

Supporting Information for: Theoretical structural and spectroscopic characterization of Peroxyacetic Acid (CH<sub>3</sub>-CO-OOH).

Study of the Far Infrared region.

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Table S4

Potential Energy Surface. Selected geometries and energies

Geometry (MP2/AVTZ) 1

Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.493941( 1)					
3	3	O	1	1.353403( 2)	2	110.565( 9)			
4	4	O	1	1.213162( 3)	2	127.314( 10)	3	180.000( 16)	0
5	5	O	3	1.439708( 4)	1	110.119( 11)	2	180.000( 17)	0
6	6	H	5	0.985653( 5)	3	99.679( 12)	1	-0.000( 18)	0
7	7	H	2	1.085075( 6)	1	111.425( 13)	3	-0.000( 19)	0
8	8	H	2	1.087577( 7)	1	108.433( 14)	7	121.362( 20)	0
9	9	H	2	1.087577( 8)	1	108.433( 15)	7	-121.362( 21)	0

-304.21180809 Energy CCSD(T)-F12/CVTA-F12

Geometry (MP2/AVTZ) 2

Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.494424( 1)					
3	3	O	1	1.353865( 2)	2	110.361( 9)			
4	4	O	1	1.213236( 3)	2	127.518( 10)	3	180.477( 16)	0
5	5	O	3	1.439634( 4)	1	110.230( 11)	2	180.000( 17)	0
6	6	H	5	0.985275( 5)	3	99.641( 12)	1	0.000( 18)	0
7	7	H	2	1.088937( 6)	1	108.597( 13)	3	90.000( 19)	0
8	8	H	2	1.085186( 7)	1	108.732( 14)	7	118.476( 20)	0
9	9	H	2	1.085820( 8)	1	110.922( 15)	7	-119.336( 21)	0

-304.21161605 Energy CCSD(T)-F12/CVTA-F12

Geometry (MP2/AVTZ) 3

Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.495062( 1)					
3	3	O	1	1.354068( 2)	2	110.185( 9)			
4	4	O	1	1.213258( 3)	2	127.720( 10)	3	180.000( 16)	0
5	5	O	3	1.439858( 4)	1	110.252( 11)	2	180.000( 17)	0
6	6	H	5	0.985046( 5)	3	99.642( 12)	1	0.000( 18)	0
7	7	H	2	1.084326( 6)	1	108.733( 13)	3	180.000( 19)	0

8 8 H 2 1.087676( 7) 1 109.767( 14) 7 120.612( 20) 0  
9 9 H 2 1.087676( 8) 1 109.767( 15) 7 -120.612( 21) 0

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-304.21140476 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 4

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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.498510( 1)  
3 3 O 1 1.365697( 2) 2 109.137( 9)  
4 4 O 1 1.206128( 3) 2 127.240( 10) 3 184.670( 16) 0  
5 5 O 3 1.438563( 4) 1 110.837( 11) 2 180.000( 17) 0  
6 6 H 5 0.973957( 5) 3 101.553( 12) 1 45.000( 18) 0  
7 7 H 2 1.085096( 6) 1 111.732( 13) 3 0.000( 19) 0  
8 8 H 2 1.087298( 7) 1 108.019( 14) 7 121.360( 20) 0  
9 9 H 2 1.087754( 8) 1 108.630( 15) 7 -121.500( 21) 0  
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-304.20708371 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 5

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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
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1 1 C  
2 2 C 1 1.498338( 1)  
3 3 O 1 1.365951( 2) 2 108.934( 9)  
4 4 O 1 1.206243( 3) 2 127.429( 10) 3 185.451( 16) 0  
5 5 O 3 1.438463( 4) 1 110.872( 11) 2 180.000( 17) 0  
6 6 H 5 0.974059( 5) 3 101.583( 12) 1 45.000( 18) 0  
7 7 H 2 1.088824( 6) 1 108.102( 13) 3 90.000( 19) 0  
8 8 H 2 1.085406( 7) 1 108.705( 14) 7 118.001( 20) 0  
9 9 H 2 1.085754( 8) 1 111.492( 15) 7 -119.538( 21) 0  
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-304.20713105 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 6

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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
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1 1 C  
2 2 C 1 1.499043( 1)  
3 3 O 1 1.366535( 2) 2 108.724( 9)  
4 4 O 1 1.206250( 3) 2 127.722( 10) 3 185.048( 16) 0  
5 5 O 3 1.438544( 4) 1 110.945( 11) 2 180.000( 17) 0  
6 6 H 5 0.973889( 5) 3 101.550( 12) 1 45.000( 18) 0  
7 7 H 2 1.084372( 6) 1 108.586( 13) 3 180.000( 19) 0  
8 8 H 2 1.087477( 7) 1 110.508( 14) 7 121.248( 20) 0  
9 9 H 2 1.087894( 8) 1 109.246( 15) 7 -119.902( 21) 0  
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-304.20687240 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 7

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.499027( 1)					
3	3	O	1	1.366567( 2)	2	108.905( 9)			
4	4	O	1	1.206101( 3)	2	127.559( 10)	3	184.166( 16)	0
5	5	O	3	1.438759( 4)	1	110.927( 11)	2	180.000( 17)	0
6	6	H	5	0.973838( 5)	3	101.501( 12)	1	45.000( 18)	0
7	7	H	2	1.089082( 6)	1	109.027( 13)	3	270.000( 19)	0
8	8	H	2	1.085828( 7)	1	110.915( 14)	7	119.389( 20)	0
9	9	H	2	1.084970( 8)	1	108.444( 15)	7	-118.555( 21)	0

-304.20683863 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 8

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502053( 1)					
3	3	O	1	1.379195( 2)	2	107.837( 9)			
4	4	O	1	1.199366( 3)	2	127.260( 10)	3	182.102( 16)	0
5	5	O	3	1.440552( 4)	1	110.635( 11)	2	180.000( 17)	0
6	6	H	5	0.969210( 5)	3	100.618( 12)	1	90.000( 18)	0
7	7	H	2	1.085068( 6)	1	112.039( 13)	3	0.000( 19)	0
8	8	H	2	1.087508( 7)	1	107.988( 14)	7	121.423( 20)	0
9	9	H	2	1.087600( 8)	1	108.442( 15)	7	-121.608( 21)	0

-304.20401907 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 9

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.501614( 1)					
3	3	O	1	1.379637( 2)	2	107.587( 9)			
4	4	O	1	1.199631( 3)	2	127.552( 10)	3	182.873( 16)	0
5	5	O	3	1.440140( 4)	1	110.718( 11)	2	180.000( 17)	0
6	6	H	5	0.969338( 5)	3	100.800( 12)	1	90.000( 18)	0
7	7	H	2	1.089015( 6)	1	108.255( 13)	3	90.000( 19)	0
8	8	H	2	1.085266( 7)	1	108.613( 14)	7	118.022( 20)	0
9	9	H	2	1.085814( 8)	1	111.553( 15)	7	-119.521( 21)	0

-304.20409026 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 10

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Z-MATRIX (ANGSTROMS AND DEGREES)  
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502079( 1)					
3	3	O	1	1.380054( 2)	2	107.354( 9)			
4	4	O	1	1.199676( 3)	2	127.856( 10)	3	182.271( 16)	0
5	5	O	3	1.440020( 4)	1	110.776( 11)	2	180.000( 17)	0
6	6	H	5	0.969229( 5)	3	100.690( 12)	1	90.000( 18)	0
7	7	H	2	1.084417( 6)	1	108.499( 13)	3	180.000( 19)	0
8	8	H	2	1.087590( 7)	1	110.307( 14)	7	120.948( 20)	0
9	9	H	2	1.087882( 8)	1	109.641( 15)	7	-120.150( 21)	0

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-304.20394275 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 11

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Z-MATRIX (ANGSTROMS AND DEGREES)  
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502063( 1)					
3	3	O	1	1.379814( 2)	2	107.614( 9)			
4	4	O	1	1.199605( 3)	2	127.572( 10)	3	181.383( 16)	0
5	5	O	3	1.440596( 4)	1	110.734( 11)	2	180.000( 17)	0
6	6	H	5	0.969195( 5)	3	100.552( 12)	1	90.000( 18)	0
7	7	H	2	1.089127( 6)	1	108.745( 13)	3	270.000( 19)	0
8	8	H	2	1.085765( 7)	1	111.357( 14)	7	119.504( 20)	0
9	9	H	2	1.085091( 8)	1	108.372( 15)	7	-118.208( 21)	0

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-304.20388912 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 12

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Z-MATRIX (ANGSTROMS AND DEGREES)  
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502822( 1)					
3	3	O	1	1.376329( 2)	2	107.719( 9)			
4	4	O	1	1.198602( 3)	2	127.237( 10)	3	179.947( 16)	0
5	5	O	3	1.448983( 4)	1	109.369( 11)	2	180.000( 17)	0
6	6	H	5	0.968512( 5)	3	98.134( 12)	1	135.000( 18)	0
7	7	H	2	1.085134( 6)	1	112.159( 13)	3	0.000( 19)	0
8	8	H	2	1.087598( 7)	1	108.035( 14)	7	121.439( 20)	0
9	9	H	2	1.087492( 8)	1	108.342( 15)	7	-121.604( 21)	0

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-304.20324815 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 13

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Z-MATRIX (ANGSTROMS AND DEGREES)  
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502733( 1)					
3	3	O	1	1.376098( 2)	2	107.477( 9)			
4	4	O	1	1.198936( 3)	2	127.514( 10)	3	180.653( 16)	0
5	5	O	3	1.448311( 4)	1	109.437( 11)	2	180.000( 17)	0
6	6	H	5	0.968477( 5)	3	98.220( 12)	1	135.000( 18)	0
7	7	H	2	1.089068( 6)	1	108.399( 13)	3	90.000( 19)	0
8	8	H	2	1.085236( 7)	1	108.466( 14)	7	118.046( 20)	0
9	9	H	2	1.085792( 8)	1	111.604( 15)	7	-119.644( 21)	0

