
H	-0.055	-3.331	-7.043	C	-8.217	0.671	-4.757
C	-1.121	-3.897	-9.526	O	-7.673	-0.501	-4.657
H	-1.688	-3.776	-10.453	O	-8.347	1.264	-5.853

C	-8.688	1.354	-3.475
H	-8.118	0.992	-2.615
H	-8.471	2.418	-3.612
Fe	-6.930	-1.629	-6.105
O	-5.432	-0.567	-6.665

^{3}IM1b

E=-3110.391515 ΔE=-0.281966

N	-10.786	-1.849	-8.255
H	-11.753	-1.640	-8.478
C	-9.940	-2.671	-8.975
C	-10.115	-1.381	-7.181
H	-10.545	-0.719	-6.447
N	-8.875	-1.867	-7.181
C	-8.754	-2.672	-8.298
H	-7.838	-3.196	-8.504
C	-4.537	-4.647	-6.639
H	-4.430	-5.514	-5.980
H	-3.564	-4.150	-6.667
C	-5.515	-3.659	-5.993
O	-6.516	-3.227	-6.688
O	-5.333	-3.276	-4.820
N	-9.454	-5.349	-4.447
H	-9.547	-6.365	-4.491
C	-10.328	-4.431	-3.887
C	-8.434	-4.671	-5.003
H	-7.630	-5.152	-5.531
N	-8.596	-3.366	-4.824
C	-9.777	-3.203	-4.127
H	-10.127	-2.218	-3.863
C	0.984	-1.197	-3.952
H	1.746	-0.517	-4.346
H	1.097	-2.166	-4.455
C	-0.407	-0.643	-4.223
C	-1.544	-1.464	-4.185
H	-1.449	-2.499	-3.866
C	-2.803	-1.003	-4.579
H	-3.659	-1.672	-4.561
C	-2.949	0.316	-5.033
O	-4.122	0.802	-5.535
H	-6.872	0.202	-6.263
C	-0.593	0.694	-4.604
H	0.259	1.370	-4.620
C	-1.842	1.173	-4.997
H	-1.963	2.201	-5.318
C	1.670	0.812	-7.947
O	2.866	0.273	-7.572
C	2.921	-1.147	-7.446
H	2.433	-1.647	-8.286
H	2.460	-1.476	-6.507
H	3.973	-1.426	-7.473
C	0.509	0.053	-8.066
H	0.485	-0.994	-7.815
C	-0.647	0.693	-8.526
C	-0.682	2.075	-8.824
C	0.496	2.831	-8.660
H	0.494	3.902	-8.849
C	1.660	2.201	-8.235
H	2.588	2.751	-8.123
N	-1.911	0.141	-8.744
C	-2.152	-1.215	-8.367
H	-2.740	-1.363	-7.468
H	-4.816	0.104	-5.644
C	-1.360	-2.210	-8.971
H	-1.029	-1.980	-9.984
C	-0.868	-3.385	-8.431
C	-0.905	-3.714	-6.965
H	-1.476	-2.995	-6.377
H	-1.284	-4.723	-6.779
H	0.123	-3.718	-6.573
C	-0.108	-4.351	-9.296
H	-0.112	-4.050	-10.347
H	-0.540	-5.356	-9.217
H	0.935	-4.450	-8.963
C	-2.746	1.178	-9.167
C	-2.024	2.344	-9.230
C	-2.646	3.592	-9.711
H	-1.877	4.277	-10.076
O	-3.413	4.204	-8.671
H	-3.935	4.894	-9.116
C	-3.564	3.310	-10.922
O	-4.371	4.481	-11.074
H	-5.332	4.298	-11.003
C	-2.741	3.217	-12.235
O	-1.551	3.533	-12.313
C	-4.215	1.149	-9.549
H	-4.779	1.612	-8.733
C	-4.805	-0.232	-9.760

H	-5.605	-0.470	-9.064
C	-4.465	-1.144	-10.684
C	-3.386	-0.972	-11.717
H	-2.625	-1.754	-11.603
H	-3.800	-1.091	-12.727
H	-2.878	-0.008	-11.666
C	-5.214	-2.447	-10.776
H	-5.948	-2.559	-9.976
H	-5.749	-2.520	-11.732
H	-4.520	-3.299	-10.737
N	-4.363	2.077	-10.759
C	-5.262	1.834	-11.766
O	-6.291	1.171	-11.666
C	-4.903	2.438	-13.128
H	-5.511	3.343	-13.270
C	-5.138	1.448	-14.283
H	-6.181	1.425	-14.603
H	-4.879	0.435	-13.964
C	-4.166	1.939	-15.366
H	-4.616	2.754	-15.938
H	-3.895	1.148	-16.066
C	-2.940	2.464	-14.596
H	-2.498	3.357	-15.047
H	-2.149	1.711	-14.505
N	-3.480	2.765	-13.261
C	-8.601	0.602	-4.658
O	-8.482	-0.674	-4.546
O	-8.340	1.237	-5.718
C	-9.039	1.377	-3.422
H	-8.468	1.026	-2.555
H	-8.776	2.423	-3.607
Fe	-7.511	-1.908	-5.729
O	-6.351	-0.623	-6.219

^{5}IM1b

E=-3110.405539 ΔE=-0.279345

N	-10.919	-1.906	-8.443
H	-11.886	-1.727	-8.698
C	-10.037	-2.736	-9.110
C	-10.275	-1.389	-7.371
H	-10.738	-0.709	-6.670
N	-9.028	-1.845	-7.315
C	-8.871	-2.688	-8.397
H	-7.937	-3.199	-8.567
C	-4.556	-4.612	-6.660
H	-4.427	-5.483	-6.010
H	-3.586	-4.111	-6.709
C	-5.506	-3.632	-5.959
O	-6.489	-3.122	-6.638
O	-5.290	-3.334	-4.773
N	-9.455	-5.314	-4.463
H	-9.541	-6.330	-4.518
C	-10.334	-4.411	-3.886
C	-8.437	-4.623	-5.002
H	-7.627	-5.090	-5.534
N	-8.605	-3.321	-4.795
C	-9.789	-3.176	-4.098
H	-10.147	-2.198	-3.820
C	1.026	-1.208	-3.938
H	1.793	-0.533	-4.330
H	1.135	-2.179	-4.439
C	-0.361	-0.646	-4.214
C	-1.504	-1.459	-4.173
H	-1.416	-2.494	-3.854
C	-2.759	-0.986	-4.561
H	-3.621	-1.649	-4.540
C	-2.894	0.334	-5.013
O	-4.067	0.829	-5.510
H	-6.831	0.277	-6.052
C	-0.535	0.693	-4.593
H	0.323	1.361	-4.611
C	-1.782	1.183	-4.982
H	-1.895	2.212	-5.303
C	1.672	0.814	-7.947
O	2.869	0.276	-7.573
C	2.927	-1.144	-7.448
H	2.437	-1.645	-8.288
H	2.468	-1.475	-6.509
H	3.979	-1.421	-7.479
C	0.512	0.055	-8.068
H	0.488	-0.993	-7.819
C	-0.644	0.695	-8.528
C	-0.680	2.077	-8.823
C	0.498	2.833	-8.658
H	0.495	3.905	-8.845
C	1.662	2.203	-8.234
H	2.590	2.754	-8.121
N	-1.909	0.142	-8.747

C	-2.150	-1.214	-8.369
H	-2.738	-1.360	-7.470
H	-4.765	0.135	-5.601
C	-1.358	-2.209	-8.971
H	-1.026	-1.980	-9.985
C	-0.868	-3.385	-8.430
C	-0.907	-3.713	-6.965
H	-1.473	-2.990	-6.376
H	-1.294	-4.720	-6.778
H	0.122	-3.723	-6.572
C	-0.112	-4.354	-9.295
H	-0.113	-4.052	-10.347
H	-0.550	-5.356	-9.218
H	0.931	-4.459	-8.961
C	-2.743	1.180	-9.171
C	-2.022	2.346	-9.230
C	-2.643	3.594	-9.714
H	-1.872	4.280	-10.074
O	-3.416	4.206	-8.678
H	-3.935	4.897	-9.127
C	-3.554	3.312	-10.929
O	-4.362	4.482	-11.089
H	-5.322	4.298	-11.005
C	-2.725	3.218	-12.238
O	-1.535	3.536	-12.310
C	-4.211	1.151	-9.559
H	-4.777	1.615	-8.745
C	-4.804	-0.228	-9.773
H	-5.614	-0.461	-9.088
C	-4.463	-1.141	-10.695
C	-3.375	-0.975	-11.720
H	-2.622	-1.763	-11.604
H	-3.784	-1.086	-12.733
H	-2.860	-0.015	-11.661
C	-5.223	-2.437	-10.797
H	-5.969	-2.543	-10.007
H	-5.746	-2.504	-11.760
H	-4.537	-3.295	-10.750
N	-4.353	2.079	-10.769
C	-5.248	1.836	-11.782
O	-6.277	1.174	-11.687
C	-4.882	2.439	-13.141
H	-5.489	3.345	-13.286
C	-5.111	1.448	-14.296
H	-6.153	1.424	-14.620
H	-4.852	0.436	-13.976
C	-4.135	1.940	-15.375
H	-4.584	2.756	-15.948
H	-3.863	1.150	-16.075
C	-2.912	2.465	-14.600
H	-2.468	3.357	-15.049
H	-2.122	1.712	-14.506
N	-3.458	2.766	-13.267
C	-8.599	0.653	-4.579
O	-8.494	-0.631	-4.465
O	-8.301	1.273	-5.631
C	-9.048	1.428	-3.352
H	-8.469	1.093	-2.485
H	-8.804	2.476	-3.547
Fe	-7.542	-1.826	-5.672
O	-6.327	-0.561	-6.102

^{7}IM1b

E=-3110.421315 ΔE=-0.277634

N	-10.971	-1.986	-8.459
H	-11.941	-1.826	-8.718
C	-10.068	-2.787	-9.135
C	-10.349	-1.469	-7.379
H	-10.820	-0.803	-6.670
N	-9.088	-1.891	-7.332
C	-8.904	-2.721	-8.422
H	-7.960	-3.217	-8.584
C	-4.542	-4.621	-6.673
H	-4.396	-5.489	-6.023
H	-3.579	-4.106	-6.727
C	-5.511	-3.659	-5.974
O	-6.535	-3.197	-6.629
O	-5.279	-3.330	-4.799
N	-9.507	-5.386	-4.382
H	-9.593	-6.400	-4.452
C	-10.392	-4.485	-3.811
C	-8.478	-4.688	-4.899
H	-7.659	-5.152	-5.421
N	-8.644	-3.387	-4.686
C	-9.836	-3.250	-4.002
H	-10.194	-2.274	-3.719
C	0.989	-1.188	-3.962
H	1.754	-0.508	-4.352

H	1.100	-2.155	-4.469	C	-2.684	3.599	-9.676
C	-0.399	-0.627	-4.239	H	-1.928	4.312	-10.011
C	-1.544	-1.437	-4.200	O	-3.500	4.178	-8.651
H	-1.461	-2.470	-3.871	H	-3.991	4.895	-9.085
C	-2.797	-0.968	-4.606	C	-3.559	3.301	-10.915
H	-3.658	-1.631	-4.585	O	-4.414	4.421	-11.124
C	-2.926	0.347	-5.074	H	-5.317	4.256	-10.765
O	-4.087	0.844	-5.598	C	-2.694	3.240	-12.204
H	-6.900	0.392	-5.714	O	-1.510	3.584	-12.245
C	-0.570	0.708	-4.634	C	-4.185	1.121	-9.574
H	0.288	1.376	-4.653	H	-4.771	1.572	-8.765
C	-1.812	1.194	-5.039	C	-4.742	-0.273	-9.797
H	-1.921	2.219	-5.376	H	-5.536	-0.537	-9.104
C	1.696	0.867	-7.958	C	-4.389	-1.176	-10.723
O	2.901	0.341	-7.596	C	-3.314	-0.982	-11.754
C	2.970	-1.077	-7.457	H	-2.541	-1.752	-11.645
H	2.471	-1.592	-8.282	H	-3.727	-1.101	-12.764
H	2.532	-1.402	-6.506	H	-2.822	-0.010	-11.696
H	4.024	-1.347	-7.504	C	-5.120	-2.489	-10.820
C	0.546	0.094	-8.081	H	-5.858	-2.612	-10.023
H	0.535	-0.957	-7.844	H	-5.649	-2.569	-11.778
C	-0.620	0.724	-8.527	H	-4.414	-3.331	-10.774
C	-0.682	2.110	-8.802	N	-4.321	2.041	-10.783
C	0.488	2.878	-8.639	C	-5.193	1.789	-11.816
H	0.472	3.951	-8.816	O	-6.205	1.102	-11.752
C	1.664	2.259	-8.230	C	-4.812	2.414	-13.159
H	2.585	2.822	-8.117	H	-5.429	3.314	-13.291
N	-1.874	0.150	-8.752	C	-5.000	1.440	-14.336
C	-2.098	-1.208	-8.371	H	-6.033	1.408	-14.687
H	-2.670	-1.357	-7.461	H	-4.738	0.426	-14.026
H	-4.803	0.170	-5.688	C	-4.007	1.963	-15.383
C	-1.309	-2.200	-8.977	H	-4.456	2.781	-15.952
H	-0.977	-1.972	-9.991	H	-3.706	1.189	-16.091
C	-0.824	-3.381	-8.439	C	-2.810	2.494	-14.573
C	-0.871	-3.716	-6.975	H	-2.368	3.398	-15.001
H	-1.426	-2.988	-6.382	H	-2.013	1.750	-14.469
H	-1.275	-4.717	-6.795	N	-3.392	2.773	-13.251
H	0.157	-3.747	-6.582	C	-8.556	0.600	-4.166
C	-0.075	-4.352	-9.307	O	-8.676	-0.665	-4.426
H	-0.073	-4.048	-10.358	O	-7.889	1.372	-4.895
H	-0.519	-5.352	-9.232	C	-9.236	1.157	-2.931
H	0.967	-4.465	-8.974	H	-9.103	0.477	-2.085
C	-2.727	1.178	-9.159	H	-8.734	2.102	-2.703
C	-2.033	2.362	-9.197	Fe	-7.647	-1.797	-5.767

O	-6.475	-0.408	-6.142

TS2

E=-2042.739796 ΔE=-0.215712

C	2.102	-2.480	-2.533
H	2.361	-1.836	-3.387
H	2.811	-3.321	-2.569
C	0.727	-3.070	-2.777
C	0.259	-4.095	-1.942
H	0.844	-4.401	-1.078
C	-0.902	-4.785	-2.249
H	-1.204	-5.630	-1.652
C	-1.641	-4.474	-3.406
O	-2.626	-5.295	-3.832
C	-0.090	-2.664	-3.847
H	0.221	-1.820	-4.459
C	-1.263	-3.349	-4.160
H	-1.864	-3.082	-5.021
C	0.437	-3.812	-7.773
O	1.758	-3.488	-7.580
C	2.456	-4.089	-6.487
H	2.576	-5.170	-6.629
H	1.940	-3.900	-5.539
H	3.442	-3.623	-6.469
C	-0.216	-4.838	-7.088
H	0.281	-5.410	-6.322
C	-1.530	-5.123	-7.474
C	-2.185	-4.401	-8.496
C	-1.522	-3.340	-9.129
H	-2.016	-2.763	-9.905
C	-0.216	-3.050	-8.767
H	0.343	-2.252	-9.246
N	-2.407	-6.121	-7.005
C	-2.150	-6.869	-5.813
H	-3.049	-7.419	-5.539
H	-2.262	-5.960	-4.743
C	-0.953	-7.769	-5.968
H	-1.080	-8.424	-6.830
C	0.215	-7.885	-5.317
C	0.668	-7.028	-4.174
H	-0.140	-6.448	-3.739
H	1.121	-7.635	-3.382
H	1.458	-6.335	-4.492
C	1.237	-8.888	-5.794
H	0.875	-9.481	-6.639
H	1.534	-9.571	-4.989
H	2.156	-8.377	-6.106
C	-3.566	-6.070	-7.793
C	-3.463	-5.025	-8.673
C	-4.493	-4.767	-9.701
H	-4.053	-4.222	-10.541
O	-5.575	-4.009	-9.150
H	-6.205	-3.884	-9.878
C	-5.008	-6.100	-10.296
O	-6.235	-5.874	-10.947
H	-6.981	-5.873	-10.299
C	-4.019	-6.601	-11.388
O	-2.997	-5.994	-11.723
C	-4.719	-7.066	-7.845
H	-5.572	-6.639	-7.311
C	-4.408	-8.402	-7.196
H	-5.004	-8.598	-6.306
C	-3.521	-9.330	-7.583
C	-2.658	-9.245	-8.816
H	-1.622	-9.530	-8.604
H	-2.998	-9.968	-9.569
H	-2.646	-8.255	-9.275
C	-3.364	-10.594	-6.785
H	-4.060	-10.647	-5.944
H	-3.518	-11.482	-7.411
H	-2.346	-10.681	-6.384
N	-5.132	-7.205	-9.301
C	-5.648	-8.373	-9.802
O	-6.144	-9.281	-9.130
C	-5.535	-8.538	-11.326
H	-6.464	-8.161	-11.768
C	-5.271	-9.992	-11.754
H	-6.206	-10.514	-11.961
H	-4.752	-10.533	-10.958
C	-4.372	-9.871	-12.995
H	-4.981	-9.754	-13.896
H	-3.749	-10.753	-13.142
C	-3.531	-8.609	-12.758
H	-3.294	-8.061	-13.674
H	-2.583	-8.836	-12.254
N	-4.385	-7.798	-11.875