-304.20323212 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 14

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503221( 1)					
3	3	O	1	1.376479( 2)	2	107.251( 9)			
4	4	O	1	1.198946( 3)	2	127.802( 10)	3	179.914( 16)	0
5	5	O	3	1.448353( 4)	1	109.473( 11)	2	180.000( 17)	0
6	6	H	5	0.968427( 5)	3	98.131( 12)	1	135.000( 18)	0
7	7	H	2	1.084526( 6)	1	108.298( 13)	3	180.000( 19)	0
8	8	H	2	1.087674( 7)	1	110.118( 14)	7	120.421( 20)	0
9	9	H	2	1.087695( 8)	1	110.057( 15)	7	-120.382( 21)	0

-304.20313172 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 15

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502733( 1)					
3	3	O	1	1.376544( 2)	2	107.489( 9)			
4	4	O	1	1.198809( 3)	2	127.556( 10)	3	179.203( 16)	0
5	5	O	3	1.448585( 4)	1	109.338( 11)	2	180.000( 17)	0
6	6	H	5	0.968467( 5)	3	98.024( 12)	1	135.000( 18)	0
7	7	H	2	1.088977( 6)	1	108.657( 13)	3	270.000( 19)	0
8	8	H	2	1.085863( 7)	1	111.567( 14)	7	119.674( 20)	0
9	9	H	2	1.085183( 8)	1	108.289( 15)	7	-118.102( 21)	0

-304.20316794 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 16

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							

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2  2 C   1  1.502494(  1)
3  3 O   1  1.370701(  2)  2 108.015(  9)
4  4 O   1  1.199486(  3)  2 127.307( 10)  3 180.000( 16)  0
5  5 O   3  1.454177(  4)  1 108.215( 11)  2 180.000( 17)  0
6  6 H   5  0.969132(  5)  3  96.851( 12)  1 180.000( 18)  0
7  7 H   2  1.085217(  6)  1 112.179( 13)  3  0.000( 19)  0
8  8 H   2  1.087527(  7)  1 108.196( 14)  7 121.502( 20)  0
9  9 H   2  1.087527(  8)  1 108.196( 15)  7 -121.502( 21)  0

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-304.20324259 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 17  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502619( 1)					
3	3	O	1	1.370539( 2)	2	107.807( 9)			
4	4	O	1	1.199793( 3)	2	127.571( 10)	3	180.682( 16)	0
5	5	O	3	1.453718( 4)	1	108.265( 11)	2	180.000( 17)	0
6	6	H	5	0.969063( 5)	3	96.841( 12)	1	180.000( 18)	0
7	7	H	2	1.088975( 6)	1	108.575( 13)	3	90.000( 19)	0
8	8	H	2	1.085262( 7)	1	108.310( 14)	7	118.059( 20)	0
9	9	H	2	1.085850( 8)	1	111.630( 15)	7	-119.778( 21)	0

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-304.20317313 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 18  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503036( 1)					
3	3	O	1	1.370922( 2)	2	107.580( 9)			
4	4	O	1	1.199829( 3)	2	127.858( 10)	3	180.000( 16)	0
5	5	O	3	1.453777( 4)	1	108.299( 11)	2	180.000( 17)	0
6	6	H	5	0.969048( 5)	3	96.833( 12)	1	180.000( 18)	0
7	7	H	2	1.084511( 6)	1	108.239( 13)	3	180.000( 19)	0
8	8	H	2	1.087697( 7)	1	110.126( 14)	7	120.343( 20)	0
9	9	H	2	1.087697( 8)	1	110.126( 15)	7	-120.343( 21)	0

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-304.20307657 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 19  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502822( 1)					
3	3	O	1	1.376329( 2)	2	107.719( 9)			
4	4	O	1	1.198602( 3)	2	127.237( 10)	3	180.053( 16)	0

5	5	O	3	1.448983( 4)	1	109.369( 11)	2	180.000( 17)	0
6	6	H	5	0.968512( 5)	3	98.134( 12)	1	225.000( 18)	0
7	7	H	2	1.085134( 6)	1	112.159( 13)	3	0.000( 19)	0
8	8	H	2	1.087492( 7)	1	108.342( 14)	7	121.604( 20)	0
9	9	H	2	1.087598( 8)	1	108.035( 15)	7	-121.439( 21)	0

-304.20324815 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 20

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502733( 1)					
3	3	O	1	1.376544( 2)	2	107.489( 9)			
4	4	O	1	1.198809( 3)	2	127.556( 10)	3	180.797( 16)	0
5	5	O	3	1.448585( 4)	1	109.338( 11)	2	180.000( 17)	0
6	6	H	5	0.968467( 5)	3	98.024( 12)	1	225.000( 18)	0
7	7	H	2	1.088977( 6)	1	108.657( 13)	3	90.000( 19)	0
8	8	H	2	1.085183( 7)	1	108.289( 14)	7	118.102( 20)	0
9	9	H	2	1.085863( 8)	1	111.567( 15)	7	-119.674( 21)	0

-304.20316794 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 21

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503221( 1)					
3	3	O	1	1.376479( 2)	2	107.251( 9)			
4	4	O	1	1.198946( 3)	2	127.802( 10)	3	180.086( 16)	0
5	5	O	3	1.448353( 4)	1	109.473( 11)	2	180.000( 17)	0
6	6	H	5	0.968427( 5)	3	98.131( 12)	1	225.000( 18)	0
7	7	H	2	1.084526( 6)	1	108.298( 13)	3	180.000( 19)	0
8	8	H	2	1.087694( 7)	1	110.057( 14)	7	120.382( 20)	0
9	9	H	2	1.087674( 8)	1	110.118( 15)	7	-120.421( 21)	0

-304.20313172 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 22

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502733( 1)					
3	3	O	1	1.376098( 2)	2	107.477( 9)			
4	4	O	1	1.198936( 3)	2	127.514( 10)	3	179.347( 16)	0
5	5	O	3	1.448311( 4)	1	109.437( 11)	2	180.000( 17)	0
6	6	H	5	0.968477( 5)	3	98.220( 12)	1	225.000( 18)	0
7	7	H	2	1.089068( 6)	1	108.399( 13)	3	270.000( 19)	0

8 8 H 2 1.085792( 7) 1 111.604( 14) 7 119.644( 20) 0  
9 9 H 2 1.085236( 8) 1 108.466( 15) 7 -118.046( 21) 0

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-304.20323212 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 23  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
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1 1 C  
2 2 C 1 1.502053( 1)  
3 3 O 1 1.379195( 2) 2 107.837( 9)  
4 4 O 1 1.199366( 3) 2 127.260( 10) 3 177.898( 16) 0  
5 5 O 3 1.440552( 4) 1 110.635( 11) 2 180.000( 17) 0  
6 6 H 5 0.969210( 5) 3 100.618( 12) 1 270.000( 18) 0  
7 7 H 2 1.085068( 6) 1 112.039( 13) 3 0.000( 19) 0  
8 8 H 2 1.087600( 7) 1 108.442( 14) 7 121.608( 20) 0  
9 9 H 2 1.087508( 8) 1 107.988( 15) 7 -121.423( 21) 0  
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-304.20401907 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 24  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
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1 1 C  
2 2 C 1 1.502063( 1)  
3 3 O 1 1.379814( 2) 2 107.614( 9)  
4 4 O 1 1.199605( 3) 2 127.572( 10) 3 178.617( 16) 0  
5 5 O 3 1.440596( 4) 1 110.734( 11) 2 180.000( 17) 0  
6 6 H 5 0.969195( 5) 3 100.552( 12) 1 270.000( 18) 0  
7 7 H 2 1.089127( 6) 1 108.745( 13) 3 90.000( 19) 0  
8 8 H 2 1.085091( 7) 1 108.372( 14) 7 118.208( 20) 0  
9 9 H 2 1.085765( 8) 1 111.357( 15) 7 -119.504( 21) 0  
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-304.20388912 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 25  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.502079( 1)  
3 3 O 1 1.380054( 2) 2 107.354( 9)  
4 4 O 1 1.199676( 3) 2 127.856( 10) 3 177.729( 16) 0  
5 5 O 3 1.440020( 4) 1 110.776( 11) 2 180.000( 17) 0  
6 6 H 5 0.969229( 5) 3 100.690( 12) 1 270.000( 18) 0  
7 7 H 2 1.084417( 6) 1 108.499( 13) 3 180.000( 19) 0  
8 8 H 2 1.087882( 7) 1 109.641( 14) 7 120.150( 20) 0  
9 9 H 2 1.087590( 8) 1 110.307( 15) 7 -120.948( 21) 0  
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-304.20394275 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 26

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.501614( 1)					
3	3	O	1	1.379637( 2)	2	107.587( 9)			
4	4	O	1	1.199631( 3)	2	127.552( 10)	3	177.127( 16)	0
5	5	O	3	1.440140( 4)	1	110.718( 11)	2	180.000( 17)	0
6	6	H	5	0.969338( 5)	3	100.800( 12)	1	270.000( 18)	0
7	7	H	2	1.089015( 6)	1	108.255( 13)	3	270.000( 19)	0
8	8	H	2	1.085814( 7)	1	111.553( 14)	7	119.521( 20)	0
9	9	H	2	1.085266( 8)	1	108.613( 15)	7	-118.022( 21)	0