IM2

E=-2042.774855 ΔE=-0.208762

C	2.018	-2.593	-2.705
H	2.300	-1.950	-3.552
H	2.715	-3.444	-2.730
C	0.627	-3.148	-2.965
C	0.154	-4.215	-2.188
H	0.770	-4.621	-1.391
C	-1.089	-4.787	-2.427
H	-1.423	-5.621	-1.833
C	-1.890	-4.308	-3.461
O	-3.067	-4.987	-3.742
C	-0.223	-2.635	-3.952
H	0.097	-1.780	-4.544
C	-1.475	-3.208	-4.208
H	-2.113	-2.815	-4.994
C	0.571	-3.603	-8.009
O	1.872	-3.216	-7.788
C	2.559	-3.797	-6.675
H	2.788	-4.855	-6.848
H	1.968	-3.700	-5.757
H	3.490	-3.242	-6.573
C	-0.008	-4.703	-7.390
H	0.528	-5.299	-6.667
C	-1.316	-5.028	-7.767
C	-2.051	-4.276	-8.711
C	-1.440	-3.155	-9.305
H	-1.979	-2.556	-10.032
C	-0.140	-2.826	-8.954
H	0.368	-1.974	-9.394
N	-2.115	-6.078	-7.301
C	-1.647	-6.892	-6.236
H	-2.089	-6.711	-5.263
H	-3.559	-4.538	-4.443
C	-0.491	-7.653	-6.429
H	-0.271	-7.936	-7.460
C	0.431	-8.008	-5.460
C	0.443	-7.351	-4.112
H	-0.552	-7.256	-3.670
H	1.081	-7.889	-3.408
H	0.848	-6.333	-4.184
C	1.581	-8.913	-5.776
H	1.526	-9.306	-6.794
H	1.616	-9.763	-5.081
H	2.540	-8.391	-5.661
C	-3.348	-5.982	-7.945
C	-3.331	-4.915	-8.805
C	-4.443	-4.718	-9.761
H	-4.090	-4.159	-10.631
O	-5.542	-4.017	-9.160
H	-6.201	-3.908	-9.864
C	-4.911	-6.090	-10.320
O	-6.158	-5.938	-10.955
H	-6.896	-5.920	-10.299
C	-3.924	-6.560	-11.426
O	-2.959	-5.899	-11.820
C	-4.566	-6.887	-7.864
H	-5.375	-6.276	-7.459
C	-4.425	-8.056	-6.913
H	-5.019	-7.919	-6.012
C	-3.657	-9.153	-6.991
C	-2.795	-9.539	-8.162
H	-1.773	-9.749	-7.831
H	-3.168	-10.465	-8.616
H	-2.743	-8.773	-8.938
C	-3.654	-10.130	-5.846
H	-4.283	-9.788	-5.020
H	-4.007	-11.116	-6.171
H	-2.636	-10.279	-5.465
N	-4.960	-7.184	-9.297
C	-5.415	-8.391	-9.752
O	-5.865	-9.306	-9.055
C	-5.311	-8.589	-11.271
H	-6.275	-8.298	-11.706
C	-4.942	-10.029	-11.665
H	-5.834	-10.645	-11.770
H	-4.298	-10.478	-10.903
C	-4.172	-9.860	-12.983
H	-4.870	-9.777	-13.821
H	-3.512	-10.702	-13.190
C	-3.391	-8.550	-12.808
H	-3.253	-7.992	-13.739
H	-2.401	-8.720	-12.371
N	-4.230	-7.789	-11.868

IM3

E=-2153.389639 ΔE=-0.211915

C	-0.979	-2.535	-3.416
H	-0.152	-2.435	-4.126

H	-1.367	-3.555	-3.490
C	-2.086	-1.539	-3.735
C	-3.396	-1.748	-3.268
H	-3.607	-2.597	-2.621
C	-4.441	-0.898	-3.617
H	-5.449	-1.074	-3.259
C	-4.209	0.194	-4.469
O	-5.292	0.923	-4.847
H	-5.081	1.607	-5.514
C	-1.859	-0.406	-4.530
H	-0.852	-0.188	-4.878
C	-2.900	0.455	-4.893
H	-2.700	1.323	-5.515
C	-2.305	-1.768	-8.638
O	-1.233	-2.572	-8.329
C	-1.392	-3.522	-7.279
H	-2.165	-4.260	-7.518
H	-1.641	-3.024	-6.335
H	-0.434	-4.037	-7.187
C	-3.552	-1.917	-8.046
H	-3.750	-2.704	-7.335
C	-4.551	-1.022	-8.448
C	-4.337	-0.021	-9.418
C	-3.067	0.089	-10.011
H	-2.874	0.843	-10.769
C	-2.059	-0.775	-9.612
H	-1.058	-0.706	-10.024
N	-5.865	-0.944	-8.001
C	-6.226	-1.741	-6.848
H	-5.358	-1.740	-6.182
O	-7.222	-0.957	-6.108
O	-7.842	-1.689	-5.213
C	-6.625	-3.145	-7.181
H	-7.116	-3.287	-8.138
C	-6.287	-4.196	-6.418
C	-5.573	-4.056	-5.095
H	-5.925	-3.194	-4.530
H	-5.747	-4.944	-4.477
H	-4.493	-3.925	-5.247
C	-6.555	-5.606	-6.855
H	-7.057	-5.630	-7.826
H	-7.164	-6.136	-6.112
H	-5.617	-6.166	-6.950
C	-6.504	0.097	-8.698
C	-5.583	0.672	-9.535
C	-5.932	1.893	-10.290
H	-5.233	2.060	-11.113
O	-5.910	3.005	-9.385
H	-5.953	3.844	-9.909
C	-7.328	1.736	-10.927
O	-7.817	2.985	-11.335
H	-8.002	3.519	-10.525
C	-7.256	0.841	-12.181
O	-6.209	0.323	-12.596
C	-7.934	0.651	-8.620
H	-7.877	1.575	-8.033
C	-8.957	-0.232	-7.932
H	-9.313	0.189	-6.998
C	-9.431	-1.438	-8.276
C	-9.139	-2.130	-9.578
H	-8.897	-3.188	-9.428
H	-10.037	-2.117	-10.209
H	-8.318	-1.675	-10.135
C	-10.368	-2.148	-7.331
H	-10.468	-1.612	-6.384
H	-11.365	-2.265	-7.769
H	-9.999	-3.157	-7.106
N	-8.309	1.063	-10.021
C	-9.589	1.021	-10.515
O	-10.611	0.935	-9.830
C	-9.700	1.067	-12.049
H	-9.928	2.100	-12.331
C	-10.757	0.103	-12.621
H	-11.741	0.570	-12.647
H	-10.826	-0.799	-12.006
C	-10.219	-0.236	-14.021
H	-10.489	0.553	-14.729
H	-10.618	-1.179	-14.399
C	-8.694	-0.284	-13.844
H	-8.135	0.056	-14.720
H	-8.333	-1.285	-13.583
N	-8.461	0.633	-12.718

TS3

E=-2153.379147 ΔE=-0.212665

C	-1.004	-2.513	-3.377
H	-0.185	-2.408	-4.097
H	-1.391	-3.533	-3.453

C	-2.116	-1.517	-3.679
C	-3.416	-1.723	-3.183
H	-3.612	-2.558	-2.513
C	-4.473	-0.892	-3.540
H	-5.474	-1.070	-3.164
C	-4.267	0.174	-4.430
O	-5.369	0.865	-4.832
H	-5.161	1.566	-5.484
C	-1.912	-0.399	-4.501
H	-0.912	-0.180	-4.868
C	-2.967	0.441	-4.872
H	-2.784	1.292	-5.523
C	-2.574	-1.859	-8.478
O	-1.510	-2.674	-8.163
C	-1.673	-3.591	-7.086
H	-2.457	-4.325	-7.299
H	-1.909	-3.062	-6.155
H	-0.723	-4.118	-6.984
C	-3.827	-1.993	-7.890
H	-4.034	-2.775	-7.177
C	-4.822	-1.089	-8.294
C	-4.565	-0.076	-9.242
C	-3.296	0.012	-9.842
H	-3.091	0.769	-10.594
C	-2.306	-0.873	-9.452
H	-1.306	-0.825	-9.870
N	-6.141	-0.982	-7.855
C	-6.505	-1.786	-6.662
H	-5.672	-1.644	-5.969
O	-7.597	-1.239	-5.944
O	-8.791	-1.871	-6.268
C	-6.656	-3.244	-7.022
H	-7.086	-3.455	-7.996
C	-6.221	-4.247	-6.246
C	-5.571	-4.017	-4.904
H	-5.977	-3.148	-4.386
H	-5.720	-4.882	-4.247
H	-4.495	-3.825	-5.016
C	-6.313	-5.682	-6.688
H	-6.774	-5.758	-7.677
H	-6.888	-6.278	-5.968
H	-5.319	-6.144	-6.755
C	-6.722	0.115	-8.516
C	-5.775	0.669	-9.345
C	-6.064	1.884	-10.138
H	-5.328	2.013	-10.936
O	-6.055	3.022	-9.267
H	-6.060	3.846	-9.816
C	-7.431	1.734	-10.835
O	-7.898	2.975	-11.286
H	-8.087	3.531	-10.493
C	-7.298	0.813	-12.069
O	-6.227	0.303	-12.429
C	-8.112	0.783	-8.499
H	-7.953	1.763	-8.040
C	-9.272	0.157	-7.775
H	-9.752	0.808	-7.050
C	-9.769	-1.122	-7.899
C	-9.338	-2.049	-9.004
H	-9.345	-3.080	-8.646
H	-10.065	-1.994	-9.822
H	-8.350	-1.822	-9.407
C	-11.090	-1.441	-7.249
H	-11.370	-0.671	-6.530
H	-11.877	-1.505	-8.003
H	-11.050	-2.409	-6.738
N	-8.450	1.080	-9.955
C	-9.694	0.963	-10.507
O	-10.749	0.825	-9.875
C	-9.744	1.004	-12.043
H	-9.972	2.037	-12.333
C	-10.765	0.028	-12.657
H	-11.756	0.477	-12.722
H	-10.843	-0.879	-12.050
C	-10.164	-0.295	-14.036
H	-10.405	0.502	-14.745
H	-10.542	-1.235	-14.442
C	-8.649	-0.338	-13.788
H	-8.050	0.003	-14.639
H	-8.297	-1.336	-13.507
N	-8.474	0.585	-12.656

IM4

E=-2153.400721 ΔE=-0.212158

C	-1.004	-2.511	-3.378
H	-0.187	-2.404	-4.098
H	-1.391	-3.532	-3.454
C	-2.119	-1.516	-3.678

C	-3.415	-1.720	-3.174	H	-5.284	-6.115	-6.741
H	-3.607	-2.552	-2.499	C	-6.696	0.125	-8.519
C	-4.475	-0.893	-3.532	C	-5.749	0.676	-9.347
H	-5.473	-1.070	-3.147	C	-6.049	1.893	-10.135
C	-4.276	0.166	-4.430	H	-5.324	2.026	-10.942
O	-5.382	0.850	-4.836	O	-6.035	3.030	-9.264
H	-5.176	1.553	-5.486	H	-6.052	3.855	-9.812
C	-1.920	-0.403	-4.507	C	-7.427	1.739	-10.817
H	-0.922	-0.184	-4.881	O	-7.900	2.977	-11.270
C	-2.978	0.433	-4.879	H	-8.091	3.535	-10.478
H	-2.800	1.279	-5.538	C	-7.306	0.814	-12.049
C	-2.568	-1.878	-8.476	O	-6.238	0.309	-12.423
O	-1.506	-2.694	-8.155	C	-8.076	0.792	-8.466
C	-1.674	-3.607	-7.077	H	-7.911	1.778	-8.021
H	-2.457	-4.341	-7.291	C	-9.195	0.169	-7.701
H	-1.913	-3.076	-6.148	H	-9.770	0.845	-7.076
H	-0.725	-4.135	-6.971	C	-9.586	-1.271	-7.671
C	-3.826	-2.011	-7.898	C	-9.274	-2.048	-8.955
H	-4.040	-2.791	-7.186	H	-9.449	-3.110	-8.777
C	-4.814	-1.102	-8.305	H	-9.952	-1.741	-9.753
C	-4.546	-0.081	-9.246	H	-8.247	-1.916	-9.302
C	-3.273	0.004	-9.835	C	-11.057	-1.419	-7.279
H	-3.057	0.766	-10.579	H	-11.273	-0.789	-6.417
C	-2.290	-0.888	-9.444	H	-11.700	-1.104	-8.096
H	-1.285	-0.840	-9.852	H	-11.282	-2.459	-7.029
N	-6.135	-0.987	-7.877	N	-8.436	1.090	-9.923
C	-6.569	-1.772	-6.695	C	-9.677	0.922	-10.454
H	-5.807	-1.590	-5.931	O	-10.709	0.714	-9.797
O	-7.733	-1.233	-6.106	C	-9.755	0.988	-11.989
O	-8.917	-1.951	-6.529	H	-9.985	2.025	-12.260
C	-6.659	-3.240	-7.032	C	-10.780	0.019	-12.608
H	-7.081	-3.472	-8.005	H	-11.771	0.470	-12.662
C	-6.214	-4.228	-6.244	H	-10.854	-0.894	-12.010
C	-5.574	-3.986	-4.900	C	-10.189	-0.291	-13.994
H	-5.974	-3.109	-4.394	H	-10.431	0.513	-14.694
H	-5.735	-4.844	-4.236	H	-10.572	-1.226	-14.406
H	-4.495	-3.807	-5.007	C	-8.673	-0.341	-13.754
C	-6.284	-5.666	-6.681	H	-8.076	-0.004	-14.605
H	-6.738	-5.754	-7.672	H	-8.327	-1.343	-13.474
H	-6.856	-6.266	-5.961	N	-8.489	0.579	-12.621

Harmonic frequencies (cm^{-1}) and normalised normal coordinates:

	1	2	3	4	5	6	7	8	9
Frequencies	-885.6525	45.5708	58.3045	71.3427	79.3486	91.1964	101.8715	108.2489	121.4090

Coord atom element:

1	C	0.00405	0.00198	0.00160	-0.00210	0.00215	-0.00790	0.00334	0.00625	0.00124
2	C	0.00205	0.00235	-0.00203	0.00191	-0.00124	0.00198	0.00040	-0.00113	-0.00047
3	C	-0.00017	0.00365	-0.00333	0.00373	-0.00096	0.00230	0.00278	0.00903	0.01833
4	H	0.00336	0.00260	-0.00014	-0.00029	0.00140	-0.00545	0.00359	0.00831	0.00804
5	H	0.00085	0.00282	-0.00360	0.00462	-0.00166	0.00493	0.00103	0.00554	0.01448
6	H	-0.00002	0.00406	-0.00519	0.00646	-0.00166	0.00565	0.00334	0.01505	0.03282
7	C	0.00289	0.00375	0.01846	-0.02168	0.01845	-0.05732	0.01873	0.03825	0.00076
8	C	0.00130	0.00265	-0.00466	0.00460	-0.00670	0.01462	-0.00706	-0.03046	-0.03828
9	C	0.00243	0.00662	-0.00509	0.00639	-0.00015	0.00052	0.00748	0.02604	0.04633
10	H	0.00170	0.00306	0.01724	-0.02200	0.01732	-0.05545	0.01670	0.03113	-0.00834
11	H	0.00098	0.00084	-0.00120	0.00114	-0.00575	0.01082	-0.00854	-0.03914	-0.05707
12	H	0.00013	0.00491	-0.00296	0.00383	0.00024	-0.00162	0.00550	0.01705	0.02913
13	H	0.00486	0.00158	0.02833	-0.02998	0.02592	-0.07636	0.02388	0.05137	0.00275
14	H	0.00258	0.00072	0.00300	-0.00165	-0.00075	-0.00006	-0.00321	-0.02000	-0.03623
15	H	0.00009	0.00635	-0.00110	0.00075	0.00532	-0.01480	0.01346	0.04404	0.06203
16	C	0.00238	0.00203	0.03116	-0.03423	0.02871	-0.08436	0.02633	0.05548	0.00253
17	C	0.00066	0.00829	-0.02630	0.02409	-0.02353	0.05462	-0.01789	-0.05927	-0.04632
18	C	0.00043	0.01598	-0.01753	0.02351	-0.00638	0.02024	0.00951	0.03760	0.08078
19	C	0.00069	0.00443	0.04208	-0.03837	0.03908	-0.10451	0.03550	0.08369	0.02243
20	C	0.00427	0.01489	-0.03744	0.03562	-0.03190	0.07222	-0.01997	-0.07096	-0.04735
21	C	-0.00411	0.02437	-0.02196	0.03144	-0.00839	0.02483	0.01350	0.04208	0.09036
22	H	-0.00224	0.00909	0.04292	-0.03581	0.04205	-0.10954	0.04025	0.09800	0.03369
23	H	-0.00290	0.01667	-0.03049	0.03232	-0.02766	0.06259	-0.01481	-0.06280	-0.04128
24	H	-0.00351	0.02177	-0.01993	0.02831	-0.00890	0.02458	0.01215	0.03524	0.08455
25	C	-0.01084	0.00059	0.05535	-0.05020	0.04711	-0.12187	0.03937	0.09139	0.02507
26	C	0.00493	0.01862	-0.05122	0.04628	-0.03990	0.08874	-0.02416	-0.07990	-0.05226
27	C	-0.00760	0.03345	-0.02955	0.04393	-0.01004	0.03178	0.01685	0.05246	0.10191
28	H	0.00506	-0.00004	0.05814	-0.05159	0.05023	-0.12645	0.04212	0.10378	0.04105
29	H	-0.00028	0.01934	-0.05264	0.04995	-0.04119	0.09377	-0.02526	-0.08349	-0.05647
30	H	-0.00719	0.03364	-0.03002	0.04790	-0.01076	0.03599	0.01585	0.04972	0.09709
31	C	0.02472	-0.00060	0.05188	-0.05273	0.03951	-0.10982	0.03331	0.06345	0.00830
32	C	0.02763	0.01791	-0.05776	0.04738	-0.04089	0.08711	-0.02668	-0.07607	-0.05896
33	C	0.01707	0.03480	-0.03116	0.04726	-0.00710	0.02729	0.01859	0.06756	0.10752
34	O	-0.02944	0.00607	0.06040	-0.06297	0.04095	-0.11934	0.04021	0.06251	0.02408
35	O	-0.03928	0.01169	-0.06563	0.05501	-0.04359	0.09433	-0.03270	-0.07706	-0.07235
36	O	-0.02042	0.03275	-0.01935	0.04940	0.00489	0.01225	0.02333	0.08661	0.10043
37	C	0.01989	-0.00085	0.03299	-0.04096	0.02794	-0.08953	0.02419	0.04275	-0.01415
38	C	-0.00398	0.01116	-0.03942	0.03330	-0.03209	0.07255	-0.02325	-0.06861	-0.04834
39	C	0.00222	0.01978	-0.02324	0.03148	-0.00797	0.02685	0.01058	0.04813	0.09619
40	H	0.00965	0.00051	0.02636	-0.03803	0.02330	-0.08116	0.02065	0.02993	-0.02589
41	H	-0.00332	0.00912	-0.03542	0.02895	-0.03022	0.06727	-0.02259	-0.06660	-0.04838
42	H	-0.00119	0.01753	-0.02184	0.02764	-0.00837	0.02410	0.00947	0.04438	0.09070
43	C	-0.00080	-0.00462	0.04456	-0.05061	0.03419	-0.10241	0.02694	0.04643	-0.01374

44	C	-0.00837	0.01504	-0.05649	0.04548	-0.04181	0.09135	-0.02856	-0.07815	-0.05260
45	C	0.00808	0.02877	-0.03290	0.04363	-0.01064	0.03408	0.01360	0.05933	0.10849
46	H	0.00160	-0.00785	0.04634	-0.05484	0.03373	-0.10167	0.02426	0.03669	-0.02205
47	H	-0.00886	0.01085	-0.05806	0.04401	-0.04194	0.09006	-0.03007	-0.07500	-0.05229
48	H	0.00530	0.02915	-0.03527	0.04598	-0.01107	0.03392	0.01443	0.06558	0.11200
49	C	0.00058	0.10346	0.04606	-0.04380	0.07624	0.00548	-0.01602	-0.08459	-0.01655
50	C	0.00212	0.04807	-0.15142	-0.04673	-0.09806	-0.06517	0.02694	0.04442	0.08827
51	C	-0.00124	0.05534	0.03247	0.05918	0.06900	0.07408	-0.00217	0.07792	0.12638
52	O	-0.00080	0.10627	0.04397	-0.04137	0.08151	0.00823	-0.01803	-0.08678	-0.03143
53	O	-0.00045	0.04990	-0.14213	-0.05863	-0.12533	-0.09082	0.04481	0.04358	0.12576
54	O	-0.00083	0.04523	0.03439	0.04971	0.07253	0.07893	-0.01091	0.07528	0.15490
55	C	-0.00017	0.10581	0.04104	-0.03967	0.06777	-0.00486	-0.00770	-0.08170	-0.03166
56	C	-0.00031	0.04739	-0.12467	-0.05236	-0.12240	-0.08661	0.04752	0.03925	0.13598
57	C	0.00043	0.04272	0.04061	0.04952	0.07788	0.08485	-0.01513	0.06889	0.15807
58	H	0.00186	0.10708	0.03711	-0.04397	0.05282	-0.01785	0.00196	-0.07992	-0.01411
59	H	0.00001	0.04772	-0.12752	-0.05360	-0.12540	-0.08933	0.04879	0.04026	0.13803
60	H	-0.00005	0.03789	0.05937	0.05722	0.09123	0.09734	-0.02008	0.06216	0.15396
61	H	-0.00050	0.10256	0.04151	-0.03381	0.06844	-0.00388	-0.00651	-0.07554	-0.03705
62	H	0.00125	0.04182	-0.10873	-0.04414	-0.10640	-0.07125	0.04044	0.03159	0.12266
63	H	0.00120	0.04262	0.03779	0.05077	0.07477	0.08210	-0.01261	0.07334	0.15789
64	H	-0.00020	0.10493	0.04330	-0.03782	0.07463	0.00105	-0.01152	-0.08199	-0.03818
65	H	0.00015	0.04713	-0.12969	-0.05567	-0.13804	-0.09912	0.05641	0.04144	0.14992
66	H	0.00103	0.04893	0.03413	0.04229	0.07672	0.08287	-0.01696	0.06612	0.16647
67	C	0.00155	0.11211	0.04398	-0.05561	0.04685	-0.02572	0.00393	-0.08459	-0.01252
68	C	0.00068	0.03793	-0.14603	-0.02510	-0.08216	-0.03826	0.01456	0.04486	0.06375
69	C	0.00086	0.04584	0.02926	0.07816	0.05551	0.07914	0.00186	0.08407	0.10044
70	H	-0.00090	0.11576	0.04213	-0.06019	0.03058	-0.04531	0.01781	-0.08475	-0.02013
71	H	0.00108	0.03520	-0.14243	-0.02589	-0.09517	-0.04219	0.01852	0.03909	0.06476
72	H	0.00352	0.04183	0.03372	0.07947	0.05589	0.08751	-0.00369	0.07892	0.10604
73	C	0.00772	0.10541	0.04482	-0.05906	0.03873	-0.02412	0.00372	-0.07867	0.00431
74	C	0.00156	0.04241	-0.15308	-0.01804	-0.05047	-0.02437	-0.00074	0.04007	0.03015
75	C	-0.00175	0.05590	0.00948	0.07826	0.03620	0.05273	0.01609	0.07894	0.05897
76	C	0.00198	0.09999	0.05271	-0.04888	0.06331	0.00676	-0.01636	-0.07895	0.01806
77	C	-0.00093	0.04213	-0.14365	-0.02203	-0.01682	-0.02856	-0.00446	0.03950	0.01205
78	C	0.00236	0.05937	0.01837	0.07459	0.04891	0.03390	0.02627	0.08013	0.03893
79	C	-0.00095	0.10497	0.05245	-0.04302	0.10140	0.03225	-0.03640	-0.08665	0.01119
80	C	-0.00128	0.03679	-0.13179	-0.03238	-0.03316	-0.03665	0.00243	0.03928	0.03242
81	C	0.00160	0.04652	0.03260	0.06389	0.05427	0.04222	0.01830	0.07731	0.06392
82	H	-0.00166	0.10459	0.04984	-0.04106	0.11735	0.04899	-0.04871	-0.08541	0.02124
83	H	-0.00106	0.03121	-0.12114	-0.03421	-0.01610	-0.03066	-0.00367	0.03201	0.02242
84	H	0.00396	0.04144	0.04438	0.06284	0.05701	0.03618	0.02195	0.07227	0.05097
85	C	-0.00100	0.10050	0.04741	-0.04024	0.10118	0.02926	-0.03448	-0.08616	-0.00876
86	C	-0.00078	0.04250	-0.13984	-0.04422	-0.07134	-0.05602	0.01800	0.04292	0.06759
87	C	0.00043	0.04828	0.03222	0.05826	0.06399	0.06025	0.00492	0.08095	0.10550

88	H	-0.00235	0.10221	0.05641	-0.03276	0.12960	0.04952	-0.04767	-0.08850	-0.01655
89	H	-0.00089	0.04087	-0.13967	-0.05286	-0.08379	-0.06595	0.02335	0.04221	0.08102
90	H	-0.00009	0.04555	0.04282	0.05355	0.07541	0.06665	-0.00189	0.07774	0.11822
91	N	0.00067	0.10843	0.03926	-0.06634	0.00856	-0.04400	0.02245	-0.06506	0.01444
92	N	-0.00335	0.03859	-0.14756	-0.00684	-0.03146	-0.01041	-0.01496	0.01907	0.00013
93	N	0.02135	0.05844	0.00605	0.08766	0.01794	0.04371	0.02359	0.05962	0.02787
94	C	0.01707	0.09843	0.03300	-0.06084	-0.00883	-0.07884	0.04803	-0.05395	0.00921
95	C	-0.04375	0.03329	-0.12273	0.00717	-0.05147	0.01496	-0.01238	-0.01893	-0.00166
96	C	-0.07757	0.05455	0.02496	0.09143	0.00994	0.06390	0.02002	0.03176	0.03022
97	H	0.01212	0.10098	0.03087	-0.05626	-0.01988	-0.08311	0.06080	-0.05886	0.01092
98	H	0.08701	0.01975	-0.11723	0.00253	-0.03557	0.02115	-0.03249	-0.00930	-0.01465
99	H	0.13150	0.03324	0.03681	0.10074	0.00722	0.05901	0.02315	0.03474	0.01349
100	H	-0.23868	0.04886	0.05427	-0.05495	0.02666	-0.10038	0.04511	0.02108	0.01273
101	H	0.45771	0.01275	-0.10065	0.02923	-0.05963	0.06634	-0.02899	-0.06125	-0.02980
102	H	0.83187	0.04528	-0.02428	0.07060	-0.00691	0.06123	0.00663	0.03397	0.05027
103	C	0.00262	0.10443	0.02746	-0.05321	-0.02917	-0.07182	0.06366	-0.07830	0.02081
104	C	-0.00547	0.04203	-0.13040	0.01189	-0.07634	0.01696	0.00658	-0.04514	0.00889
105	C	-0.00867	0.06514	0.02752	0.08952	-0.00253	0.09671	0.01605	-0.01595	0.03442
106	H	0.03304	0.10484	0.01831	-0.06011	-0.04285	-0.06829	0.06572	-0.10303	0.02013
107	H	-0.00644	0.03320	-0.13465	0.00720	-0.06971	0.00161	0.00181	-0.02512	0.00308
108	H	-0.02176	0.07241	0.03211	0.09407	-0.00499	0.10658	0.01908	-0.02579	0.03721
109	C	0.00179	0.10329	0.03150	-0.04309	-0.02689	-0.06710	0.06533	-0.07045	0.02407
110	C	-0.00308	0.04735	-0.12612	0.02426	-0.09146	0.04096	0.01436	-0.07804	0.02037
111	C	-0.00041	0.06669	0.02041	0.07458	-0.01005	0.09369	0.01613	-0.03822	0.03265
112	C	-0.00155	0.09362	0.03324	-0.03410	-0.01647	-0.06829	0.06122	-0.04169	0.02330
113	C	-0.00121	0.04989	-0.11157	0.03000	-0.09177	0.05477	0.01552	-0.09354	0.02208
114	C	-0.00134	0.06955	0.00921	0.06615	-0.01443	0.08395	0.01797	-0.04028	0.03248
115	H	0.00080	0.08430	0.02866	-0.02991	-0.01298	-0.06642	0.05607	-0.02925	0.02160
116	H	0.00405	0.04545	-0.11540	0.03293	-0.09136	0.05680	0.01162	-0.08995	0.01880
117	H	-0.00323	0.06015	0.00677	0.07118	-0.00831	0.08525	0.01356	-0.02297	0.03354
118	H	0.00003	0.08310	0.04267	-0.02562	-0.00791	-0.05847	0.05552	-0.03160	0.02215
119	H	0.00170	0.05027	-0.09822	0.03326	-0.08856	0.06110	0.01556	-0.09929	0.02203
120	H	-0.00007	0.07549	0.01303	0.06352	-0.01744	0.08308	0.02120	-0.05096	0.03263
121	H	-0.00142	0.09246	0.02446	-0.03535	-0.01925	-0.06977	0.05964	-0.04108	0.02285
122	H	0.00096	0.05288	-0.10589	0.02763	-0.09062	0.05288	0.01790	-0.09711	0.02223
123	H	0.00132	0.07918	-0.00127	0.05886	-0.02185	0.07602	0.02224	-0.05052	0.03446
124	C	0.00060	0.10158	0.03288	-0.04032	-0.03300	-0.05497	0.06812	-0.09165	0.02936
125	C	-0.00067	0.04554	-0.11845	0.03374	-0.09160	0.05414	0.01600	-0.08772	0.02625
126	C	0.00061	0.07013	0.01396	0.05958	-0.02000	0.08766	0.01984	-0.06291	0.03352
127	H	0.00281	0.09913	0.03356	-0.04287	-0.03612	-0.05298	0.07061	-0.10547	0.03226
128	H	-0.00114	0.04722	-0.11703	0.03396	-0.08907	0.05056	0.01652	-0.08103	0.02487
129	H	0.00039	0.06968	0.01258	0.05983	-0.02008	0.08817	0.01829	-0.06172	0.03312
130	H	0.00307	0.09936	0.04434	-0.02948	-0.02576	-0.04333	0.06509	-0.08739	0.03159
131	H	-0.00022	0.04395	-0.12033	0.03218	-0.09373	0.05553	0.01506	-0.09350	0.02716