-304.20409025 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 27

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498510( 1)					
3	3	O	1	1.365697( 2)	2	109.137( 9)			
4	4	O	1	1.206128( 3)	2	127.240( 10)	3	175.330( 16)	0
5	5	O	3	1.438563( 4)	1	110.837( 11)	2	180.000( 17)	0
6	6	H	5	0.973957( 5)	3	101.553( 12)	1	315.000( 18)	0
7	7	H	2	1.085096( 6)	1	111.732( 13)	3	0.000( 19)	0
8	8	H	2	1.087754( 7)	1	108.630( 14)	7	121.500( 20)	0
9	9	H	2	1.087298( 8)	1	108.019( 15)	7	-121.360( 21)	0

-304.20708371 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 28

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.499027( 1)					
3	3	O	1	1.366567( 2)	2	108.905( 9)			
4	4	O	1	1.206101( 3)	2	127.559( 10)	3	175.834( 16)	0
5	5	O	3	1.438759( 4)	1	110.927( 11)	2	180.000( 17)	0
6	6	H	5	0.973838( 5)	3	101.501( 12)	1	315.000( 18)	0
7	7	H	2	1.089082( 6)	1	109.027( 13)	3	90.000( 19)	0
8	8	H	2	1.084970( 7)	1	108.444( 14)	7	118.555( 20)	0
9	9	H	2	1.085828( 8)	1	110.915( 15)	7	-119.389( 21)	0

-304.20683863 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 29

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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.499043( 1)					
3	3	O	1	1.366535( 2)	2	108.724( 9)			
4	4	O	1	1.206250( 3)	2	127.722( 10)	3	174.952( 16)	0
5	5	O	3	1.438544( 4)	1	110.945( 11)	2	180.000( 17)	0
6	6	H	5	0.973889( 5)	3	101.550( 12)	1	315.000( 18)	0
7	7	H	2	1.084372( 6)	1	108.586( 13)	3	180.000( 19)	0
8	8	H	2	1.087894( 7)	1	109.246( 14)	7	119.902( 20)	0
9	9	H	2	1.087477( 8)	1	110.508( 15)	7	-121.248( 21)	0

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-304.20687240 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 30

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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498338( 1)					
3	3	O	1	1.365951( 2)	2	108.934( 9)			
4	4	O	1	1.206243( 3)	2	127.429( 10)	3	174.549( 16)	0
5	5	O	3	1.438463( 4)	1	110.872( 11)	2	180.000( 17)	0
6	6	H	5	0.974059( 5)	3	101.583( 12)	1	315.000( 18)	0
7	7	H	2	1.088824( 6)	1	108.102( 13)	3	270.000( 19)	0
8	8	H	2	1.085754( 7)	1	111.492( 14)	7	119.538( 20)	0
9	9	H	2	1.085406( 8)	1	108.705( 15)	7	-118.001( 21)	0

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-304.20713105 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 31

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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502565( 1)					
3	3	O	1	1.372908( 2)	2	111.383( 9)			
4	4	O	1	1.208984( 3)	2	125.142( 10)	3	166.151( 16)	0
5	5	O	3	1.449600( 4)	1	110.548( 11)	2	135.000( 17)	0
6	6	H	5	0.976867( 5)	3	101.317( 12)	1	0.000( 18)	0
7	7	H	2	1.083865( 6)	1	111.712( 13)	3	0.000( 19)	0
8	8	H	2	1.087273( 7)	1	111.469( 14)	7	124.838( 20)	0
9	9	H	2	1.088253( 8)	1	105.026( 15)	7	-118.580( 21)	0

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-304.19246888 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 32

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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503802( 1)					
3	3	O	1	1.374021( 2)	2	111.383( 9)			
4	4	O	1	1.209182( 3)	2	125.343( 10)	3	166.120( 16)	0
5	5	O	3	1.449392( 4)	1	110.505( 11)	2	135.000( 17)	0
6	6	H	5	0.976696( 5)	3	101.376( 12)	1	0.000( 18)	0
7	7	H	2	1.089617( 6)	1	111.590( 13)	3	90.000( 19)	0
8	8	H	2	1.085215( 7)	1	107.087( 14)	7	118.079( 20)	0
9	9	H	2	1.084359( 8)	1	109.736( 15)	7	-120.761( 21)	0

-304.19193678 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 33

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498508( 1)					
3	3	O	1	1.374022( 2)	2	110.351( 9)			
4	4	O	1	1.208949( 3)	2	125.772( 10)	3	164.698( 16)	0
5	5	O	3	1.448611( 4)	1	110.509( 11)	2	135.000( 17)	0
6	6	H	5	0.977054( 5)	3	101.336( 12)	1	0.000( 18)	0
7	7	H	2	1.084381( 6)	1	109.394( 13)	3	180.000( 19)	0
8	8	H	2	1.088564( 7)	1	105.890( 14)	7	118.413( 20)	0
9	9	H	2	1.087690( 8)	1	112.495( 15)	7	-124.059( 21)	0

-304.19394472 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 34

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.497701( 1)					
3	3	O	1	1.372995( 2)	2	110.437( 9)			
4	4	O	1	1.208730( 3)	2	125.620( 10)	3	164.903( 16)	0
5	5	O	3	1.448913( 4)	1	110.472( 11)	2	135.000( 17)	0
6	6	H	5	0.977131( 5)	3	101.285( 12)	1	0.000( 18)	0
7	7	H	2	1.089428( 6)	1	104.818( 13)	3	270.000( 19)	0
8	8	H	2	1.085447( 7)	1	112.300( 14)	7	118.355( 20)	0
9	9	H	2	1.085798( 8)	1	110.500( 15)	7	-117.030( 21)	0

-304.19433352 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 35

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							

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2  2 C   1  1.498264( 1)
3  3 O   1  1.379150( 2)  2 111.904( 9)
4  4 O   1  1.206831( 3)  2 126.235( 10)  3 172.156( 16)  0
5  5 O   3  1.446949( 4)  1 108.704( 11)  2 135.000( 17)  0
6  6 H   5  0.976616( 5)  3 100.794( 12)  1  45.000( 18)  0
7  7 H   2  1.083923( 6)  1 111.671( 13)  3  0.000( 19)  0
8  8 H   2  1.087088( 7)  1 111.036( 14)  7 124.731( 20)  0
9  9 H   2  1.088894( 8)  1 105.499( 15)  7 -118.595( 21)  0

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-304.19731969 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 36  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.499016( 1)					
3	3	O	1	1.380518( 2)	2	111.896( 9)			
4	4	O	1	1.207003( 3)	2	126.459( 10)	3	172.469( 16)	0
5	5	O	3	1.446808( 4)	1	108.593( 11)	2	135.000( 17)	0
6	6	H	5	0.976504( 5)	3	100.760( 12)	1	45.000( 18)	0
7	7	H	2	1.089836( 6)	1	110.728( 13)	3	90.000( 19)	0
8	8	H	2	1.085611( 7)	1	107.477( 14)	7	117.690( 20)	0
9	9	H	2	1.084283( 8)	1	110.210( 15)	7	-120.732( 21)	0

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-304.19687817 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 37  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.494286( 1)					
3	3	O	1	1.380584( 2)	2	110.806( 9)			
4	4	O	1	1.206623( 3)	2	127.169( 10)	3	171.304( 16)	0
5	5	O	3	1.446312( 4)	1	108.616( 11)	2	135.000( 17)	0
6	6	H	5	0.976456( 5)	3	100.762( 12)	1	45.000( 18)	0
7	7	H	2	1.084371( 6)	1	109.569( 13)	3	180.000( 19)	0
8	8	H	2	1.088565( 7)	1	106.729( 14)	7	119.187( 20)	0
9	9	H	2	1.088189( 8)	1	111.586( 15)	7	-123.376( 21)	0

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-304.19862142 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 38  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.493814( 1)					
3	3	O	1	1.379355( 2)	2	110.902( 9)			
4	4	O	1	1.206519( 3)	2	126.920( 10)	3	171.267( 16)	0

5	5	O	3	1.446598( 4)	1	108.705( 11)	2	135.000( 17)	0
6	6	H	5	0.976561( 5)	3	100.778( 12)	1	45.000( 18)	0
7	7	H	2	1.089995( 6)	1	105.444( 13)	3	270.000( 19)	0
8	8	H	2	1.085730( 7)	1	111.807( 14)	7	118.037( 20)	0
9	9	H	2	1.085473( 8)	1	110.448( 15)	7	-117.511( 21)	0

-304.19896823 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 39

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.500150( 1)					
3	3	O	1	1.394183( 2)	2	110.635( 9)			
4	4	O	1	1.200390( 3)	2	126.622( 10)	3	175.432( 16)	0
5	5	O	3	1.443146( 4)	1	108.510( 11)	2	135.000( 17)	0
6	6	H	5	0.970126( 5)	3	101.533( 12)	1	90.000( 18)	0
7	7	H	2	1.084009( 6)	1	111.900( 13)	3	0.000( 19)	0
8	8	H	2	1.087074( 7)	1	110.531( 14)	7	124.449( 20)	0
9	9	H	2	1.089051( 8)	1	105.982( 15)	7	-118.911( 21)	0

-304.19589793 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 40

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.500566( 1)					
3	3	O	1	1.395538( 2)	2	110.606( 9)			
4	4	O	1	1.200534( 3)	2	126.883( 10)	3	176.006( 16)	0
5	5	O	3	1.442822( 4)	1	108.336( 11)	2	135.000( 17)	0
6	6	H	5	0.970026( 5)	3	101.453( 12)	1	90.000( 18)	0
7	7	H	2	1.089979( 6)	1	110.143( 13)	3	90.000( 19)	0
8	8	H	2	1.085795( 7)	1	107.660( 14)	7	117.391( 20)	0
9	9	H	2	1.084207( 8)	1	110.763( 15)	7	-120.703( 21)	0

-304.19556039 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 41

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.496414( 1)					
3	3	O	1	1.395550( 2)	2	109.461( 9)			
4	4	O	1	1.200195( 3)	2	127.680( 10)	3	174.789( 16)	0
5	5	O	3	1.442594( 4)	1	108.439( 11)	2	135.000( 17)	0
6	6	H	5	0.969929( 5)	3	101.444( 12)	1	90.000( 18)	0
7	7	H	2	1.084418( 6)	1	109.471( 13)	3	180.000( 19)	0

8 8 H 2 1.088341( 7) 1 107.462( 14) 7 119.569( 20) 0  
9 9 H 2 1.088479( 8) 1 111.168( 15) 7 -122.881( 21) 0

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-304.19716128 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 42  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.496116( 1)  
3 3 O 1 1.394232( 2) 2 109.559( 9)  
4 4 O 1 1.200116( 3) 2 127.393( 10) 3 174.535( 16) 0  
5 5 O 3 1.442968( 4) 1 108.567( 11) 2 135.000( 17) 0  
6 6 H 5 0.970055( 5) 3 101.506( 12) 1 90.000( 18) 0  
7 7 H 2 1.090072( 6) 1 106.020( 13) 3 270.000( 19) 0  
8 8 H 2 1.085914( 7) 1 111.715( 14) 7 118.073( 20) 0  
9 9 H 2 1.085347( 8) 1 110.202( 15) 7 -117.723( 21) 0  
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-304.19744366 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 43  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.502139( 1)  
3 3 O 1 1.396282( 2) 2 109.975( 9)  
4 4 O 1 1.198282( 3) 2 126.429( 10) 3 174.783( 16) 0  
5 5 O 3 1.450700( 4) 1 107.674( 11) 2 135.000( 17) 0  
6 6 H 5 0.968253( 5) 3 99.512( 12) 1 135.000( 18) 0  
7 7 H 2 1.083969( 6) 1 112.080( 13) 3 0.000( 19) 0  
8 8 H 2 1.087040( 7) 1 110.507( 14) 7 124.592( 20) 0  
9 9 H 2 1.089041( 8) 1 105.876( 15) 7 -118.862( 21) 0  
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-304.19288664 Energy CCSD(T)-F12/CVTA-F12  
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=====  
Geometry (MP2/AVTZ) 44  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.502863( 1)  
3 3 O 1 1.397008( 2) 2 109.931( 9)  
4 4 O 1 1.198521( 3) 2 126.661( 10) 3 175.346( 16) 0  
5 5 O 3 1.450558( 4) 1 107.553( 11) 2 135.000( 17) 0  
6 6 H 5 0.968149( 5) 3 99.430( 12) 1 135.000( 18) 0  
7 7 H 2 1.090048( 6) 1 110.214( 13) 3 90.000( 19) 0  
8 8 H 2 1.085807( 7) 1 107.456( 14) 7 117.168( 20) 0  
9 9 H 2 1.084046( 8) 1 110.928( 15) 7 -120.939( 21) 0  
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-304.19253599 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 45

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498486( 1)					
3	3	O	1	1.397328( 2)	2	108.755( 9)			
4	4	O	1	1.198127( 3)	2	127.493( 10)	3	173.952( 16)	0
5	5	O	3	1.449980( 4)	1	107.632( 11)	2	135.000( 17)	0
6	6	H	5	0.968114( 5)	3	99.424( 12)	1	135.000( 18)	0
7	7	H	2	1.084451( 6)	1	109.331( 13)	3	180.000( 19)	0
8	8	H	2	1.088288( 7)	1	107.435( 14)	7	119.383( 20)	0
9	9	H	2	1.088433( 8)	1	111.377( 15)	7	-122.925( 21)	0

-304.19420019 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 46

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498002( 1)					
3	3	O	1	1.396494( 2)	2	108.861( 9)			
4	4	O	1	1.197969( 3)	2	127.214( 10)	3	173.768( 16)	0
5	5	O	3	1.450319( 4)	1	107.709( 11)	2	135.000( 17)	0
6	6	H	5	0.968221( 5)	3	99.453( 12)	1	135.000( 18)	0
7	7	H	2	1.089958( 6)	1	106.008( 13)	3	270.000( 19)	0
8	8	H	2	1.085903( 7)	1	111.896( 14)	7	118.209( 20)	0
9	9	H	2	1.085396( 8)	1	110.073( 15)	7	-117.621( 21)	0

-304.19449019 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 47

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503019( 1)					
3	3	O	1	1.391710( 2)	2	110.299( 9)			
4	4	O	1	1.198370( 3)	2	126.286( 10)	3	173.878( 16)	0
5	5	O	3	1.461502( 4)	1	106.609( 11)	2	135.000( 17)	0
6	6	H	5	0.968707( 5)	3	97.122( 12)	1	180.000( 18)	0
7	7	H	2	1.083983( 6)	1	112.178( 13)	3	0.000( 19)	0
8	8	H	2	1.087040( 7)	1	110.648( 14)	7	124.736( 20)	0
9	9	H	2	1.089002( 8)	1	105.681( 15)	7	-118.762( 21)	0

-304.19087433 Energy CCSD(T)-F12/CVTA-F12

Geometry (MP2/AVTZ) 48

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Z-MATRIX (ANGSTROMS AND DEGREES)  
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503453( 1)					
3	3	O	1	1.393380( 2)	2	110.238( 9)			
4	4	O	1	1.198448( 3)	2	126.611( 10)	3	174.411( 16)	0
5	5	O	3	1.461291( 4)	1	106.436( 11)	2	135.000( 17)	0
6	6	H	5	0.968675( 5)	3	97.108( 12)	1	180.000( 18)	0
7	7	H	2	1.089954( 6)	1	110.413( 13)	3	90.000( 19)	0
8	8	H	2	1.085754( 7)	1	107.427( 14)	7	117.346( 20)	0
9	9	H	2	1.084165( 8)	1	110.834( 15)	7	-120.964( 21)	0

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-304.19050532 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 49

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Z-MATRIX (ANGSTROMS AND DEGREES)  
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498806( 1)					
3	3	O	1	1.393494( 2)	2	109.017( 9)			
4	4	O	1	1.198098( 3)	2	127.446( 10)	3	173.043( 16)	0
5	5	O	3	1.460319( 4)	1	106.507( 11)	2	135.000( 17)	0
6	6	H	5	0.968646( 5)	3	97.142( 12)	1	180.000( 18)	0
7	7	H	2	1.084466( 6)	1	109.372( 13)	3	180.000( 19)	0
8	8	H	2	1.088300( 7)	1	107.359( 14)	7	119.356( 20)	0
9	9	H	2	1.088533( 8)	1	111.416( 15)	7	-122.905( 21)	0

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-304.19227939 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 50

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Z-MATRIX (ANGSTROMS AND DEGREES)  
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498688( 1)					
3	3	O	1	1.391387( 2)	2	109.190( 9)			
4	4	O	1	1.198211( 3)	2	127.013( 10)	3	172.723( 16)	0
5	5	O	3	1.460795( 4)	1	106.667( 11)	2	135.000( 17)	0
6	6	H	5	0.968706( 5)	3	97.154( 12)	1	180.000( 18)	0
7	7	H	2	1.089951( 6)	1	105.787( 13)	3	270.000( 19)	0
8	8	H	2	1.085888( 7)	1	112.080( 14)	7	118.325( 20)	0
9	9	H	2	1.085494( 8)	1	110.096( 15)	7	-117.450( 21)	0

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-304.19257972 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 51

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Z-MATRIX (ANGSTROMS AND DEGREES)  
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503217( 1)					
3	3	O	1	1.395128( 2)	2	110.528( 9)			
4	4	O	1	1.197564( 3)	2	126.302( 10)	3	174.855( 16)	0
5	5	O	3	1.459502( 4)	1	107.269( 11)	2	135.000( 17)	0
6	6	H	5	0.968608( 5)	3	96.970( 12)	1	225.000( 18)	0
7	7	H	2	1.084091( 6)	1	112.227( 13)	3	0.000( 19)	0
8	8	H	2	1.087118( 7)	1	110.545( 14)	7	124.452( 20)	0
9	9	H	2	1.089014( 8)	1	105.849( 15)	7	-119.067( 21)	0

-304.19061259 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 52

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503476( 1)					
3	3	O	1	1.396625( 2)	2	110.484( 9)			
4	4	O	1	1.197705( 3)	2	126.614( 10)	3	175.505( 16)	0
5	5	O	3	1.459270( 4)	1	107.050( 11)	2	135.000( 17)	0
6	6	H	5	0.968605( 5)	3	97.039( 12)	1	225.000( 18)	0
7	7	H	2	1.089979( 6)	1	110.238( 13)	3	90.000( 19)	0
8	8	H	2	1.085827( 7)	1	107.523( 14)	7	117.278( 20)	0
9	9	H	2	1.084281( 8)	1	111.053( 15)	7	-120.844( 21)	0

-304.19028700 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 53

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498904( 1)					
3	3	O	1	1.396805( 2)	2	109.252( 9)			
4	4	O	1	1.197343( 3)	2	127.487( 10)	3	174.167( 16)	0
5	5	O	3	1.458335( 4)	1	107.151( 11)	2	135.000( 17)	0
6	6	H	5	0.968606( 5)	3	97.103( 12)	1	225.000( 18)	0
7	7	H	2	1.084520( 6)	1	109.405( 13)	3	180.000( 19)	0
8	8	H	2	1.088401( 7)	1	107.612( 14)	7	119.430( 20)	0
9	9	H	2	1.088575( 8)	1	111.280( 15)	7	-122.798( 21)	0

-304.19202635 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 54

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							

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2  2 C   1  1.498902(  1)
3  3 O   1  1.394913(  2)  2 109.388(  9)
4  4 O   1  1.197391(  3)  2 127.095( 10)  3 173.816( 16)  0
5  5 O   3  1.459027(  4)  1 107.327( 11)  2 135.000( 17)  0
6  6 H   5  0.968634(  5)  3  97.022( 12)  1 225.000( 18)  0
7  7 H   2  1.090092(  6)  1 105.965( 13)  3 270.000( 19)  0
8  8 H   2  1.085962(  7)  1 112.007( 14)  7 118.430( 20)  0
9  9 H   2  1.085495(  8)  1 110.106( 15)  7 -117.444( 21)  0