132	H	-0.00054	0.06913	0.00780	0.05328	-0.02463	0.08301	0.02037	-0.06902	0.03291
133	H	0.00032	0.10211	0.02745	-0.04389	-0.03489	-0.06017	0.06791	-0.08998	0.02745
134	H	-0.00018	0.04297	-0.10987	0.03748	-0.08902	0.06157	0.01689	-0.09364	0.02929
135	H	0.00158	0.06926	0.01096	0.05375	-0.02316	0.08190	0.02215	-0.06990	0.03397
136	C	-0.00921	0.11631	0.03486	-0.07082	0.00723	-0.01773	0.00978	-0.05858	0.03769
137	C	0.00474	0.02639	-0.12685	-0.00134	0.02197	-0.01620	-0.02184	0.01249	-0.03176
138	C	0.00351	0.05241	0.01117	0.08554	0.02180	0.00826	0.03702	0.05289	-0.01463
139	C	-0.00034	0.10141	0.04877	-0.05693	0.03900	0.00595	-0.01387	-0.06997	0.04453
140	C	-0.00199	0.03518	-0.12504	-0.00814	0.03888	-0.02157	-0.01705	0.02311	-0.03044
141	C	0.00458	0.05854	0.01424	0.08066	0.04470	0.00598	0.04126	0.06614	-0.01342
142	C	-0.00023	0.09668	0.04955	-0.03866	0.03891	0.01875	-0.02379	-0.04595	0.05647
143	C	-0.00037	0.02457	-0.10476	-0.00707	0.09409	-0.01568	-0.01368	0.00986	-0.03085
144	C	0.00033	0.05881	0.01659	0.06277	0.05691	-0.00765	0.05065	0.04015	-0.02737
145	H	0.00150	0.08801	0.05340	-0.02096	0.04318	0.02640	-0.02103	-0.02938	0.06103
146	H	-0.00161	0.02658	-0.10584	-0.02124	0.10089	-0.01243	-0.03427	0.00911	-0.02402
147	H	0.00168	0.05532	0.01998	0.06227	0.06388	-0.00137	0.03786	0.04694	-0.01962
148	O	0.00044	0.08550	0.05400	-0.03584	0.05222	0.01693	-0.00571	-0.05932	0.05523
149	O	-0.00052	0.01704	-0.09607	0.01136	0.10364	-0.01622	0.01328	0.00816	-0.03353
150	O	0.00011	0.05649	0.01545	0.03435	0.07361	-0.00805	0.04382	0.00806	-0.01762
151	H	-0.00033	0.09696	0.05836	-0.02997	0.05415	0.01971	-0.00533	-0.05208	0.05767
152	H	-0.00013	0.01549	-0.09230	0.00385	0.10729	-0.01380	0.01196	0.00124	-0.02724
153	H	0.00068	0.04652	0.01228	0.02824	0.07238	-0.01013	0.04319	0.00066	-0.01882
154	C	-0.00024	0.09687	0.03422	-0.03196	-0.00655	0.01138	-0.05646	0.00127	0.02805
155	C	-0.00000	0.02036	-0.09714	-0.01142	0.12419	-0.01007	-0.01000	-0.00365	-0.01618
156	C	0.00004	0.06311	0.01325	0.07001	0.02751	-0.01886	0.07104	0.03248	-0.04606
157	O	0.00006	0.08944	0.03300	-0.01490	0.00005	0.00776	-0.04643	0.01102	0.01100
158	O	0.00022	0.01744	-0.08899	-0.00978	0.18279	-0.00132	0.01246	-0.03547	0.01252
159	O	0.00029	0.07228	0.01272	0.04244	0.03395	-0.01247	0.06657	0.00566	-0.01138
160	H	-0.00130	0.08722	0.03699	-0.02665	-0.01275	0.01101	-0.05481	0.00562	0.02163
161	H	0.00011	0.01111	-0.06021	-0.00244	0.11540	-0.00280	0.01752	-0.02407	0.00753
162	H	-0.00109	0.06865	0.01503	0.02907	0.02279	-0.00903	0.05965	-0.00150	0.00089
163	C	-0.00024	0.08892	0.03080	-0.01115	-0.02687	0.00236	-0.08601	0.05012	-0.02663
164	C	-0.00018	0.02420	-0.09204	-0.01585	0.12074	-0.00848	-0.04597	0.02089	-0.01576
165	C	-0.00010	0.05318	0.00608	0.09272	0.01443	-0.02880	0.07207	0.06275	-0.10065
166	O	-0.00026	0.07431	0.02362	-0.00234	-0.01595	0.00224	-0.06384	0.04415	-0.03023
167	O	0.00037	0.03450	-0.08453	-0.01748	0.10526	-0.01018	-0.07984	0.04152	-0.02454
168	O	0.00056	0.02892	-0.00096	0.11525	0.02041	-0.03255	0.07393	0.08817	-0.13294
169	C	-0.00172	0.11288	0.01941	-0.08094	-0.02403	0.00868	0.01428	-0.01760	0.02531
170	C	-0.00077	0.02701	-0.10434	0.00781	0.05959	-0.03561	-0.02677	-0.02580	-0.02677
171	C	-0.00008	0.06142	0.01196	0.09016	0.00348	-0.02638	0.06526	0.02695	-0.04643
172	H	-0.00324	0.11358	0.02467	-0.08775	-0.01123	-0.00290	0.03545	-0.03651	0.02335
173	H	-0.00410	0.03711	-0.08888	0.01973	0.06502	-0.07528	-0.05076	-0.07210	-0.00396
174	H	0.00012	0.05372	0.01025	0.06673	0.01702	-0.01168	0.11769	0.03474	-0.06592
175	C	0.00133	0.10390	0.00812	-0.10719	-0.05157	0.06658	0.07014	0.04153	-0.02599

176	C	0.00051	0.02761	-0.10415	0.01916	0.03813	-0.04644	-0.04382	-0.03520	-0.02546
177	C	0.00099	0.06471	0.01480	0.12767	-0.02909	-0.08079	-0.00093	-0.02200	-0.01450
178	H	0.00134	0.09663	0.01006	-0.12050	-0.05091	0.08594	0.09544	0.06162	-0.04113
179	H	0.00017	0.02690	-0.10018	0.04654	0.03507	-0.09854	-0.09800	-0.08096	0.01508
180	H	0.00049	0.05867	0.01612	0.12699	-0.02872	-0.08102	0.00364	-0.01906	-0.01582
181	C	0.00024	0.10938	0.00810	-0.11799	-0.06568	0.09550	0.09478	0.06335	-0.05304
182	C	-0.00041	0.02884	-0.10532	-0.00455	0.03252	0.00014	0.00171	0.00303	-0.06600
183	C	0.00027	0.07433	0.01802	0.16123	-0.04751	-0.12893	-0.05786	-0.06717	0.02228
184	C	0.00015	0.11691	0.00899	-0.10076	-0.07278	0.08489	0.06869	0.04886	-0.04060
185	C	0.00025	0.02827	-0.11004	-0.03890	0.03850	0.06390	0.06246	0.05249	-0.11839
186	C	0.00046	0.08110	0.01825	0.17504	-0.05246	-0.13614	-0.07508	-0.07692	0.02967
187	H	0.00047	0.11699	0.00958	-0.10863	-0.07257	0.09492	0.07934	0.05528	-0.04623
188	H	0.00120	0.03257	-0.10586	-0.05303	0.03398	0.08856	0.08183	0.06291	-0.12644
189	H	0.00033	0.08571	0.01912	0.18785	-0.05957	-0.14307	-0.09670	-0.09070	0.04412
190	H	0.00205	0.12309	0.01061	-0.10494	-0.07795	0.10379	0.07467	0.05527	-0.04670
191	H	0.00017	0.02580	-0.10940	-0.03916	0.04115	0.06619	0.06588	0.05809	-0.12324
192	H	0.00041	0.07935	0.01815	0.17527	-0.05235	-0.14563	-0.08146	-0.08409	0.03788
193	H	-0.00115	0.11738	0.00829	-0.08172	-0.07344	0.05706	0.03835	0.03146	-0.02401
194	H	0.00073	0.02743	-0.10849	-0.04178	0.03896	0.07116	0.06977	0.05970	-0.12451
195	H	0.00036	0.07845	0.01860	0.16381	-0.04914	-0.11553	-0.05614	-0.05807	0.01184
196	C	0.00016	0.10083	0.00746	-0.14092	-0.07014	0.13479	0.14162	0.09918	-0.09435
197	C	0.00018	0.02934	-0.09731	0.01797	0.02135	-0.03019	-0.02393	-0.02112	-0.04722
198	C	-0.00005	0.07614	0.02362	0.19736	-0.06245	-0.18119	-0.10600	-0.11096	0.05679
199	H	0.00030	0.09308	0.00440	-0.15586	-0.06407	0.15319	0.15735	0.11450	-0.10659
200	H	0.00046	0.03224	-0.09561	0.03633	0.01647	-0.06143	-0.05688	-0.04909	-0.02194
201	H	-0.00007	0.06935	0.02060	0.18575	-0.05737	-0.16752	-0.09450	-0.09994	0.04780
202	H	0.00001	0.10189	0.01060	-0.13377	-0.07427	0.13018	0.14202	0.09671	-0.09506
203	H	0.00063	0.02942	-0.10087	0.00627	0.02691	-0.01374	-0.01061	-0.00733	-0.05728
204	H	0.00015	0.07493	0.02652	0.21069	-0.06769	-0.20199	-0.12463	-0.12895	0.07049
205	H	0.00035	0.09727	0.00635	-0.14645	-0.06855	0.14282	0.14939	0.10603	-0.10070
206	H	0.00109	0.02568	-0.09484	0.02211	0.01523	-0.03251	-0.01813	-0.01972	-0.05544
207	H	-0.00054	0.08414	0.02778	0.21329	-0.06857	-0.20222	-0.12498	-0.12879	0.07232
208	N	0.00038	0.11573	0.02259	-0.05857	-0.03586	0.01039	-0.07184	0.00242	0.04349
209	N	0.00010	0.01704	-0.09737	-0.00575	0.10799	-0.01427	0.00215	-0.01075	-0.02661
210	N	0.00016	0.06031	0.00918	0.07761	0.00296	-0.02717	0.08430	0.02400	-0.05736
211	C	-0.00017	0.10448	0.02956	-0.02860	-0.07194	0.00190	-0.09348	0.04322	-0.00698
212	C	-0.00044	0.01886	-0.09534	-0.00913	0.12913	-0.01087	0.01098	-0.02117	-0.00867
213	C	-0.00015	0.06235	0.00211	0.06669	-0.01344	-0.02847	0.09686	0.01061	-0.06027
214	O	0.00019	0.10088	0.02666	-0.02491	-0.09273	0.00250	-0.07190	0.04552	-0.01637
215	O	0.00014	0.01791	-0.09406	-0.02506	0.13134	-0.00621	0.00119	-0.03008	0.00261
216	O	-0.00001	0.05744	0.00186	0.05041	-0.02727	-0.02267	0.09964	0.00029	-0.05291
217	C	-0.00026	0.09559	0.02731	-0.01541	-0.06018	-0.00301	-0.14654	0.09124	-0.05850
218	C	-0.00008	0.02285	-0.08853	-0.00885	0.14020	-0.00718	-0.00295	-0.01109	0.00703
219	C	0.00002	0.06105	0.00287	0.06957	-0.01498	-0.02967	0.09805	0.01484	-0.07062

220	H	-0.00016	0.08806	0.02545	-0.01195	-0.04949	-0.00292	-0.14009	0.09028	-0.06160
221	H	-0.00023	0.01967	-0.08698	-0.01170	0.15345	-0.00336	0.01348	-0.02844	0.03073
222	H	0.00026	0.07231	0.00805	0.06175	-0.02593	-0.02699	0.10408	-0.00064	-0.04183
223	C	-0.00004	0.09363	0.02315	-0.01099	-0.06577	-0.00652	-0.18598	0.13091	-0.09974
224	C	-0.00006	0.02380	-0.08598	-0.00846	0.13827	-0.00664	-0.01419	-0.00182	0.00569
225	C	0.00009	0.05445	-0.00391	0.07063	-0.01562	-0.03296	0.11349	0.01022	-0.09462
226	H	0.00002	0.09301	0.01951	-0.00949	-0.06248	-0.00751	-0.19835	0.14299	-0.11183
227	H	0.00006	0.02264	-0.07775	-0.00976	0.13182	-0.00465	0.00351	-0.01771	0.02300
228	H	0.00052	0.05981	-0.00315	0.06654	-0.02116	-0.03216	0.11907	-0.00109	-0.08417
229	H	-0.00029	0.10300	0.02196	-0.01064	-0.06963	-0.00788	-0.19252	0.13347	-0.09919
230	H	0.00021	0.01979	-0.09157	-0.01027	0.14045	-0.00704	-0.01732	0.00126	-0.00743
231	H	0.00020	0.04602	-0.00656	0.06817	-0.01235	-0.03199	0.11307	0.01130	-0.10322
232	C	-0.00003	0.08170	0.01823	-0.00724	-0.05297	-0.00711	-0.19059	0.14290	-0.11756
233	C	0.00002	0.03173	-0.08586	-0.00392	0.13696	-0.00813	-0.05021	0.03140	-0.00898
234	C	-0.00024	0.04341	-0.00572	0.07185	-0.00790	-0.03215	0.10409	0.02217	-0.10661
235	H	0.00017	0.07352	0.01578	-0.00566	-0.04505	-0.00686	-0.19580	0.15074	-0.12621
236	H	0.00025	0.03941	-0.08296	0.00558	0.13776	-0.01192	-0.04721	0.04243	-0.02139
237	H	-0.00009	0.04876	-0.00446	0.07159	-0.01115	-0.03245	0.10894	0.01657	-0.09974
238	H	-0.00005	0.08013	0.01665	-0.00752	-0.05514	-0.00743	-0.20390	0.15371	-0.12531
239	H	0.00025	0.03220	-0.08529	-0.00362	0.13280	-0.00839	-0.06210	0.04107	-0.01490
240	H	0.00007	0.03441	-0.00583	0.06949	-0.00799	-0.03125	0.11051	0.01512	-0.10807
241	C	0.00004	0.08295	0.02078	-0.00595	-0.04855	-0.00663	-0.16205	0.12020	-0.10031
242	C	0.00006	0.03013	-0.08771	-0.00602	0.13238	-0.00796	-0.06260	0.03997	-0.01612
243	C	-0.00019	0.04393	-0.00617	0.08417	0.00012	-0.03586	0.08688	0.05274	-0.13110
244	H	0.00035	0.08046	0.01731	-0.00037	-0.04527	-0.00983	-0.15507	0.12653	-0.11832
245	H	0.00021	0.03207	-0.08579	-0.00591	0.13502	-0.00652	-0.08070	0.05221	-0.01423
246	H	0.00011	0.04395	-0.00546	0.08424	0.00231	-0.03526	0.07537	0.06141	-0.13279
247	H	-0.00015	0.08350	0.02154	-0.00871	-0.04838	-0.00487	-0.16111	0.11306	-0.08753
248	H	0.00001	0.02866	-0.08648	-0.00929	0.12234	-0.00750	-0.07731	0.05010	-0.02757
249	H	0.00002	0.04074	-0.00750	0.08630	-0.00432	-0.03829	0.07978	0.06821	-0.15713
250	N	0.00001	0.08333	0.02398	-0.01238	-0.04028	-0.00153	-0.13225	0.08367	-0.05666
251	N	-0.00013	0.02808	-0.08825	-0.00736	0.12926	-0.00827	-0.03400	0.01800	-0.01032
252	N	0.00016	0.04785	-0.00058	0.07679	0.00610	-0.02892	0.07693	0.04207	-0.09272

		10	11	12	13	14	15	16	17	18
Frequencies		126.3147	127.7241	142.4266	146.2905	154.9642	171.0315	183.0569	188.7230	192.0949
Coord atom element:										
1	C	0.00911	-0.00295	-0.01244	-0.01826	0.01510	0.00944	-0.00331	-0.01710	-0.01122
2	C	-0.00027	0.00013	-0.00505	-0.00688	0.00633	0.00817	-0.00895	-0.01915	-0.02278
3	C	0.02492	-0.00858	0.01516	0.01764	0.00072	0.00136	0.00436	-0.01622	0.00830
4	H	0.01640	-0.00555	-0.00328	-0.00664	0.01113	0.00705	-0.00024	-0.01675	-0.00439
5	H	0.01777	-0.00689	0.01403	0.01772	-0.00185	0.00026	0.00248	-0.01048	0.00542
6	H	0.04237	-0.01489	0.03456	0.04243	-0.00790	-0.00658	0.01535	-0.00794	0.03534
7	C	0.04663	-0.01433	-0.06882	-0.10052	0.07474	0.03441	0.00428	-0.04806	-0.00524

8	C	-0.06066	0.02065	-0.03817	-0.04478	0.01113	0.02676	-0.04916	-0.04767	-0.11600
9	C	0.06535	-0.02276	0.04003	0.04656	-0.00184	-0.00501	0.02182	-0.01615	0.04817
10	H	0.04274	-0.01123	-0.07780	-0.11230	0.08443	0.03628	0.01456	-0.05064	0.02325
11	H	-0.08793	0.03001	-0.05878	-0.07030	0.01484	0.03298	-0.06547	-0.05101	-0.15528
12	H	0.04241	-0.01461	0.02128	0.02364	0.00379	0.00043	0.01231	-0.01971	0.02599
13	H	0.05517	-0.01799	-0.07831	-0.11533	0.08001	0.03211	0.00700	-0.03565	-0.00274
14	H	-0.05459	0.01768	-0.04473	-0.05478	0.01391	0.02438	-0.04721	-0.03656	-0.11481
15	H	0.10345	-0.03409	0.04455	0.04757	0.00959	-0.01069	0.05064	-0.00473	0.11634
16	C	0.06113	-0.01944	-0.08564	-0.12621	0.08825	0.03541	0.00920	-0.04242	0.00096
17	C	-0.08149	0.02890	-0.02888	-0.02691	0.00937	0.03858	-0.05901	-0.08288	-0.13137
18	C	0.09483	-0.03521	0.07487	0.09290	-0.01397	0.00200	0.00271	-0.04875	0.00028
19	C	0.07622	-0.02336	-0.08199	-0.11968	0.07959	0.04173	-0.01647	-0.05688	-0.05999
20	C	-0.07443	0.02055	-0.02962	-0.03112	0.02608	0.04464	-0.05776	-0.09394	-0.13091
21	C	0.11374	-0.04769	0.07436	0.08828	0.00161	0.01185	-0.00854	-0.06729	-0.03053
22	H	0.08860	-0.02603	-0.08320	-0.12037	0.08157	0.05137	-0.03298	-0.07159	-0.09694
23	H	-0.06562	0.01259	-0.02870	-0.03333	0.02912	0.04533	-0.06658	-0.09969	-0.15626
24	H	0.10867	-0.04849	0.07534	0.08756	0.00150	0.00547	-0.00044	-0.05914	-0.01422
25	C	0.07020	-0.02283	-0.07708	-0.11439	0.06444	0.03537	-0.02409	-0.05668	-0.08095
26	C	-0.06621	0.02057	-0.03769	-0.04084	0.04599	0.04970	-0.03935	-0.09039	-0.08332
27	C	0.13368	-0.05587	0.07015	0.08327	0.01732	0.02610	-0.02498	-0.08018	-0.06824
28	H	0.07721	-0.02528	-0.05915	-0.09134	0.04315	0.03366	-0.03729	-0.05769	-0.11476
29	H	-0.06392	0.01717	-0.04394	-0.04894	0.06007	0.04863	-0.03435	-0.08467	-0.07273
30	H	0.13276	-0.05884	0.06195	0.07300	0.03096	0.02718	-0.02727	-0.07703	-0.07646
31	C	0.05057	-0.02125	-0.07244	-0.11258	0.06345	0.02399	-0.00837	-0.05245	-0.04664
32	C	-0.06662	0.03334	-0.05606	-0.05653	0.05405	0.06134	-0.03016	-0.09181	-0.05187
33	C	0.14146	-0.05123	0.06088	0.07743	0.01940	0.03592	-0.03253	-0.07914	-0.07982
34	O	0.04762	-0.03022	-0.04144	-0.08039	0.03284	0.01481	-0.02629	-0.07057	-0.09309
35	O	-0.06478	0.04172	-0.07725	-0.07484	0.07448	0.06704	-0.00815	-0.07707	0.00876
36	O	0.14339	-0.05153	0.03092	0.04218	0.04113	0.04188	-0.04065	-0.06169	-0.09281
37	C	0.05667	-0.01957	-0.09913	-0.14751	0.10274	0.02821	0.03433	-0.02596	0.05862
38	C	-0.09093	0.03936	-0.02987	-0.02173	0.01011	0.05313	-0.06407	-0.11454	-0.13553
39	C	0.10109	-0.03355	0.08275	0.10788	-0.02044	0.01520	-0.01862	-0.07802	-0.04777
40	H	0.05705	-0.01758	-0.10875	-0.16118	0.11685	0.02881	0.05313	-0.01987	0.10580
41	H	-0.09847	0.04295	-0.02820	-0.01868	0.00267	0.05232	-0.07000	-0.12026	-0.14787
42	H	0.09062	-0.02789	0.08045	0.10601	-0.02357	0.01473	-0.01755	-0.08398	-0.04201
43	C	0.05031	-0.02094	-0.09350	-0.14191	0.09131	0.01835	0.03085	-0.02106	0.04652
44	C	-0.08483	0.04265	-0.03754	-0.02884	0.02564	0.06388	-0.04990	-0.11891	-0.09591
45	C	0.12062	-0.03880	0.07736	0.10251	-0.00712	0.03488	-0.03836	-0.09884	-0.09267
46	H	0.04504	-0.02150	-0.09299	-0.14430	0.09161	0.00743	0.04870	-0.00341	0.08607
47	H	-0.08547	0.04792	-0.03998	-0.02872	0.02491	0.06599	-0.04337	-0.12038	-0.07897
48	H	0.12143	-0.03585	0.07390	0.10139	-0.00684	0.04340	-0.04805	-0.11067	-0.11367
49	C	0.05057	0.04510	0.02634	0.01562	0.01597	0.02126	0.01337	-0.04454	0.04681
50	C	-0.08282	0.05016	0.01316	0.00422	0.04356	0.01035	-0.00899	0.03118	0.01099
51	C	-0.04715	0.08327	-0.02702	-0.08995	-0.06678	-0.00181	0.01855	0.01365	0.01237

52	O	0.06938	0.03978	0.02157	0.01863	0.01405	0.05724	-0.00273	-0.01544	0.04385
53	O	-0.15796	0.04751	0.04253	0.02548	0.09604	-0.08444	0.00333	-0.05409	0.02108
54	O	-0.05619	0.11536	-0.02542	-0.11981	-0.10167	-0.07530	0.08568	-0.05184	0.03460
55	C	0.04905	0.02447	0.02964	0.03799	0.05392	0.07573	-0.04167	-0.00055	0.04200
56	C	-0.18052	0.04573	0.06006	0.03944	0.11991	-0.13554	0.00983	-0.12963	0.03235
57	C	-0.05533	0.12247	-0.02080	-0.12111	-0.11086	-0.11231	0.11349	-0.10127	0.04339
58	H	0.01349	0.02415	0.04608	0.05079	0.08450	0.03749	-0.04331	-0.04399	0.05195
59	H	-0.18440	0.04584	0.06113	0.04088	0.12334	-0.13587	0.00820	-0.12883	0.03294
60	H	-0.04975	0.12116	-0.01697	-0.11822	-0.11348	-0.13713	0.12659	-0.14366	0.04773
61	H	0.05456	0.01797	0.02312	0.03681	0.05592	0.10668	-0.06155	0.03345	0.03478
62	H	-0.15955	0.04449	0.05637	0.03532	0.10496	-0.13849	0.02012	-0.14485	0.03111
63	H	-0.05699	0.11912	-0.02298	-0.12085	-0.10629	-0.09581	0.10026	-0.08066	0.03956
64	H	0.06337	0.02569	0.02217	0.02999	0.03878	0.08907	-0.03877	0.01631	0.03792
65	H	-0.21177	0.04318	0.07508	0.05392	0.15130	-0.16559	0.00384	-0.16544	0.04050
66	H	-0.05789	0.13295	-0.01918	-0.12585	-0.12150	-0.12955	0.13281	-0.11455	0.04773
67	C	-0.00051	0.01777	0.04085	0.04351	0.05529	-0.00428	-0.00566	-0.04161	0.03355
68	C	-0.02745	0.04611	-0.00327	-0.00560	0.01672	0.05393	-0.01369	0.03656	0.00271
69	C	-0.02678	0.05101	-0.03305	-0.07020	-0.05216	0.03574	-0.01477	0.02699	-0.01314
70	H	-0.02722	-0.00832	0.05041	0.06398	0.08494	-0.00719	-0.02922	-0.02767	0.02517
71	H	-0.03312	0.03579	0.00348	0.00100	0.02664	0.04135	-0.01622	0.01438	-0.00324
72	H	-0.01602	0.06059	-0.03285	-0.07486	-0.05893	0.02564	-0.00274	0.00063	-0.01222
73	C	-0.01176	0.02327	0.03897	0.03263	0.04178	-0.01906	0.00733	-0.04254	0.02678
74	C	0.02404	0.05695	-0.01841	-0.01228	-0.00308	0.08965	-0.01051	0.05090	0.01424
75	C	-0.02467	0.01228	-0.02786	-0.03137	-0.00742	0.06454	-0.05377	0.04739	-0.01923
76	C	0.02258	0.05049	0.03289	0.00927	0.02362	-0.01698	0.01835	-0.05290	0.02811
77	C	0.01485	0.05339	-0.01716	-0.01266	-0.01066	0.07648	-0.00876	0.07398	0.02268
78	C	-0.05521	-0.01134	-0.02333	-0.02074	-0.00590	0.05648	-0.06168	0.07174	-0.01731
79	C	0.07382	0.08671	0.02222	-0.01574	-0.01463	-0.00108	0.04800	-0.07544	0.05614
80	C	-0.01520	0.05211	-0.01097	-0.01369	-0.00234	0.06166	-0.01197	0.09193	0.01684
81	C	-0.06218	0.01226	-0.02523	-0.04286	-0.02788	0.04240	-0.04215	0.08448	-0.01038
82	H	0.09682	0.11380	0.01411	-0.03762	-0.04187	0.00432	0.07050	-0.08678	0.06957
83	H	-0.00173	0.05852	-0.01410	-0.02192	-0.01817	0.06297	-0.00344	0.09972	0.02495
84	H	-0.06978	-0.00275	-0.02271	-0.03403	-0.02215	0.03912	-0.05055	0.09705	-0.01444
85	C	0.08322	0.07481	0.01875	-0.00997	-0.01573	0.01357	0.04184	-0.06501	0.05565
86	C	-0.06186	0.05024	0.00341	-0.00483	0.02702	0.03518	-0.01737	0.08085	0.01097
87	C	-0.05799	0.05872	-0.02926	-0.07627	-0.05529	0.02235	-0.00973	0.06915	0.00291
88	H	0.11449	0.08928	0.01060	-0.02415	-0.03814	0.02228	0.05316	-0.07092	0.06045
89	H	-0.08442	0.05161	0.00968	-0.00360	0.03675	0.01797	-0.01680	0.08433	0.01180
90	H	-0.06011	0.07524	-0.02873	-0.08845	-0.06504	0.00469	0.00371	0.06848	0.00839
91	N	-0.04379	0.00227	0.03286	0.03144	0.02626	-0.01312	-0.00030	-0.01545	0.00645
92	N	0.07337	0.06288	-0.01903	-0.00738	0.00454	0.08197	0.00006	0.00523	0.02681
93	N	0.00161	-0.01247	-0.02546	-0.01309	0.01532	0.05539	-0.06207	0.00514	-0.02358
94	C	-0.05592	-0.03987	0.02705	-0.01038	-0.05537	-0.02187	-0.04651	-0.01162	-0.04863
95	C	0.07612	0.02030	-0.01749	-0.01389	0.02716	0.05373	0.01088	-0.03118	0.01121

96	C	0.00616	-0.03359	-0.02120	-0.00272	0.04959	0.02615	-0.05306	-0.02002	-0.03481
97	H	-0.06028	-0.06860	0.02997	-0.03642	-0.09732	-0.02721	-0.05818	-0.00440	-0.06263
98	H	0.08828	0.06623	-0.03799	0.01524	0.08532	0.05588	0.02831	-0.05115	0.02159
99	H	0.00763	-0.04192	-0.04605	-0.02732	0.03167	0.01452	-0.06256	-0.04272	-0.06614
100	H	-0.00874	-0.02260	-0.00912	-0.03213	-0.01911	0.00384	-0.04556	-0.04720	-0.07333
101	H	0.02832	0.02004	-0.04546	-0.04670	0.06917	0.05062	0.01050	-0.07796	-0.01356
102	H	0.06148	-0.01994	-0.01183	-0.00628	0.06499	0.05336	-0.04058	-0.04940	-0.06231
103	C	-0.05857	-0.10095	0.04237	-0.06191	-0.10356	-0.04486	-0.05009	0.01199	-0.05659
104	C	0.07622	-0.04651	-0.00096	-0.07887	-0.04091	0.04474	0.01881	-0.00562	0.01722
105	C	0.01199	-0.07103	-0.01810	-0.01306	0.13365	-0.05022	-0.01945	0.01424	-0.01170
106	H	-0.04558	-0.13112	0.04202	-0.09592	-0.10046	-0.08819	-0.01782	0.05142	-0.03496
107	H	0.07890	-0.01626	-0.01532	-0.06423	-0.06072	0.06122	0.01210	-0.00567	0.00549
108	H	0.00971	-0.08683	-0.01016	-0.01677	0.14628	-0.05753	-0.01914	0.00907	-0.00683
109	C	-0.06052	-0.10224	0.04577	-0.06373	-0.12898	-0.01689	-0.06561	-0.01142	-0.06803
110	C	0.08298	-0.10842	0.02396	-0.13391	-0.06214	0.04065	0.05886	0.00282	0.06015
111	C	0.01531	-0.08701	-0.01892	-0.02446	0.17517	-0.10989	0.01030	0.06067	0.00867
112	C	-0.06165	-0.07573	0.03707	-0.03397	-0.13722	0.01772	-0.11699	-0.05060	-0.11481
113	C	0.07577	-0.12838	0.03988	-0.13629	-0.05087	0.03365	0.07605	-0.00168	0.08046
114	C	0.01902	-0.08568	-0.02433	-0.03593	0.16801	-0.12015	0.01325	0.07806	0.00702
115	H	-0.05915	-0.06206	0.03297	-0.02209	-0.14055	0.03437	-0.13241	-0.06522	-0.12887
116	H	0.06810	-0.11623	0.04339	-0.12022	-0.06764	0.05545	0.05542	-0.02591	0.06229
117	H	0.02711	-0.07255	-0.03379	-0.02696	0.17693	-0.11405	0.00146	0.07436	-0.00644
118	H	-0.05811	-0.06938	0.02919	-0.02444	-0.10474	0.00669	-0.10864	-0.04212	-0.10706
119	H	0.06879	-0.13557	0.04596	-0.13168	-0.03816	0.02552	0.08703	-0.00079	0.09300
120	H	0.01251	-0.09507	-0.01488	-0.03952	0.15813	-0.11908	0.01804	0.07373	0.01362
121	H	-0.06115	-0.06987	0.03939	-0.03180	-0.15352	0.03101	-0.12519	-0.06150	-0.12259
122	H	0.07746	-0.13534	0.03557	-0.14594	-0.03393	0.01375	0.09225	0.01904	0.09532
123	H	0.02350	-0.09403	-0.02593	-0.05626	0.15762	-0.12951	0.02478	0.09408	0.01611
124	C	-0.05464	-0.14046	0.05855	-0.10682	-0.13918	-0.03956	-0.02905	0.01669	-0.03350
125	C	0.08889	-0.13516	0.03134	-0.16944	-0.08337	0.04214	0.08832	0.01475	0.08973
126	C	0.01239	-0.11209	-0.00787	-0.03988	0.19904	-0.15681	0.03386	0.09345	0.02837
127	H	-0.05215	-0.16505	0.06547	-0.13302	-0.14369	-0.06146	-0.00635	0.03859	-0.01429
128	H	0.08722	-0.12514	0.02866	-0.16198	-0.09396	0.05737	0.07670	0.00334	0.07956
129	H	0.01222	-0.10822	-0.00860	-0.03377	0.20683	-0.15784	0.03194	0.09172	0.02705
130	H	-0.05439	-0.14084	0.05663	-0.10779	-0.13491	-0.03485	-0.02455	0.01394	-0.02771
131	H	0.08917	-0.14263	0.03449	-0.17378	-0.07402	0.02866	0.09711	0.02471	0.09783
132	H	0.01276	-0.11755	-0.00402	-0.04450	0.20046	-0.16685	0.03938	0.10145	0.03305
133	H	-0.05479	-0.13416	0.05638	-0.09891	-0.13453	-0.04065	-0.03612	0.01568	-0.04109
134	H	0.09032	-0.15133	0.03679	-0.19111	-0.09499	0.03805	0.10607	0.02421	0.10754
135	H	0.01249	-0.12379	-0.00307	-0.05435	0.18650	-0.16512	0.04126	0.10461	0.03416
136	C	-0.02369	0.02997	0.02429	0.02552	0.03101	0.01609	0.01585	-0.00937	0.01045
137	C	0.06676	0.05702	-0.01339	-0.00966	-0.00814	0.02194	-0.00549	0.00623	0.02965
138	C	-0.02321	-0.03433	-0.01768	0.00308	0.00431	0.02783	-0.05918	0.00009	-0.00879
139	C	0.00765	0.05306	0.03155	0.00597	0.02937	-0.00149	0.00720	-0.02464	0.01179