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-304.19229997 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 55  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1		1 C							
2	2 C	1	1.504129( 1)						
3	3 O	1	1.401054( 2)	2	110.236( 9)				
4	4 O	1	1.197409( 3)	2	126.165( 10)	3	174.719( 16)	0	
5	5 O	3	1.450058( 4)	1	109.187( 11)	2	135.000( 17)	0	
6	6 H	5	0.968861( 5)	3	99.207( 12)	1	270.000( 18)	0	
7	7 H	2	1.084115( 6)	1	112.210( 13)	3	0.000( 19)	0	
8	8 H	2	1.087223( 7)	1	110.406( 14)	7	124.181( 20)	0	
9	9 H	2	1.089062( 8)	1	106.084( 15)	7	-119.441( 21)	0	

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-304.18959268 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 56  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1		1 C							
2	2 C	1	1.504230( 1)						
3	3 O	1	1.402176( 2)	2	110.172( 9)				
4	4 O	1	1.197593( 3)	2	126.470( 10)	3	175.436( 16)	0	
5	5 O	3	1.449582( 4)	1	108.982( 11)	2	135.000( 17)	0	
6	6 H	5	0.968955( 5)	3	99.348( 12)	1	270.000( 18)	0	
7	7 H	2	1.090097( 6)	1	110.057( 13)	3	90.000( 19)	0	
8	8 H	2	1.085864( 7)	1	107.637( 14)	7	117.164( 20)	0	
9	9 H	2	1.084393( 8)	1	111.208( 15)	7	-120.596( 21)	0	

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-304.18932765 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 57  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1		1 C							
2	2 C	1	1.499895( 1)						
3	3 O	1	1.402090( 2)	2	108.971( 9)				
4	4 O	1	1.197285( 3)	2	127.290( 10)	3	174.003( 16)	0	

5	5	O	3	1.448834( 4)	1	109.106( 11)	2	135.000( 17)	0
6	6	H	5	0.968987( 5)	3	99.414( 12)	1	270.000( 18)	0
7	7	H	2	1.084536( 6)	1	109.398( 13)	3	180.000( 19)	0
8	8	H	2	1.088611( 7)	1	107.801( 14)	7	119.459( 20)	0
9	9	H	2	1.088466( 8)	1	111.268( 15)	7	-122.885( 21)	0

-304.19098542 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 58

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.499882( 1)					
3	3	O	1	1.401039( 2)	2	109.085( 9)			
4	4	O	1	1.197151( 3)	2	126.980( 10)	3	173.696( 16)	0
5	5	O	3	1.449705( 4)	1	109.271( 11)	2	135.000( 17)	0
6	6	H	5	0.968898( 5)	3	99.301( 12)	1	270.000( 18)	0
7	7	H	2	1.090261( 6)	1	106.231( 13)	3	270.000( 19)	0
8	8	H	2	1.085908( 7)	1	111.927( 14)	7	118.494( 20)	0
9	9	H	2	1.085481( 8)	1	110.066( 15)	7	-117.399( 21)	0

-304.19121603 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 59

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.505203( 1)					
3	3	O	1	1.390625( 2)	2	110.246( 9)			
4	4	O	1	1.201617( 3)	2	125.616( 10)	3	170.489( 16)	0
5	5	O	3	1.449786( 4)	1	110.930( 11)	2	135.000( 17)	0
6	6	H	5	0.970513( 5)	3	101.786( 12)	1	315.000( 18)	0
7	7	H	2	1.083841( 6)	1	112.071( 13)	3	0.000( 19)	0
8	8	H	2	1.087259( 7)	1	110.755( 14)	7	124.516( 20)	0
9	9	H	2	1.088785( 8)	1	105.663( 15)	7	-119.163( 21)	0

-304.18766941 Energy CCSD(T)-F12/CVTA-F12

=====  
 Geometry (MP2/AVTZ) 60

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.505460( 1)					
3	3	O	1	1.391926( 2)	2	110.178( 9)			
4	4	O	1	1.201793( 3)	2	125.945( 10)	3	170.895( 16)	0
5	5	O	3	1.449171( 4)	1	110.784( 11)	2	135.000( 17)	0
6	6	H	5	0.970626( 5)	3	101.875( 12)	1	315.000( 18)	0
7	7	H	2	1.089903( 6)	1	110.674( 13)	3	90.000( 19)	0

8 8 H 2 1.085664( 7) 1 107.390( 14) 7 117.449( 20) 0  
9 9 H 2 1.084326( 8) 1 110.635( 15) 7 -120.649( 21) 0

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-304.18732843 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 61

-----  
Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.500820( 1)  
3 3 O 1 1.391328( 2) 2 109.064( 9)  
4 4 O 1 1.201581( 3) 2 126.560( 10) 3 169.320( 16) 0  
5 5 O 3 1.448279( 4) 1 110.843( 11) 2 135.000( 17) 0  
6 6 H 5 0.970752( 5) 3 101.911( 12) 1 315.000( 18) 0  
7 7 H 2 1.084474( 6) 1 109.326( 13) 3 180.000( 19) 0  
8 8 H 2 1.088559( 7) 1 107.117( 14) 7 119.135( 20) 0  
9 9 H 2 1.088173( 8) 1 111.807( 15) 7 -123.327( 21) 0  
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-304.18913653 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 62

-----  
Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.500641( 1)  
3 3 O 1 1.390397( 2) 2 109.187( 9)  
4 4 O 1 1.201413( 3) 2 126.260( 10) 3 169.283( 16) 0  
5 5 O 3 1.448965( 4) 1 110.957( 11) 2 135.000( 17) 0  
6 6 H 5 0.970638( 5) 3 101.822( 12) 1 315.000( 18) 0  
7 7 H 2 1.089886( 6) 1 105.753( 13) 3 270.000( 19) 0  
8 8 H 2 1.085619( 7) 1 112.165( 14) 7 118.460( 20) 0  
9 9 H 2 1.085628( 8) 1 110.120( 15) 7 -117.170( 21) 0  
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-----  
-304.18940149 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 63

-----  
Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.503818( 1)  
3 3 O 1 1.414320( 2) 2 113.863( 9)  
4 4 O 1 1.199197( 3) 2 125.677( 10) 3 182.123( 16) 0  
5 5 O 3 1.470227( 4) 1 107.367( 11) 2 90.000( 17) 0  
6 6 H 5 0.971606( 5) 3 104.321( 12) 1 0.000( 18) 0  
7 7 H 2 1.083676( 6) 1 111.579( 13) 3 0.000( 19) 0  
8 8 H 2 1.088634( 7) 1 107.985( 14) 7 121.094( 20) 0  
9 9 H 2 1.088866( 8) 1 109.338( 15) 7 -122.651( 21) 0  
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-304.17141615 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 64

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.499511( 1)					
3	3	O	1	1.415632( 2)	2	112.775( 9)			
4	4	O	1	1.198733( 3)	2	126.611( 10)	3	183.050( 16)	0
5	5	O	3	1.468754( 4)	1	107.249( 11)	2	90.000( 17)	0
6	6	H	5	0.971802( 5)	3	104.350( 12)	1	0.000( 18)	0
7	7	H	2	1.090781( 6)	1	107.282( 13)	3	90.000( 19)	0
8	8	H	2	1.086280( 7)	1	110.054( 14)	7	117.062( 20)	0
9	9	H	2	1.085437( 8)	1	111.185( 15)	7	-118.633( 21)	0

-304.17284777 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 65

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.495979( 1)					
3	3	O	1	1.416722( 2)	2	112.025( 9)			
4	4	O	1	1.198757( 3)	2	127.335( 10)	3	182.182( 16)	0
5	5	O	3	1.469308( 4)	1	107.624( 11)	2	90.000( 17)	0
6	6	H	5	0.971575( 5)	3	104.254( 12)	1	0.000( 18)	0
7	7	H	2	1.084493( 6)	1	110.584( 13)	3	180.000( 19)	0
8	8	H	2	1.089267( 7)	1	109.761( 14)	7	122.919( 20)	0
9	9	H	2	1.089350( 8)	1	108.154( 15)	7	-120.985( 21)	0

-304.17368331 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 66

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.500271( 1)					
3	3	O	1	1.415349( 2)	2	113.146( 9)			
4	4	O	1	1.199195( 3)	2	126.354( 10)	3	180.775( 16)	0
5	5	O	3	1.470244( 4)	1	107.818( 11)	2	90.000( 17)	0
6	6	H	5	0.971333( 5)	3	104.221( 12)	1	0.000( 18)	0
7	7	H	2	1.091378( 6)	1	108.584( 13)	3	270.000( 19)	0
8	8	H	2	1.084627( 7)	1	110.905( 14)	7	119.195( 20)	0
9	9	H	2	1.085825( 8)	1	109.364( 15)	7	-117.217( 21)	0

-304.17223358 Energy CCSD(T)-F12/CVTA-F12

Geometry (MP2/AVTZ) 67

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                Z-MATRIX (ANGSTROMS AND DEGREES)
  CD  Cent  Atom  N1   Length/X    N2   Alpha/Y    N3   Beta/Z    J
-----
  1   1  C
  2   2  C    1  1.499076( 1)
  3   3  O    1  1.417498( 2)  2  114.288( 9)
  4   4  O    1  1.200411( 3)  2  126.146( 10)  3  179.553( 16)  0
  5   5  O    3  1.462940( 4)  1  103.793( 11)  2  90.000( 17)  0
  6   6  H    5  0.973289( 5)  3  101.632( 12)  1  45.000( 18)  0
  7   7  H    2  1.083315( 6)  1  111.415( 13)  3  0.000( 19)  0
  8   8  H    2  1.088623( 7)  1  108.567( 14)  7  121.665( 20)  0
  9   9  H    2  1.088296( 8)  1  108.617( 15)  7 -121.744( 21)  0
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-304.17972766 Energy CCSD(T)-F12/CVTA-F12

=====  
 Geometry (MP2/AVTZ) 68

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                Z-MATRIX (ANGSTROMS AND DEGREES)
  CD  Cent  Atom  N1   Length/X    N2   Alpha/Y    N3   Beta/Z    J
-----
  1   1  C
  2   2  C    1  1.494811( 1)
  3   3  O    1  1.418868( 2)  2  113.187( 9)
  4   4  O    1  1.200026( 3)  2  127.142( 10)  3  180.503( 16)  0
  5   5  O    3  1.461663( 4)  1  103.795( 11)  2  90.000( 17)  0
  6   6  H    5  0.973170( 5)  3  101.738( 12)  1  45.000( 18)  0
  7   7  H    2  1.090996( 6)  1  107.832( 13)  3  90.000( 19)  0
  8   8  H    2  1.085994( 7)  1  109.779( 14)  7  117.290( 20)  0
  9   9  H    2  1.084700( 8)  1  110.550( 15)  7 -119.092( 21)  0
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-304.18110252 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 69

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                Z-MATRIX (ANGSTROMS AND DEGREES)
  CD  Cent  Atom  N1   Length/X    N2   Alpha/Y    N3   Beta/Z    J
-----
  1   1  C
  2   2  C    1  1.491211( 1)
  3   3  O    1  1.420043( 2)  2  112.329( 9)
  4   4  O    1  1.199920( 3)  2  127.910( 10)  3  178.826( 16)  0
  5   5  O    3  1.461884( 4)  1  104.241( 11)  2  90.000( 17)  0
  6   6  H    5  0.973243( 5)  3  101.688( 12)  1  45.000( 18)  0
  7   7  H    2  1.084465( 6)  1  110.671( 13)  3  180.000( 19)  0
  8   8  H    2  1.089081( 7)  1  108.112( 14)  7  121.879( 20)  0
  9   9  H    2  1.088906( 8)  1  109.028( 15)  7 -121.890( 21)  0
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-304.18214082 Energy CCSD(T)-F12/CVTA-F12

=====  
 Geometry (MP2/AVTZ) 70

-----  
 Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.495587( 1)					
3	3	O	1	1.418277( 2)	2	113.514( 9)			
4	4	O	1	1.200269( 3)	2	126.816( 10)	3	178.150( 16)	0
5	5	O	3	1.462630( 4)	1	104.314( 11)	2	90.000( 17)	0
6	6	H	5	0.973334( 5)	3	101.587( 12)	1	45.000( 18)	0
7	7	H	2	1.090550( 6)	1	107.429( 13)	3	270.000( 19)	0
8	8	H	2	1.084527( 7)	1	111.112( 14)	7	118.810( 20)	0
9	9	H	2	1.085895( 8)	1	109.720( 15)	7	-117.315( 21)	0

-304.18071072 Energy CCSD(T)-F12/CVTA-F12

=====  
=====

Geometry (MP2/AVTZ) 71

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498248( 1)					
3	3	O	1	1.423455( 2)	2	113.939( 9)			
4	4	O	1	1.198291( 3)	2	126.343( 10)	3	182.130( 16)	0
5	5	O	3	1.461085( 4)	1	101.314( 11)	2	90.000( 17)	0
6	6	H	5	0.970747( 5)	3	99.375( 12)	1	90.000( 18)	0
7	7	H	2	1.083384( 6)	1	111.565( 13)	3	0.000( 19)	0
8	8	H	2	1.088359( 7)	1	108.430( 14)	7	121.726( 20)	0
9	9	H	2	1.088301( 8)	1	108.598( 15)	7	-121.586( 21)	0

-304.18510391 Energy CCSD(T)-F12/CVTA-F12

=====  
=====

Geometry (MP2/AVTZ) 72

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.494095( 1)					
3	3	O	1	1.424721( 2)	2	112.853( 9)			
4	4	O	1	1.197923( 3)	2	127.271( 10)	3	183.056( 16)	0
5	5	O	3	1.460107( 4)	1	101.227( 11)	2	90.000( 17)	0
6	6	H	5	0.970688( 5)	3	99.422( 12)	1	90.000( 18)	0
7	7	H	2	1.090869( 6)	1	107.616( 13)	3	90.000( 19)	0
8	8	H	2	1.085937( 7)	1	109.709( 14)	7	117.200( 20)	0
9	9	H	2	1.084600( 8)	1	110.900( 15)	7	-119.264( 21)	0

-304.18646657 Energy CCSD(T)-F12/CVTA-F12

=====  
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Geometry (MP2/AVTZ) 73