140	C	0.03590	0.04409	-0.01168	-0.00646	-0.01435	0.03518	0.00215	0.03496	0.03265
141	C	-0.05680	-0.04761	-0.01539	0.00560	0.00087	0.03470	-0.05816	0.03082	-0.00597
142	C	0.00599	0.05082	0.02997	-0.00803	0.03488	0.01376	-0.03098	0.02791	-0.01898
143	C	0.00397	0.00414	0.00003	0.00508	-0.00405	0.00757	0.02823	0.02301	0.00241
144	C	-0.06866	-0.05786	-0.00824	0.02720	0.00175	0.01765	-0.01559	-0.01798	0.01854
145	H	-0.00073	0.03782	0.02765	-0.01617	0.03606	0.01673	-0.05312	0.05913	-0.04496
146	H	0.00128	-0.00305	0.00396	0.00147	-0.00022	0.00129	0.02272	0.02978	-0.01199
147	H	-0.07429	-0.06959	-0.00680	0.02142	0.00478	0.01421	-0.02890	0.00014	-0.00475
148	O	-0.00359	0.04156	0.03118	0.00269	0.03706	0.00432	-0.00847	0.00085	-0.01553
149	O	-0.00750	-0.00503	-0.00281	0.01288	-0.00437	0.00708	0.04082	0.01233	0.00400
150	O	-0.06633	-0.05351	-0.00077	0.03620	0.00871	0.00170	0.01511	-0.05604	0.02101
151	H	-0.00651	0.04237	0.03131	-0.00075	0.03880	0.01195	-0.02208	0.01851	-0.02021
152	H	-0.01042	-0.00604	-0.00028	0.01462	-0.00062	0.00509	0.04782	0.00724	-0.00070
153	H	-0.06415	-0.05401	-0.00025	0.03952	0.00782	-0.00506	0.02764	-0.07168	0.02453
154	C	0.00802	0.03941	0.02863	-0.01554	0.02817	0.03160	-0.06118	0.07392	-0.01193
155	C	-0.01179	-0.01387	0.00467	0.00847	0.00352	-0.00563	0.03285	0.01681	-0.02242
156	C	-0.04759	-0.02540	-0.00457	0.03199	-0.00025	0.02707	-0.00166	-0.03134	0.05423
157	O	0.00355	0.03695	0.04544	-0.02401	0.02783	0.02344	-0.07582	0.08504	-0.00484
158	O	-0.02569	-0.01519	0.01697	0.00541	0.01575	-0.02088	0.01638	0.02311	-0.03939
159	O	-0.04613	-0.02494	-0.03833	0.05399	0.00149	0.04065	0.03269	-0.06207	0.04362
160	H	0.00960	0.04107	0.03797	-0.02264	0.02769	0.02736	-0.07157	0.08159	-0.00727
161	H	-0.01569	-0.00664	0.00617	0.00732	0.00929	-0.00711	0.01738	0.01527	-0.02445
162	H	-0.04060	-0.02228	-0.04925	0.05747	0.00070	0.04502	0.04190	-0.06952	0.04018
163	C	0.00346	0.02540	0.06965	-0.03849	0.02326	0.01717	-0.09214	0.10497	0.01495
164	C	-0.04429	-0.07835	-0.03798	0.03739	-0.00835	-0.00451	0.06653	-0.03791	-0.02577
165	C	-0.03937	-0.00803	0.05415	0.00182	0.00082	0.01397	-0.03619	0.01608	0.09006
166	O	0.00867	0.04019	0.08833	-0.05149	0.02678	0.01750	-0.14579	0.15332	0.05145
167	O	-0.05690	-0.10941	-0.05705	0.05175	-0.01625	-0.01109	0.12005	-0.09765	-0.05158
168	O	-0.04980	-0.02510	0.07927	-0.01310	-0.00472	0.00293	-0.09987	0.05381	0.15618
169	C	-0.01808	0.02147	-0.01543	0.04178	0.02137	0.06332	0.05078	0.01938	0.00828
170	C	0.06411	0.06320	0.01742	-0.02451	-0.00444	-0.04585	-0.03662	-0.02045	0.01571
171	C	-0.01906	-0.00842	-0.00756	0.02108	0.00016	0.01292	-0.02275	-0.03005	0.03205
172	H	-0.03192	0.02751	0.00842	0.04351	0.02671	0.05462	0.06621	0.01175	0.01483
173	H	0.06309	0.07999	0.04063	-0.03265	0.00134	-0.08013	-0.06564	-0.04665	0.02664
174	H	-0.04166	-0.01357	0.01078	0.03189	0.00440	0.03037	0.02861	-0.01992	0.03310
175	C	-0.00039	0.00681	-0.07086	0.06109	-0.00643	0.05828	0.07693	0.04309	-0.00611
176	C	0.08777	0.07164	-0.01291	-0.02325	-0.02107	-0.08301	-0.06237	-0.02651	0.01084
177	C	0.01344	0.01395	-0.04895	0.02748	-0.01755	-0.02539	-0.04181	-0.03016	0.02334
178	H	-0.00661	0.00011	-0.06903	0.06141	-0.01170	0.06310	0.07681	0.04319	-0.00562
179	H	0.08716	0.08261	-0.01542	-0.01809	-0.01973	-0.06981	-0.04627	-0.01303	0.00393
180	H	0.00958	0.01274	-0.04733	0.02846	-0.02048	-0.01921	-0.03879	-0.02802	0.02292
181	C	0.02095	-0.00173	-0.12191	0.07219	-0.03134	-0.00316	0.06150	0.06711	-0.04866
182	C	0.10461	0.06183	-0.03825	-0.02623	-0.04075	-0.14505	-0.10665	-0.03428	-0.00580
183	C	0.02663	0.02063	-0.10304	0.05396	-0.02930	-0.03220	0.00845	0.03149	-0.02849

184	C	0.02675	-0.00786	-0.13172	0.07161	-0.02341	-0.00804	0.08777	0.09788	-0.07662
185	C	0.11957	0.04928	-0.02933	-0.05246	-0.04804	-0.22884	-0.20434	-0.08841	0.00455
186	C	0.03180	0.01471	-0.11151	0.05262	-0.02487	-0.04240	0.02065	0.04994	-0.04811
187	H	0.02613	-0.00984	-0.13222	0.07174	-0.02418	-0.01245	0.08251	0.09304	-0.07506
188	H	0.11727	0.03475	-0.03479	-0.05269	-0.04525	-0.24057	-0.19847	-0.08294	-0.00839
189	H	0.03274	0.00508	-0.11323	0.04916	-0.01457	-0.03663	0.05168	0.07845	-0.07108
190	H	0.03082	-0.02227	-0.13590	0.06540	-0.01759	-0.02823	0.09500	0.11142	-0.10095
191	H	0.12090	0.05162	-0.02387	-0.05727	-0.04931	-0.23973	-0.23229	-0.10391	0.01492
192	H	0.02621	0.01775	-0.11231	0.06019	-0.02497	-0.01899	0.04728	0.05899	-0.04679
193	H	0.02842	0.00259	-0.12820	0.07227	-0.02003	0.01054	0.09904	0.10901	-0.07089
194	H	0.11966	0.04741	-0.02689	-0.05539	-0.04837	-0.23812	-0.22064	-0.09771	0.00850
195	H	0.03574	0.01268	-0.10325	0.04179	-0.02593	-0.07030	-0.02417	0.02387	-0.03730
196	C	0.03775	-0.00896	-0.16627	0.08163	-0.06684	-0.07671	0.02705	0.08686	-0.09518
197	C	0.11051	0.06665	-0.08085	-0.00273	-0.05757	-0.15594	-0.07207	0.01796	-0.05185
198	C	0.03676	0.03214	-0.16444	0.08962	-0.04917	-0.03537	0.07455	0.11619	-0.09653
199	H	0.03779	-0.01318	-0.16005	0.07528	-0.07022	-0.08773	0.00884	0.07609	-0.09200
200	H	0.11237	0.07580	-0.09394	0.00909	-0.05624	-0.14044	-0.03867	0.04594	-0.06686
201	H	0.03745	0.02983	-0.15950	0.08445	-0.05163	-0.04405	0.06111	0.10849	-0.09457
202	H	0.04109	-0.01136	-0.19123	0.09290	-0.07862	-0.09402	0.03624	0.11577	-0.12637
203	H	0.10601	0.06298	-0.05360	-0.01746	-0.04693	-0.14712	-0.09542	-0.01932	-0.01797
204	H	0.04248	0.03760	-0.19522	0.10665	-0.06130	-0.04452	0.10293	0.15983	-0.13551
205	H	0.03839	-0.01095	-0.16605	0.07939	-0.07004	-0.08429	0.01840	0.08373	-0.09629
206	H	0.12135	0.06779	-0.12338	0.01473	-0.08207	-0.19500	-0.06498	0.06092	-0.10348
207	H	0.03676	0.03766	-0.17317	0.09897	-0.04496	-0.02219	0.09933	0.13318	-0.10380
208	N	0.00608	0.01761	-0.03554	0.02433	0.01819	0.05882	-0.00712	0.03108	-0.01150
209	N	0.01323	0.01980	0.03095	-0.01106	0.00811	-0.01793	0.01504	0.02408	-0.02694
210	N	-0.02158	0.00490	0.00521	0.02392	0.00012	0.01906	0.00135	-0.03433	0.04995
211	C	0.01159	-0.00164	-0.05693	0.02930	-0.01141	0.02002	-0.03140	-0.06015	0.09095
212	C	-0.00147	0.01364	0.04019	-0.01039	0.02149	-0.00114	0.02291	0.07020	-0.07418
213	C	0.00573	0.04175	0.00598	0.02134	-0.00045	0.01745	0.02582	-0.04500	0.04360
214	O	0.02093	-0.00859	-0.13349	0.06844	-0.04279	0.01289	-0.05262	-0.15348	0.23291
215	O	0.00585	0.03121	0.07401	-0.03043	0.03675	0.00394	0.04404	0.12259	-0.15328
216	O	0.02303	0.06072	-0.00791	0.02440	-0.00407	0.01706	0.03663	-0.04920	0.04769
217	C	-0.00227	-0.01778	0.03691	-0.02026	0.00044	-0.00958	0.00077	-0.01497	-0.00658
218	C	-0.03584	-0.04197	-0.01372	0.02369	0.00958	0.01257	-0.01487	0.04817	-0.00016
219	C	0.00850	0.05102	0.02336	0.01390	0.00215	0.01577	0.04429	-0.04216	0.02757
220	H	-0.00442	-0.01330	0.05852	-0.03099	0.00612	-0.00981	-0.00752	0.01387	-0.01802
221	H	-0.04080	-0.04273	-0.03008	0.03154	0.01193	0.02812	-0.06837	0.07436	0.04537
222	H	0.00871	0.04240	-0.03746	0.04489	-0.00751	0.03154	0.01431	-0.07778	0.09236
223	C	-0.01516	-0.05061	0.05539	-0.02654	-0.00854	-0.03816	0.07249	-0.05637	-0.05692
224	C	-0.04631	-0.06325	-0.03002	0.03358	0.00338	0.01291	-0.02240	0.03258	0.02332
225	C	0.03409	0.09956	0.08726	-0.01993	0.01574	0.00031	0.11831	-0.01184	-0.07848
226	H	-0.02165	-0.06398	0.05988	-0.02676	-0.01142	-0.04637	0.09203	-0.06745	-0.06894
227	H	-0.03912	-0.04569	-0.03395	0.03312	0.00737	0.02627	-0.05536	0.04887	0.04853

228	H	0.04538	0.11421	0.07883	-0.01866	0.01761	0.00255	0.11458	-0.00540	-0.08903
229	H	-0.01533	-0.05862	0.03609	-0.01685	-0.01268	-0.04025	0.07031	-0.06828	-0.05231
230	H	-0.03845	-0.05337	-0.00788	0.02128	0.00604	-0.00102	0.01963	0.03850	-0.03096
231	H	0.03910	0.10971	0.11288	-0.03409	0.01990	-0.00833	0.14672	0.00020	-0.11787
232	C	-0.02422	-0.05659	0.08902	-0.04082	-0.00567	-0.04609	0.09678	-0.04675	-0.07856
233	C	-0.07505	-0.11967	-0.06298	0.05512	-0.01200	0.00905	-0.03120	-0.01393	0.07506
234	C	0.02404	0.08723	0.10638	-0.02773	0.01547	-0.00553	0.13453	-0.00928	-0.08811
235	H	-0.03176	-0.06461	0.10519	-0.04773	-0.00520	-0.05038	0.10485	-0.04107	-0.08364
236	H	-0.08407	-0.12660	-0.05770	0.05679	-0.01210	0.01474	-0.05343	-0.00468	0.10953
237	H	0.02713	0.09040	0.09350	-0.02128	0.01495	-0.00100	0.12295	-0.01141	-0.07718
238	H	-0.03012	-0.07252	0.08208	-0.03673	-0.01152	-0.05417	0.12139	-0.07445	-0.08819
239	H	-0.08009	-0.13324	-0.07021	0.05941	-0.01704	0.00388	-0.01751	-0.03544	0.07400
240	H	0.03383	0.10587	0.13017	-0.04206	0.02061	-0.01234	0.16297	-0.00034	-0.13108
241	C	-0.01335	-0.02740	0.09619	-0.04608	0.00450	-0.03003	0.04894	0.00154	-0.05683
242	C	-0.07602	-0.12878	-0.06679	0.05664	-0.01663	-0.00053	0.00284	-0.04207	0.05104
243	C	-0.00270	0.04877	0.11004	-0.02346	0.00854	-0.00819	0.12079	-0.01756	-0.04397
244	H	-0.01271	-0.01933	0.12199	-0.05596	0.00726	-0.03418	0.07457	0.00827	-0.07288
245	H	-0.09247	-0.15956	-0.08692	0.06729	-0.02309	0.00084	-0.02642	-0.05208	0.09030
246	H	-0.01258	0.03127	0.10340	-0.01922	0.00511	-0.00859	0.10925	-0.02226	-0.02473
247	H	-0.01316	-0.02986	0.07978	-0.03958	0.00339	-0.02602	0.03226	0.00051	-0.04637
248	H	-0.07388	-0.13345	-0.06180	0.05324	-0.02040	-0.01331	0.04655	-0.07007	0.01615
249	H	-0.00172	0.05112	0.13967	-0.03615	0.00879	-0.02075	0.17076	-0.02794	-0.07879
250	N	-0.00446	-0.00700	0.06903	-0.03690	0.01124	-0.00647	-0.02357	0.04149	-0.01816
251	N	-0.05169	-0.08093	-0.03953	0.03960	-0.00517	0.00368	0.01476	-0.00916	0.01391
252	N	-0.01551	0.02244	0.05870	-0.00224	0.00432	0.00812	0.03335	-0.00830	0.02429