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							

```

2  2 C   1  1.490270(  1)
3  3 O   1  1.425978(  2)  2 111.910(  9)
4  4 O   1  1.197779(  3)  2 128.176( 10)  3 181.831( 16)  0
5  5 O   3  1.459640(  4)  1 101.773( 11)  2  90.000( 17)  0
6  6 H   5  0.970659(  5)  3  99.549( 12)  1  90.000( 18)  0
7  7 H   2  1.084491(  6)  1 110.576( 13)  3 180.000( 19)  0
8  8 H   2  1.088796(  7)  1 108.559( 14)  7 121.976( 20)  0
9  9 H   2  1.089085(  8)  1 108.672( 15)  7 -121.522( 21)  0

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-304.18761873 Energy CCSD(T)-F12/CVTA-F12  
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=====  
Geometry (MP2/AVTZ) 74  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.494373( 1)					
3	3	O	1	1.424102( 2)	2	113.091( 9)			
4	4	O	1	1.198243( 3)	2	127.122( 10)	3	180.776( 16)	0
5	5	O	3	1.460569( 4)	1	101.852( 11)	2	90.000( 17)	0
6	6	H	5	0.970718( 5)	3	99.515( 12)	1	90.000( 18)	0
7	7	H	2	1.090692( 6)	1	107.481( 13)	3	270.000( 19)	0
8	8	H	2	1.084587( 7)	1	111.093( 14)	7	118.921( 20)	0
9	9	H	2	1.085779( 8)	1	109.583( 15)	7	-117.315( 21)	0

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-304.18620710 Energy CCSD(T)-F12/CVTA-F12  
=====

=====  
Geometry (MP2/AVTZ) 75  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.499394( 1)					
3	3	O	1	1.424662( 2)	2	113.568( 9)			
4	4	O	1	1.196178( 3)	2	126.278( 10)	3	183.730( 16)	0
5	5	O	3	1.469824( 4)	1	101.423( 11)	2	90.000( 17)	0
6	6	H	5	0.968101( 5)	3	97.833( 12)	1	135.000( 18)	0
7	7	H	2	1.083432( 6)	1	111.619( 13)	3	0.000( 19)	0
8	8	H	2	1.088189( 7)	1	108.434( 14)	7	121.897( 20)	0
9	9	H	2	1.088672( 8)	1	108.579( 15)	7	-121.432( 21)	0

-----  
-304.18263540 Energy CCSD(T)-F12/CVTA-F12  
=====

=====  
Geometry (MP2/AVTZ) 76  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.495293( 1)					
3	3	O	1	1.426181( 2)	2	112.455( 9)			
4	4	O	1	1.195703( 3)	2	127.185( 10)	3	184.627( 16)	0



5	5	O	3	1.468913( 4)	1	101.270( 11)	2	90.000( 17)	0
6	6	H	5	0.968083( 5)	3	97.892( 12)	1	135.000( 18)	0
7	7	H	2	1.090666( 6)	1	107.577( 13)	3	90.000( 19)	0
8	8	H	2	1.086123( 7)	1	109.644( 14)	7	117.110( 20)	0
9	9	H	2	1.084793( 8)	1	111.037( 15)	7	-119.407( 21)	0

-304.18401082 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 77

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.491086( 1)					
3	3	O	1	1.427367( 2)	2	111.466( 9)			
4	4	O	1	1.195686( 3)	2	128.130( 10)	3	183.658( 16)	0
5	5	O	3	1.468891( 4)	1	101.497( 11)	2	90.000( 17)	0
6	6	H	5	0.968110( 5)	3	97.965( 12)	1	135.000( 18)	0
7	7	H	2	1.084496( 6)	1	110.563( 13)	3	180.000( 19)	0
8	8	H	2	1.089045( 7)	1	108.858( 14)	7	122.171( 20)	0
9	9	H	2	1.089165( 8)	1	108.443( 15)	7	-121.369( 21)	0

-304.18522400 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 78

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.495084( 1)					
3	3	O	1	1.425899( 2)	2	112.636( 9)			
4	4	O	1	1.196083( 3)	2	127.148( 10)	3	182.486( 16)	0
5	5	O	3	1.469365( 4)	1	101.688( 11)	2	90.000( 17)	0
6	6	H	5	0.968098( 5)	3	97.981( 12)	1	135.000( 18)	0
7	7	H	2	1.091093( 6)	1	107.666( 13)	3	270.000( 19)	0
8	8	H	2	1.084594( 7)	1	111.001( 14)	7	118.928( 20)	0
9	9	H	2	1.085766( 8)	1	109.548( 15)	7	-117.355( 21)	0

-304.18381484 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 79

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.499848( 1)					
3	3	O	1	1.423599( 2)	2	113.742( 9)			
4	4	O	1	1.195605( 3)	2	126.252( 10)	3	184.219( 16)	0
5	5	O	3	1.474971( 4)	1	100.904( 11)	2	90.000( 17)	0
6	6	H	5	0.968173( 5)	3	97.324( 12)	1	180.000( 18)	0
7	7	H	2	1.083432( 6)	1	111.637( 13)	3	0.000( 19)	0

8 8 H 2 1.088214( 7) 1 108.255( 14) 7 121.721( 20) 0  
9 9 H 2 1.088530( 8) 1 108.772( 15) 7 -121.571( 21) 0

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-304.18069286 Energy CCSD(T)-F12/CVTA-F12  
=====

=====  
Geometry (MP2/AVTZ) 80  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.495837( 1)  
3 3 O 1 1.425130( 2) 2 112.641( 9)  
4 4 O 1 1.195145( 3) 2 127.165( 10) 3 185.173( 16) 0  
5 5 O 3 1.473511( 4) 1 100.975( 11) 2 90.000( 17) 0  
6 6 H 5 0.968148( 5) 3 97.411( 12) 1 180.000( 18) 0  
7 7 H 2 1.090642( 6) 1 107.480( 13) 3 90.000( 19) 0  
8 8 H 2 1.086145( 7) 1 109.712( 14) 7 117.122( 20) 0  
9 9 H 2 1.084584( 8) 1 111.039( 15) 7 -119.456( 21) 0  
-----

-----  
-304.18208192 Energy CCSD(T)-F12/CVTA-F12  
=====

=====  
Geometry (MP2/AVTZ) 81  
-----

Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.492051( 1)  
3 3 O 1 1.426539( 2) 2 111.722( 9)  
4 4 O 1 1.195070( 3) 2 128.070( 10) 3 184.193( 16) 0  
5 5 O 3 1.473837( 4) 1 101.292( 11) 2 90.000( 17) 0  
6 6 H 5 0.968090( 5) 3 97.419( 12) 1 180.000( 18) 0  
7 7 H 2 1.084542( 6) 1 110.502( 13) 3 180.000( 19) 0  
8 8 H 2 1.088555( 7) 1 108.973( 14) 7 122.250( 20) 0  
9 9 H 2 1.089233( 8) 1 108.373( 15) 7 -121.077( 21) 0  
-----

-----  
-304.18312408 Energy CCSD(T)-F12/CVTA-F12  
=====

=====  
Geometry (MP2/AVTZ) 82  
-----

Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.496003( 1)  
3 3 O 1 1.424692( 2) 2 112.914( 9)  
4 4 O 1 1.195580( 3) 2 127.044( 10) 3 182.978( 16) 0  
5 5 O 3 1.475282( 4) 1 101.208( 11) 2 90.000( 17) 0  
6 6 H 5 0.968106( 5) 3 97.341( 12) 1 180.000( 18) 0  
7 7 H 2 1.090745( 6) 1 107.891( 13) 3 270.000( 19) 0  
8 8 H 2 1.084680( 7) 1 110.992( 14) 7 119.046( 20) 0  
9 9 H 2 1.085736( 8) 1 109.396( 15) 7 -117.463( 21) 0  
-----

-304.18169855 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 83

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.500612( 1)					
3	3	O	1	1.424044( 2)	2	114.074( 9)			
4	4	O	1	1.195573( 3)	2	126.019( 10)	3	184.604( 16)	0
5	5	O	3	1.468402( 4)	1	100.663( 11)	2	90.000( 17)	0
6	6	H	5	0.968866( 5)	3	98.636( 12)	1	225.000( 18)	0
7	7	H	2	1.083791( 6)	1	111.894( 13)	3	0.000( 19)	0
8	8	H	2	1.088242( 7)	1	108.013( 14)	7	121.255( 20)	0
9	9	H	2	1.088213( 8)	1	109.016( 15)	7	-122.022( 21)	0

-304.18201058 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 84

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.496598( 1)					
3	3	O	1	1.425417( 2)	2	113.109( 9)			
4	4	O	1	1.195229( 3)	2	126.823( 10)	3	185.709( 16)	0
5	5	O	3	1.466669( 4)	1	100.945( 11)	2	90.000( 17)	0
6	6	H	5	0.968804( 5)	3	98.767( 12)	1	225.000( 18)	0
7	7	H	2	1.090564( 6)	1	107.345( 13)	3	90.000( 19)	0
8	8	H	2	1.086062( 7)	1	109.756( 14)	7	117.164( 20)	0
9	9	H	2	1.084568( 8)	1	111.487( 15)	7	-119.437( 21)	0

-304.18329668 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 85

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.493386( 1)					
3	3	O	1	1.426780( 2)	2	112.216( 9)			
4	4	O	1	1.195123( 3)	2	127.746( 10)	3	184.804( 16)	0
5	5	O	3	1.466777( 4)	1	101.526( 11)	2	90.000( 17)	0
6	6	H	5	0.968674( 5)	3	98.603( 12)	1	225.000( 18)	0
7	7	H	2	1.084578( 6)	1	110.341( 13)	3	180.000( 19)	0
8	8	H	2	1.088209( 7)	1	109.395( 14)	7	121.929( 20)	0
9	9	H	2	1.089259( 8)	1	108.382( 15)	7	-120.850( 21)	0

-304.18420564 Energy CCSD(T)-F12/CVTA-F12

=====  
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Geometry (MP2/AVTZ) 86

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-----
                Z-MATRIX (ANGSTROMS AND DEGREES)
  CD  Cent  Atom  N1   Length/X   N2   Alpha/Y   N3   Beta/Z   J
-----
  1   1  C
  2   2  C   1  1.497355( 1)
  3   3  O   1  1.425082( 2)  2  113.288( 9)
  4   4  O   1  1.195567( 3)  2  126.819( 10)  3  183.479( 16)  0
  5   5  O   3  1.468881( 4)  1  101.219( 11)  2  90.000( 17)  0
  6   6  H   5  0.968722( 5)  3  98.492( 12)  1  225.000( 18)  0
  7   7  H   2  1.090315( 6)  1  108.238( 13)  3  270.000( 19)  0
  8   8  H   2  1.085096( 7)  1  111.027( 14)  7  119.524( 20)  0
  9   9  H   2  1.085709( 8)  1  109.212( 15)  7 -117.472( 21)  0
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-304.18288432 Energy CCSD(T)-F12/CVTA-F12

=====  
 Geometry (MP2/AVTZ) 87

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-----
                Z-MATRIX (ANGSTROMS AND DEGREES)
  CD  Cent  Atom  N1   Length/X   N2   Alpha/Y   N3   Beta/Z   J
-----
  1   1  C
  2   2  C   1  1.503138( 1)
  3   3  O   1  1.423185( 2)  2  113.939( 9)
  4   4  O   1  1.195624( 3)  2  125.647( 10)  3  184.728( 16)  0
  5   5  O   3  1.459444( 4)  1  102.494( 11)  2  90.000( 17)  0
  6   6  H   5  0.970945( 5)  3  100.844( 12)  1  270.000( 18)  0
  7   7  H   2  1.084966( 6)  1  112.192( 13)  3  0.000( 19)  0
  8   8  H   2  1.088249( 7)  1  107.844( 14)  7  120.578( 20)  0
  9   9  H   2  1.088337( 8)  1  109.321( 15)  7 -122.815( 21)  0
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-304.18095542 Energy CCSD(T)-F12/CVTA-F12

=====  
 Geometry (MP2/AVTZ) 88

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-----
                Z-MATRIX (ANGSTROMS AND DEGREES)
  CD  Cent  Atom  N1   Length/X   N2   Alpha/Y   N3   Beta/Z   J