		19	20	21	22	23	24	25	26	27
Frequencies		192.6477	201.2446	211.3821	233.4880	235.7760	241.6896	248.8824	253.6330	256.8386
Coord atom element:										
1	C	-0.00992	0.00571	0.00778	-0.00146	-0.00431	0.00153	0.00231	-0.00031	-0.00087
2	C	-0.00571	-0.01324	0.01179	-0.00188	-0.00885	0.00152	0.00845	0.00455	0.00221
3	C	-0.01806	0.06594	0.03100	-0.00730	-0.02403	-0.00393	0.01931	0.00936	-0.00559
4	H	-0.01284	0.02539	0.01494	-0.00295	-0.01011	0.00007	0.00740	0.00342	0.00008
5	H	-0.01149	0.04327	0.02043	-0.00431	-0.01636	-0.00229	0.01389	0.00807	-0.00027
6	H	-0.02372	0.12114	0.04080	-0.01007	-0.03208	-0.00778	0.02535	0.01314	-0.00825
7	C	-0.04199	0.06623	0.01326	-0.00432	-0.00317	0.00398	-0.00650	-0.01197	-0.01196
8	C	0.01470	-0.18646	-0.00155	0.00373	-0.00094	0.01113	0.00901	0.00750	0.01833
9	C	-0.03738	0.17301	0.05571	-0.01398	-0.04204	-0.01000	0.03105	0.01449	-0.01360
10	H	-0.05687	0.14960	0.02780	-0.00992	-0.01660	-0.00212	0.00062	-0.00835	-0.01825
11	H	0.03007	-0.28513	-0.02162	0.00908	0.01429	0.01736	-0.00029	0.00231	0.02420
12	H	-0.02982	0.12111	0.04434	-0.01127	-0.03385	-0.00692	0.02557	0.01111	-0.01168
13	H	-0.03337	0.03216	-0.00884	0.00047	0.01540	0.00751	-0.02183	-0.02187	-0.01219
14	H	0.02306	-0.21877	-0.02101	0.00822	0.01537	0.01446	-0.00408	-0.00087	0.01817
15	H	-0.05989	0.31800	0.06919	-0.01973	-0.05104	-0.01772	0.03092	0.01147	-0.02843

16	C	-0.04068	0.05639	-0.00037	-0.00159	0.00811	0.00607	-0.01637	-0.01942	-0.01559
17	C	-0.00718	-0.12133	0.04382	-0.00613	-0.03675	0.00545	0.03660	0.02377	0.01798
18	C	-0.04247	0.13273	0.07967	-0.01548	-0.05542	-0.00604	0.04295	0.01786	-0.01374
19	C	-0.02403	-0.06859	-0.01821	0.00404	0.03478	0.01760	-0.04706	-0.07827	-0.10376
20	C	-0.01641	-0.10254	0.05582	-0.00777	-0.06235	-0.00128	0.07329	0.10294	0.15333
21	C	-0.04311	0.08395	0.08174	-0.01370	-0.06901	-0.00761	0.06727	0.07729	0.09602
22	H	-0.01903	-0.13486	-0.03071	0.00779	0.05569	0.02559	-0.07178	-0.11702	-0.15564
23	H	-0.00879	-0.15968	0.05628	-0.00657	-0.07561	-0.00264	0.09705	0.15018	0.23361
24	H	-0.04383	0.10920	0.09052	-0.01603	-0.08751	-0.01367	0.09181	0.11935	0.15820
25	C	-0.01363	-0.11298	-0.00916	0.00230	0.02242	0.01913	-0.02955	-0.06960	-0.10847
26	C	-0.03622	0.00299	0.05443	-0.00886	-0.05638	-0.00737	0.05712	0.09184	0.14564
27	C	-0.03560	-0.00364	0.05272	-0.00467	-0.04252	-0.00179	0.04285	0.07121	0.12381
28	H	0.00113	-0.19745	-0.02200	0.00694	0.04142	0.03216	-0.04569	-0.10453	-0.16385
29	H	-0.03621	0.00966	0.05027	-0.00782	-0.06441	-0.01612	0.06761	0.13057	0.22392
30	H	-0.02912	-0.04242	0.04013	-0.00106	-0.04380	-0.00696	0.04880	0.10646	0.20375
31	C	-0.02501	-0.02179	0.03481	-0.00765	-0.03199	0.00314	0.03140	0.01503	-0.00477
32	C	-0.05375	0.09366	0.04321	-0.00853	-0.01563	-0.00024	-0.00141	-0.00975	-0.01277
33	C	-0.03010	-0.04012	0.01843	0.00234	0.00677	0.01011	-0.01308	-0.00827	0.02015
34	O	-0.01494	-0.07696	0.08415	-0.01263	-0.07760	-0.00092	0.07573	0.04437	-0.00466
35	O	-0.07230	0.20574	0.01360	-0.00682	0.01992	0.00031	-0.04219	-0.04522	-0.03708
36	O	-0.00973	-0.13605	-0.04155	0.00976	0.03679	0.01077	-0.03125	0.00502	0.07693
37	C	-0.05412	0.16100	0.01176	-0.00662	-0.01651	-0.00469	0.01805	0.04538	0.07932
38	C	-0.03259	-0.03595	0.07658	-0.01331	-0.04023	0.00665	0.01512	-0.04955	-0.12226
39	C	-0.04485	0.08765	0.08548	-0.01461	-0.03860	0.00353	0.00914	-0.06031	-0.14075
40	H	-0.07084	0.26504	0.02326	-0.01049	-0.03103	-0.01332	0.03372	0.08119	0.13549
41	H	-0.03221	-0.04530	0.08335	-0.01598	-0.04028	0.00871	0.00807	-0.08282	-0.19107
42	H	-0.05312	0.12722	0.10096	-0.02006	-0.04516	0.00215	0.00632	-0.08969	-0.20955
43	C	-0.04391	0.12317	0.01946	-0.00874	-0.03259	-0.00756	0.03967	0.06776	0.09856
44	C	-0.05554	0.07615	0.07909	-0.01434	-0.02870	0.00565	-0.00702	-0.07509	-0.15241
45	C	-0.04116	0.00789	0.06217	-0.00596	-0.00790	0.01408	-0.02102	-0.08318	-0.14071
46	H	-0.04770	0.18054	0.02762	-0.01179	-0.05076	-0.01483	0.06382	0.10967	0.15587
47	H	-0.06537	0.13371	0.08608	-0.01699	-0.02235	0.00689	-0.02677	-0.12323	-0.23596
48	H	-0.04144	-0.01197	0.05847	-0.00489	0.00737	0.01911	-0.04428	-0.12667	-0.20507
49	C	-0.00750	-0.01783	-0.00137	0.09521	-0.00026	0.00249	-0.01627	0.00264	0.00700
50	C	0.04504	0.00308	0.03035	0.05345	-0.02028	0.02630	0.00576	-0.02380	0.00858
51	C	0.02911	0.00898	0.00182	0.06236	-0.04273	0.03195	0.00264	-0.02063	0.01038
52	O	0.02821	-0.01104	0.00014	0.12521	-0.01899	0.01477	-0.01780	-0.00715	0.00918
53	O	-0.05821	-0.00552	-0.05877	0.01337	-0.02061	0.00298	-0.00196	-0.01033	0.01145
54	O	-0.04039	-0.02080	0.08039	0.01413	0.03585	0.00510	0.01192	0.01049	0.00474
55	C	0.04304	0.00630	-0.09464	0.18930	-0.09270	0.04278	-0.03194	-0.03506	0.02659
56	C	-0.14356	-0.01752	-0.15255	-0.00133	-0.00690	-0.03377	-0.03717	0.01905	0.00926
57	C	-0.09360	-0.03971	0.09268	-0.02857	0.09154	-0.03297	0.00133	0.04434	-0.00643
58	H	-0.00841	0.00393	-0.17199	0.19429	-0.10618	0.03433	-0.04833	-0.02551	0.03142
59	H	-0.14282	-0.01652	-0.15782	0.00284	-0.01173	-0.03021	-0.03639	0.01702	0.01083

60	H	-0.13942	-0.05199	0.07229	-0.05267	0.12126	-0.06489	-0.01696	0.06934	-0.01413
61	H	0.08129	0.01909	-0.10623	0.22493	-0.13065	0.06715	-0.02988	-0.05855	0.03521
62	H	-0.15838	-0.02534	-0.13635	-0.02408	0.02268	-0.05517	-0.04469	0.03534	-0.00008
63	H	-0.07101	-0.03081	0.08247	-0.00546	0.06440	-0.01591	0.00395	0.02850	-0.00023
64	H	0.06286	0.00720	-0.05839	0.18302	-0.08445	0.04539	-0.02371	-0.03744	0.02356
65	H	-0.18680	-0.01844	-0.22911	0.00965	-0.02469	-0.04010	-0.05476	0.02459	0.01583
66	H	-0.10748	-0.04864	0.13084	-0.05813	0.12461	-0.04443	0.00994	0.05784	-0.01396
67	C	-0.01808	-0.00774	-0.03650	0.05182	-0.02944	0.00674	0.01001	0.00320	-0.00512
68	C	0.05743	0.00049	0.03557	0.05303	0.02768	-0.00167	-0.03553	-0.02006	0.01970
69	C	0.03835	0.01820	-0.04311	0.02772	-0.01487	0.00065	-0.03423	-0.02148	0.01715
70	H	-0.01361	0.00237	-0.06943	0.03311	-0.05905	0.01241	0.02626	0.00374	-0.01214
71	H	0.03006	0.00009	0.00881	0.02987	0.04479	-0.01699	-0.05006	-0.02176	0.02381
72	H	0.01530	0.01170	-0.04302	0.02442	0.01459	-0.01463	-0.05608	-0.02446	0.02502
73	C	-0.02264	-0.00808	-0.01100	0.03501	-0.02237	0.01085	0.01566	-0.00311	-0.00815
74	C	0.07951	-0.00570	0.05683	0.06556	0.04444	-0.01116	-0.03833	-0.00040	0.01849
75	C	0.05564	0.02505	-0.08402	0.00843	-0.01576	-0.01454	-0.03208	-0.00309	0.01383
76	C	-0.03628	-0.01411	-0.01505	0.02727	-0.00506	0.00728	-0.00442	-0.01352	0.00541
77	C	0.09201	-0.00462	0.07532	0.05493	0.01006	0.00770	-0.00142	0.01194	-0.00078
78	C	0.06959	0.03147	-0.07399	-0.00294	-0.05243	-0.00093	0.00563	0.01111	-0.00838
79	C	-0.03818	-0.03351	0.02766	0.08141	0.03929	-0.00574	-0.03300	-0.00115	0.01613
80	C	0.10511	0.00613	0.07869	0.06729	-0.04555	0.04538	0.03332	-0.00899	-0.00597
81	C	0.08821	0.03446	-0.03953	0.04573	-0.10771	0.04880	0.04074	-0.01170	-0.01087
82	H	-0.03775	-0.04323	0.05859	0.11534	0.05955	-0.00704	-0.04666	-0.00061	0.02341
83	H	0.11561	0.00496	0.10210	0.08703	-0.06210	0.06062	0.04883	-0.00772	-0.01097
84	H	0.09605	0.04034	-0.04552	0.03824	-0.13493	0.06175	0.06165	-0.01162	-0.01950
85	C	-0.02722	-0.03265	0.03427	0.08026	0.04735	-0.01397	-0.03515	0.00869	0.01256
86	C	0.09210	0.01229	0.05699	0.06893	-0.07056	0.06190	0.04393	-0.02915	-0.00193
87	C	0.07990	0.02666	-0.00410	0.07837	-0.11368	0.07117	0.04590	-0.02932	-0.00220
88	H	-0.03093	-0.03955	0.04880	0.07505	0.07508	-0.02867	-0.05161	0.01641	0.01545
89	H	0.09242	0.01688	0.05664	0.07620	-0.10507	0.08531	0.06900	-0.03910	-0.00576
90	H	0.07644	0.02580	0.00962	0.08327	-0.13830	0.09347	0.06826	-0.03691	-0.00528
91	N	0.01500	0.00432	0.04108	0.03365	-0.01321	0.01293	0.02171	0.00064	-0.01556
92	N	0.03159	-0.01914	0.02283	0.04421	0.06756	-0.03113	-0.04580	0.01034	0.02327
93	N	0.02685	0.01947	-0.09827	-0.01052	0.02888	-0.03952	-0.04585	0.01216	0.02089
94	C	0.05004	0.02720	0.10307	0.00374	0.00410	-0.01646	0.00003	0.01550	-0.01166
95	C	-0.01525	0.00534	0.02697	0.03621	0.07511	-0.00060	-0.04935	-0.01155	0.03487
96	C	-0.00060	0.03586	-0.09367	-0.01406	0.03747	-0.00853	-0.04670	-0.00571	0.03516
97	H	0.05913	0.03682	0.11426	-0.00891	0.00941	-0.02897	-0.01590	0.01350	-0.00465
98	H	-0.04048	-0.00755	0.02029	0.04863	0.05757	0.01863	-0.01757	-0.00716	0.01322
99	H	-0.02035	0.04568	-0.07119	-0.03211	0.02150	-0.01065	-0.03561	-0.00421	0.01768
100	H	0.01252	-0.00982	0.09612	-0.01120	-0.06566	-0.02189	0.05844	0.04624	-0.01802
101	H	-0.06179	0.08123	0.04423	0.01443	0.05191	0.02213	-0.04106	-0.04387	-0.00713
102	H	-0.00832	-0.04455	-0.06431	0.00484	0.05687	0.01228	-0.05159	-0.02112	0.02782
103	C	0.06721	0.03261	0.11017	-0.01556	0.01256	-0.03200	-0.03054	-0.00056	0.00752

104	C	-0.01338	-0.00382	0.01390	0.01836	0.05999	-0.03486	-0.07487	-0.02843	0.05139
105	C	0.02977	0.02697	-0.05670	-0.00483	0.09244	0.06647	-0.03858	-0.01119	0.03637
106	H	0.08226	-0.00221	0.15985	-0.01941	-0.04116	-0.09075	-0.03600	-0.02073	0.00104
107	H	-0.01619	-0.00841	0.04855	0.01802	0.00664	-0.15345	-0.12912	-0.06848	0.08073
108	H	0.02766	0.03579	-0.09192	-0.00349	0.13961	0.16374	0.00886	0.01951	0.01527
109	C	0.04193	0.05514	0.04452	-0.02187	0.04031	0.00046	-0.03334	-0.00268	0.02340
110	C	-0.04975	-0.03585	-0.07077	0.00563	0.00619	0.01674	-0.00336	-0.00309	0.00054
111	C	0.07862	-0.01350	0.05593	-0.00023	0.04551	0.02126	-0.03140	-0.00478	0.00527
112	C	0.03175	0.12203	-0.02548	-0.01738	0.22191	0.14001	-0.07578	0.01153	0.09683
113	C	-0.07165	-0.04615	-0.12531	0.00962	0.01556	0.18511	0.12252	0.09077	-0.09944
114	C	0.10273	-0.02801	0.12951	-0.00702	-0.02482	-0.15395	-0.11209	-0.07671	0.05966
115	H	0.02468	0.14456	-0.05411	-0.01481	0.28854	0.19318	-0.09043	0.01913	0.12574
116	H	-0.08594	-0.01329	-0.16493	0.01347	0.09458	0.28756	0.13699	0.12297	-0.09380
117	H	0.10846	-0.01765	0.13167	-0.00855	0.00329	-0.18967	-0.16447	-0.10477	0.12025
118	H	0.03333	0.11101	-0.03025	-0.01589	0.21138	0.14381	-0.06480	0.01595	0.08841
119	H	-0.08196	-0.05566	-0.15106	0.01315	0.00955	0.27557	0.20019	0.14441	-0.16854
120	H	0.09248	-0.02956	0.11059	-0.00528	-0.02444	-0.08477	-0.05644	-0.03702	0.00889
121	H	0.02591	0.13429	-0.03349	-0.01660	0.24612	0.15492	-0.08447	0.01238	0.11259
122	H	-0.05827	-0.07162	-0.08907	0.00660	-0.05527	0.09440	0.10969	0.06141	-0.10865
123	H	0.11851	-0.04877	0.18613	-0.01257	-0.10449	-0.30328	-0.16369	-0.13588	0.08342
124	C	0.03903	0.01082	0.05049	-0.04001	-0.08705	-0.08697	-0.00770	-0.02030	-0.02298
125	C	-0.07336	-0.07126	-0.10459	-0.01431	-0.12871	-0.12285	-0.01668	-0.06085	0.00009
126	C	0.11516	-0.04233	0.12532	0.00786	0.04794	0.12596	0.05547	0.07717	-0.09926
127	H	0.04725	-0.01718	0.06946	-0.04861	-0.15601	-0.12355	0.01573	-0.02043	-0.06390
128	H	-0.08027	-0.05937	-0.11442	-0.01530	-0.12467	-0.16108	-0.05135	-0.08724	0.03864
129	H	0.11648	-0.03874	0.12457	0.01226	0.07395	0.16721	0.06957	0.09518	-0.10857
130	H	0.02333	0.00600	0.01796	-0.04898	-0.13051	-0.14562	-0.02370	-0.05664	-0.00225
131	H	-0.06616	-0.08132	-0.09336	-0.01257	-0.12693	-0.08232	0.01572	-0.03361	-0.03594
132	H	0.12439	-0.04837	0.14373	0.01178	0.06242	0.17720	0.08748	0.11113	-0.13539
133	H	0.04797	0.01884	0.06714	-0.03284	-0.04677	-0.04346	-0.00209	0.00103	-0.02695
134	H	-0.08501	-0.09324	-0.12183	-0.02980	-0.22120	-0.21785	-0.02448	-0.10015	-0.00242
135	H	0.12159	-0.05471	0.14463	0.00318	0.01376	0.09744	0.05911	0.07541	-0.11537
136	C	0.01132	-0.00004	0.02264	0.03905	-0.01284	0.01403	0.01135	-0.01380	-0.00351
137	C	0.03194	-0.01736	0.02628	0.00015	0.04315	-0.02278	-0.01195	0.02988	-0.00336
138	C	0.02229	0.01731	-0.07051	-0.02741	0.02290	-0.05108	-0.01047	0.04244	-0.01362
139	C	-0.01754	-0.00351	-0.01945	0.01780	-0.02225	0.01800	-0.00167	-0.03047	0.01026
140	C	0.04518	-0.01631	0.05255	0.00661	0.02568	-0.01006	0.00161	0.03345	-0.01188
141	C	0.03341	0.02075	-0.05874	-0.02570	-0.00807	-0.03397	0.00572	0.04128	-0.02290
142	C	-0.01351	0.01100	-0.06585	-0.08566	-0.02762	0.00202	0.00276	-0.02035	0.00456
143	C	0.00671	-0.00994	0.02512	-0.07571	0.00334	0.01032	0.00137	0.00152	0.00196
144	C	0.00363	0.00661	-0.03078	0.03021	-0.01474	-0.01501	0.00570	0.01615	-0.01509
145	H	-0.00738	0.02212	-0.08876	-0.16025	-0.02821	-0.00248	0.00174	-0.01626	0.00694
146	H	0.00112	-0.00369	0.01948	-0.06729	0.00598	0.00024	0.00560	0.01506	-0.00986
147	H	0.00329	0.01612	-0.04799	-0.00309	-0.01388	-0.02294	0.00755	0.02582	-0.02083

148	O	-0.02487	0.00839	-0.07331	-0.10204	-0.05228	0.03228	-0.00768	-0.06747	0.03224
149	O	0.00666	-0.01136	0.01728	-0.13451	-0.01706	0.03984	-0.01002	-0.04175	0.03311
150	O	-0.01353	0.00351	-0.03574	0.06831	-0.03598	0.00578	0.00000	-0.01802	-0.00220
151	H	-0.02216	0.01185	-0.07928	-0.12880	-0.04874	0.02527	-0.00603	-0.05758	0.02792
152	H	0.00034	-0.00938	0.00798	-0.14676	-0.02920	0.04921	-0.01283	-0.05842	0.04005
153	H	-0.01758	0.00062	-0.03196	0.08916	-0.04063	0.01331	-0.00197	-0.02920	0.00263
154	C	-0.02315	0.00709	-0.04015	-0.08144	0.01623	-0.04911	0.02627	0.05023	-0.04294
155	C	-0.00360	-0.00092	0.00269	-0.09909	-0.01206	0.02341	-0.00610	-0.02009	0.01469
156	C	-0.00752	-0.01093	-0.00334	0.05143	0.00314	-0.02122	0.01081	0.01703	-0.01746
157	O	-0.04798	0.00321	-0.03033	-0.09939	0.00562	-0.03260	0.01802	0.03588	-0.03200
158	O	-0.02460	0.00790	-0.03566	-0.18434	-0.07739	0.08862	-0.03692	-0.10539	0.07339
159	O	0.03862	-0.00388	-0.03087	0.06449	0.00525	-0.03561	0.02049	0.02089	-0.02382
160	H	-0.03702	0.00446	-0.03286	-0.08873	0.01253	-0.04175	0.02230	0.04442	-0.03830
161	H	-0.01132	0.00400	-0.02137	-0.12114	-0.04273	0.05062	-0.01994	-0.06155	0.04276
162	H	0.05424	-0.00198	-0.03398	0.07976	0.01246	-0.04536	0.02513	0.02951	-0.03023
163	C	-0.09046	-0.01064	0.00841	-0.08265	0.02115	-0.03167	0.01873	0.04210	-0.03467
164	C	0.03126	0.00655	-0.01105	-0.01988	0.00524	-0.00865	0.00438	0.01328	-0.01071
165	C	-0.09713	-0.03648	0.06209	0.04788	0.00419	0.01411	-0.00185	-0.01339	0.00659
166	O	-0.16224	-0.02890	0.04796	-0.08965	0.01976	-0.00745	0.01452	0.00892	-0.01074
167	O	0.09391	0.02118	-0.04044	0.01456	0.00804	-0.02919	0.00534	0.04315	-0.03125
168	O	-0.20321	-0.06774	0.13409	0.09845	0.00293	0.05539	-0.01481	-0.06263	0.04422
169	C	0.00861	-0.00983	0.02770	0.00519	0.02081	-0.01227	0.01770	0.00860	-0.01278
170	C	0.03806	-0.00104	0.00898	-0.01707	0.00678	-0.00112	-0.00230	0.01215	-0.00563
171	C	0.00494	-0.00039	-0.02789	0.00253	0.01958	-0.04300	0.01243	0.03389	-0.02479
172	H	-0.00027	-0.01358	0.04962	0.02714	0.00187	0.01439	0.01476	-0.01528	-0.00175
173	H	0.05633	0.00594	0.00997	0.02501	-0.01637	0.01184	0.00692	0.00044	-0.00926
174	H	-0.02383	-0.01275	0.00686	0.00244	0.00943	-0.01196	0.00121	0.00637	-0.00490
175	C	-0.03618	-0.01878	0.03699	-0.02229	0.02341	-0.00143	-0.00746	0.01181	-0.00127
176	C	0.04163	0.00472	0.00507	0.00096	-0.00485	0.00511	-0.00565	0.01442	-0.00775
177	C	0.00980	0.00519	-0.02766	0.03000	0.00466	-0.03520	0.01439	0.03502	-0.03021
178	H	-0.04610	-0.02061	0.04368	-0.01964	0.00206	0.00610	-0.06154	0.06434	-0.02002
179	H	0.04272	0.00166	0.02236	0.00360	-0.02033	0.01739	-0.03580	0.04166	-0.01854
180	H	0.00411	0.00304	-0.01930	0.03213	-0.01331	-0.02747	-0.02948	0.07751	-0.04553
181	C	-0.07366	-0.00643	0.01032	-0.00881	0.00712	0.00731	0.00773	-0.01658	0.01148
182	C	0.03017	0.01859	-0.02828	0.02133	-0.02091	0.00266	0.00531	0.00634	-0.00817
183	C	-0.03510	0.00420	-0.01474	0.01778	-0.00133	-0.00967	0.02432	-0.00738	-0.00456
184	C	-0.08023	-0.00217	0.00172	-0.01356	0.08653	-0.01713	0.16771	-0.18448	0.08049
185	C	0.06527	0.04468	-0.09653	0.07724	0.00318	-0.04242	0.12086	-0.06531	-0.00104
186	C	-0.03710	0.00896	-0.02592	0.01892	0.05686	-0.03048	0.14746	-0.13317	0.04544
187	H	-0.08037	-0.00088	-0.00123	-0.01004	0.07650	-0.01274	0.14918	-0.16509	0.07219
188	H	0.05811	0.04940	-0.10507	0.08387	0.01138	-0.03711	0.13463	-0.08707	0.00959
189	H	-0.04446	0.00998	-0.02416	0.00983	0.11778	-0.04384	0.25136	-0.25356	0.09933
190	H	-0.08217	0.00653	-0.01816	-0.00201	0.14197	-0.03746	0.28532	-0.30349	0.12705
191	H	0.07814	0.04859	-0.11102	0.08693	0.00911	-0.05847	0.15249	-0.07918	-0.00310

192	H	-0.04893	0.00030	-0.00163	0.00259	0.02565	-0.00464	0.06037	-0.06362	0.02599
193	H	-0.08095	-0.00900	0.01575	-0.03064	0.10538	-0.02189	0.19624	-0.21561	0.09477
194	H	0.07166	0.04807	-0.10805	0.08506	0.00993	-0.05214	0.14633	-0.08200	0.00115
195	H	-0.01772	0.01879	-0.05424	0.03922	0.07042	-0.05441	0.20543	-0.16758	0.04750
196	C	-0.13072	0.00818	-0.02078	0.04036	-0.09252	0.03699	-0.12624	0.11002	-0.04059
197	C	-0.02068	0.01662	-0.01459	0.02379	-0.07451	0.04359	-0.07822	0.05822	-0.01903
198	C	-0.10986	-0.00162	0.01491	0.01068	-0.06562	0.05072	-0.08341	0.04974	-0.01062
199	H	-0.13081	0.01093	-0.03080	0.05082	-0.11230	0.03844	-0.15990	0.14965	-0.05845
200	H	-0.03432	0.01035	0.00628	0.00623	-0.07972	0.06445	-0.09567	0.05490	-0.01037
201	H	-0.11029	0.00047	0.00812	0.01804	-0.08274	0.05328	-0.11291	0.08285	-0.02509
202	H	-0.16496	0.01105	-0.02395	0.05828	-0.12304	0.05130	-0.16387	0.13619	-0.04881
203	H	0.01591	0.01695	-0.02242	0.01904	-0.03624	0.01592	-0.01892	0.02001	-0.01012
204	H	-0.15164	-0.00309	0.02588	0.01322	-0.11170	0.08610	-0.15739	0.09707	-0.02113
205	H	-0.13373	0.01032	-0.02593	0.04698	-0.10521	0.03834	-0.14679	0.13225	-0.05027
206	H	-0.07909	0.02221	-0.02061	0.05400	-0.14981	0.07656	-0.18275	0.13970	-0.04702
207	H	-0.11420	-0.00578	0.02748	-0.00139	-0.04778	0.05445	-0.05269	0.00906	0.00885
208	N	0.04342	0.00813	-0.04136	-0.03802	0.05368	-0.08866	0.04800	0.08572	-0.06785
209	N	-0.00556	0.00038	0.00583	-0.10322	-0.00279	0.01453	-0.00640	-0.00481	0.00552
210	N	0.00129	-0.01154	0.00053	0.02305	0.01449	-0.02784	0.01178	0.02757	-0.02330
211	C	0.07006	-0.01704	-0.00693	-0.12953	0.00223	-0.01263	0.00890	0.02788	-0.02202
212	C	-0.03234	0.01267	-0.01100	-0.06609	0.02192	-0.02517	0.01468	0.02413	-0.01902
213	C	0.03808	-0.01100	-0.00014	-0.02691	0.01639	-0.02862	0.01542	0.03722	-0.03112
214	O	0.11637	-0.05670	0.03720	-0.32096	-0.05204	0.07624	-0.02926	-0.03642	0.02768
215	O	-0.04467	0.03268	-0.03394	-0.00588	0.04923	-0.06788	0.03500	0.06081	-0.04684
216	O	0.05869	-0.01351	0.00235	-0.09213	0.01044	-0.01841	0.01361	0.03612	-0.03016
217	C	0.02282	0.00593	-0.01663	-0.01742	0.00748	-0.02473	0.00896	0.03324	-0.02541
218	C	-0.05810	-0.00744	0.00881	-0.07190	0.01767	-0.01444	0.01077	0.01628	-0.01457
219	C	0.04523	-0.00796	-0.00356	-0.04174	0.01464	-0.02793	0.01773	0.03762	-0.03262
220	H	-0.00689	0.00537	-0.01045	-0.02496	0.00589	-0.01944	0.00383	0.03158	-0.02287
221	H	-0.09692	-0.02234	0.02435	-0.12812	0.01314	-0.00444	-0.00066	0.02010	-0.01435
222	H	0.07118	-0.02087	-0.00144	-0.07307	0.01683	-0.03230	0.01977	0.04632	-0.03899
223	C	0.04733	0.02062	-0.02215	0.09619	0.00288	-0.01539	0.01340	-0.00088	-0.00421
224	C	-0.06377	-0.01367	0.01721	-0.04651	0.01985	-0.01464	0.01076	0.01666	-0.01533
225	C	0.07456	0.01779	-0.03187	-0.08614	0.01418	-0.03101	0.03120	0.03103	-0.03188
226	H	0.04932	0.02330	-0.02142	0.12891	0.00062	-0.00935	0.01286	-0.01407	0.00469
227	H	-0.07270	-0.02093	0.02190	-0.09811	0.01551	-0.01067	-0.00109	0.02961	-0.02007
228	H	0.08973	0.02348	-0.04928	-0.09558	0.03515	-0.06682	0.06341	0.05693	-0.05903
229	H	0.05659	0.02261	-0.03067	0.13720	0.02659	-0.05130	0.04748	0.01781	-0.02734
230	H	-0.04914	0.00018	0.00200	-0.03948	0.02180	-0.01708	0.02550	0.00216	-0.01010
231	H	0.07711	0.02613	-0.03630	-0.10412	0.00088	-0.01025	0.02023	0.00821	-0.01310
232	C	0.02669	0.02078	-0.00603	0.08486	-0.03294	0.04478	-0.03399	-0.05065	0.04362
233	C	-0.07192	-0.02590	0.03758	0.05286	0.02409	-0.01585	0.01176	0.01180	-0.01325
234	C	0.05837	0.01595	-0.01781	-0.08801	-0.01187	0.01451	-0.00316	-0.00675	0.00389
235	H	0.00933	0.01851	0.00747	0.07791	-0.05706	0.08619	-0.06597	-0.08524	0.07649

236	H	-0.10562	-0.04040	0.06204	0.04701	0.02365	-0.00720	0.00289	0.01323	-0.01222
237	H	0.06385	0.01462	-0.02335	-0.08373	0.00513	-0.01287	0.01757	0.01766	-0.01884
238	H	0.04876	0.02651	-0.01135	0.12826	-0.03741	0.04835	-0.03419	-0.06291	0.05189
239	H	-0.05772	-0.02360	0.03497	0.08934	0.02352	-0.01657	0.01405	0.00658	-0.01055
240	H	0.07290	0.02755	-0.02940	-0.11797	-0.03029	0.03860	-0.02060	-0.03036	0.02577
241	C	-0.00948	0.01060	0.00265	0.00427	-0.02449	0.03528	-0.03144	-0.02604	0.02620
242	C	-0.03758	-0.01520	0.02329	0.08991	0.02165	-0.01849	0.01641	0.00418	-0.00924
243	C	0.01192	-0.00211	0.02272	-0.04658	-0.03296	0.05967	-0.03765	-0.04425	0.03844
244	H	-0.01592	0.00939	0.01536	-0.02909	-0.04641	0.07590	-0.06017	-0.05851	0.05649
245	H	-0.06135	-0.02515	0.03765	0.13999	0.02554	-0.02150	0.01690	0.00513	-0.01079
246	H	-0.00346	-0.00839	0.03374	-0.02439	-0.03630	0.06837	-0.04479	-0.05191	0.04538
247	H	-0.00762	0.01094	-0.00402	0.01868	-0.01135	0.01173	-0.01467	-0.00738	0.00868
248	H	-0.00154	-0.00247	0.00779	0.12928	0.01629	-0.01520	0.01777	-0.01055	0.00062
249	H	0.02510	0.00329	0.02807	-0.05622	-0.05933	0.10442	-0.06771	-0.08577	0.07541
250	N	-0.03398	0.00235	-0.00361	-0.04519	0.00485	-0.01429	0.00044	0.02934	-0.02064
251	N	-0.02298	-0.00707	0.00981	-0.00608	0.01465	-0.01209	0.01155	0.00802	-0.00953
252	N	-0.02057	-0.01445	0.02382	-0.00694	-0.00140	0.00570	-0.00362	0.00575	-0.00581