-----
  1   1  C
  2   2  C   1  1.499309( 1)
  3   3  O   1  1.423336( 2)  2  113.219( 9)
  4   4  O   1  1.195515( 3)  2  126.196( 10)  3  186.039( 16)  0
  5   5  O   3  1.457944( 4)  1  102.753( 11)  2  90.000( 17)  0
  6   6  H   5  0.970641( 5)  3  100.999( 12)  1  270.000( 18)  0
  7   7  H   2  1.090627( 6)  1  107.055( 13)  3  90.000( 19)  0
  8   8  H   2  1.085798( 7)  1  109.909( 14)  7  117.254( 20)  0
  9   9  H   2  1.085824( 8)  1  112.396( 15)  7 -118.744( 21)  0
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-304.18203121 Energy CCSD(T)-F12/CVTA-F12

=====  
 Geometry (MP2/AVTZ) 89

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 Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.496296( 1)					
3	3	O	1	1.425553( 2)	2	112.412( 9)			
4	4	O	1	1.195368( 3)	2	127.131( 10)	3	185.304( 16)	0
5	5	O	3	1.457455( 4)	1	103.558( 11)	2	90.000( 17)	0
6	6	H	5	0.970110( 5)	3	100.806( 12)	1	270.000( 18)	0
7	7	H	2	1.084564( 6)	1	110.186( 13)	3	180.000( 19)	0
8	8	H	2	1.088947( 7)	1	110.486( 14)	7	121.661( 20)	0
9	9	H	2	1.089281( 8)	1	108.312( 15)	7	-120.750( 21)	0

-304.18279675 Energy CCSD(T)-F12/CVTA-F12

=====  
=====

Geometry (MP2/AVTZ) 90

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.499955( 1)					
3	3	O	1	1.424706( 2)	2	113.179( 9)			
4	4	O	1	1.195630( 3)	2	126.487( 10)	3	183.775( 16)	0
5	5	O	3	1.459642( 4)	1	103.224( 11)	2	90.000( 17)	0
6	6	H	5	0.970409( 5)	3	100.682( 12)	1	270.000( 18)	0
7	7	H	2	1.091023( 6)	1	108.771( 13)	3	270.000( 19)	0
8	8	H	2	1.085642( 7)	1	110.989( 14)	7	120.071( 20)	0
9	9	H	2	1.085633( 8)	1	109.157( 15)	7	-117.197( 21)	0

-304.18173355 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 91

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.505861( 1)					
3	3	O	1	1.418288( 2)	2	113.549( 9)			
4	4	O	1	1.196647( 3)	2	125.525( 10)	3	184.268( 16)	0
5	5	O	3	1.462184( 4)	1	105.838( 11)	2	90.000( 17)	0
6	6	H	5	0.972763( 5)	3	103.127( 12)	1	315.000( 18)	0
7	7	H	2	1.084861( 6)	1	111.995( 13)	3	0.000( 19)	0
8	8	H	2	1.088497( 7)	1	107.608( 14)	7	120.262( 20)	0
9	9	H	2	1.088895( 8)	1	109.711( 15)	7	-123.538( 21)	0

-304.17455093 Energy CCSD(T)-F12/CVTA-F12

=====  
=====

Geometry (MP2/AVTZ) 92

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							

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2  2 C   1  1.501787(  1)
3  3 O   1  1.418512(  2)  2 112.672(  9)
4  4 O   1  1.196355(  3)  2 126.170( 10)  3 185.495( 16)  0
5  5 O   3  1.460866(  4)  1 105.779( 11)  2  90.000( 17)  0
6  6 H   5  0.972862(  5)  3 103.136( 12)  1 315.000( 18)  0
7  7 H   2  1.090634(  6)  1 106.839( 13)  3  90.000( 19)  0
8  8 H   2  1.085976(  7)  1 110.170( 14)  7 117.169( 20)  0
9  9 H   2  1.086754(  8)  1 112.311( 15)  7 -118.067( 21)  0

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-304.17584456 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 93  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498813( 1)					
3	3	O	1	1.419944( 2)	2	112.074( 9)			
4	4	O	1	1.196432( 3)	2	126.876( 10)	3	185.093( 16)	0
5	5	O	3	1.460738( 4)	1	106.537( 11)	2	90.000( 17)	0
6	6	H	5	0.971723( 5)	3	103.101( 12)	1	315.000( 18)	0
7	7	H	2	1.084453( 6)	1	110.277( 13)	3	180.000( 19)	0
8	8	H	2	1.089883( 7)	1	111.321( 14)	7	122.683( 20)	0
9	9	H	2	1.089390( 8)	1	107.863( 15)	7	-120.531( 21)	0

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-304.17640237 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 94  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502666( 1)					
3	3	O	1	1.419744( 2)	2	112.906( 9)			
4	4	O	1	1.196699( 3)	2	126.246( 10)	3	183.479( 16)	0
5	5	O	3	1.462387( 4)	1	106.537( 11)	2	90.000( 17)	0
6	6	H	5	0.971678( 5)	3	103.031( 12)	1	315.000( 18)	0
7	7	H	2	1.091976( 6)	1	109.458( 13)	3	270.000( 19)	0
8	8	H	2	1.085170( 7)	1	110.817( 14)	7	120.089( 20)	0
9	9	H	2	1.085729( 8)	1	109.040( 15)	7	-116.978( 21)	0

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-304.17517832 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 95  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.508027( 1)					
3	3	O	1	1.381618( 2)	2	117.168( 9)			
4	4	O	1	1.201923( 3)	2	124.481( 10)	3	190.696( 16)	0

5	5	O	3	1.459015( 4)	1	113.480( 11)	2	45.000( 17)	0
6	6	H	5	0.970098( 5)	3	103.924( 12)	1	0.000( 18)	0
7	7	H	2	1.086023( 6)	1	113.629( 13)	3	0.000( 19)	0
8	8	H	2	1.087236( 7)	1	105.807( 14)	7	119.783( 20)	0
9	9	H	2	1.088819( 8)	1	110.293( 15)	7	-124.287( 21)	0

-304.18277253 Energy CCSD(T)-F12/CVTA-F12

Geometry (MP2/AVTZ) 96

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.506811( 1)					
3	3	O	1	1.382158( 2)	2	117.868( 9)			
4	4	O	1	1.201929( 3)	2	123.939( 10)	3	192.284( 16)	0
5	5	O	3	1.458716( 4)	1	114.532( 11)	2	45.000( 17)	0
6	6	H	5	0.969127( 5)	3	103.773( 12)	1	0.000( 18)	0
7	7	H	2	1.089920( 6)	1	105.224( 13)	3	90.000( 19)	0
8	8	H	2	1.085135( 7)	1	109.220( 14)	7	116.559( 20)	0
9	9	H	2	1.086193( 8)	1	116.025( 15)	7	-118.024( 21)	0

-304.18221895 Energy CCSD(T)-F12/CVTA-F12

Geometry (MP2/AVTZ) 97

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.506453( 1)					
3	3	O	1	1.383020( 2)	2	117.072( 9)			
4	4	O	1	1.202126( 3)	2	124.743( 10)	3	192.490( 16)	0
5	5	O	3	1.459229( 4)	1	114.380( 11)	2	45.000( 17)	0
6	6	H	5	0.968657( 5)	3	103.888( 12)	1	0.000( 18)	0
7	7	H	2	1.084362( 6)	1	107.917( 13)	3	180.000( 19)	0
8	8	H	2	1.089337( 7)	1	114.933( 14)	7	120.598( 20)	0
9	9	H	2	1.088555( 8)	1	107.658( 15)	7	-119.551( 21)	0

-304.18257549 Energy CCSD(T)-F12/CVTA-F12

Geometry (MP2/AVTZ) 98

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.507745( 1)					
3	3	O	1	1.381510( 2)	2	116.219( 9)			
4	4	O	1	1.202199( 3)	2	125.330( 10)	3	190.848( 16)	0
5	5	O	3	1.459506( 4)	1	113.092( 11)	2	45.000( 17)	0
6	6	H	5	0.969735( 5)	3	103.977( 12)	1	0.000( 18)	0
7	7	H	2	1.091678( 6)	1	111.976( 13)	3	270.000( 19)	0

8 8 H 2 1.087012( 7) 1 110.424( 14) 7 121.394( 20) 0  
9 9 H 2 1.084705( 8) 1 107.209( 15) 7 -117.597( 21) 0

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-304.18331272 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 99  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.503378( 1)  
3 3 O 1 1.390659( 2) 2 116.574( 9)  
4 4 O 1 1.201801( 3) 2 125.627( 10) 3 189.382( 16) 0  
5 5 O 3 1.456469( 4) 1 111.010( 11) 2 45.000( 17) 0  
6 6 H 5 0.970023( 5) 3 102.220( 12) 1 45.000( 18) 0  
7 7 H 2 1.083512( 6) 1 112.280( 13) 3 0.000( 19) 0  
8 8 H 2 1.087678( 7) 1 106.154( 14) 7 121.012( 20) 0  
9 9 H 2 1.088701( 8) 1 110.142( 15) 7 -122.980( 21) 0  
-----

-----  
-304.18784429 Energy CCSD(T)-F12/CVTA-F12  
=====

=====  
Geometry (MP2/AVTZ) 100  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.501277( 1)  
3 3 O 1 1.391605( 2) 2 116.828( 9)  
4 4 O 1 1.201839( 3) 2 125.522( 10) 3 190.675( 16) 0  
5 5 O 3 1.456540( 4) 1 112.056( 11) 2 45.000( 17) 0  
6 6 H 5 0.969939( 5) 3 102.138( 12) 1 45.000( 18) 0  
7 7 H 2 1.090090( 6) 1 105.607( 13) 3 90.000( 19) 0  
8 8 H 2 1.085573( 7) 1 109.480( 14) 7 116.576( 20) 0  
9 9 H 2 1.083722( 8) 1 113.436( 15) 7 -118.420( 21) 0  
-----

-----  
-304.18775033 Energy CCSD(T)-F12/CVTA-F12  
=====

=====  
Geometry (MP2/AVTZ) 101  
-----

Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.500999( 1)  
3 3 O 1 1.391771( 2) 2 116.294( 9)  
4 4 O 1 1.201937( 3) 2 126.030( 10) 3 190.772( 16) 0  
5 5 O 3 1.457116( 4) 1 111.756( 11) 2 45.000( 17) 0  
6 6 H 5 0.969743( 5) 3 102.121( 12) 1 45.000( 18) 0  
7 7 H 2 1.084273( 6) 1 108.553( 13) 3 180.000( 19) 0  
8 8 H 2 1.086032( 7) 1 113.193( 14) 7 122.721( 20) 0  
9 9 H 2 1.089139( 8) 1 107.255( 15) 7 -119.288( 21) 0  
-----



-304.18788649 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 102

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.502849( 1)					
3	3	O	1	1.390982( 2)	2	115.863( 9)			
4	4	O	1	1.201829( 3)	2	126.242( 10)	3	189.267( 16)	0
5	5	O	3	1.457222( 4)	1	110.536( 11)	2	45.000( 17)	0
6	6	H	5	0.969786( 5)	3	102.214( 12)	1	45.000( 18)	0
7	7	H	2	1.089623( 6)	1	111.324( 13)	3	270.000( 19)	0
8	8	H	2	1.085567( 7)	1	110.175( 14)	7	119.856( 20)	0
9	9	H	2	1.085149( 8)	1	107.483( 15)	7	-118.316( 21)	0

=====  
-304.18814319 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 103

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.500261( 1)					
3	3	O	1	1.395440( 2)	2	116.540( 9)			
4	4	O	1	1.201449( 3)	2	125.816( 10)	3	189.576( 16)	0
5	5	O	3	1.454689( 4)	1	108.730( 11)	2	45.000( 17)	0
6	6	H	5	0.969432( 5)	3	99.304( 12)	1	90.000( 18)	0
7	7	H	2	1.082694( 6)	1	112.356( 13)	3	0.000( 19)	0
8	8	H	2	1.087732( 7)	1	106.450( 14)	7	121.657( 20)	0
9	9	H	2	1.088195( 8)	1	109.666( 15)	7	-122.068( 21)	0

=====  
-304.19386043 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 104

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.497984( 1)					
3	3	O	1	1.396823( 2)	2	116.632( 9)			
4	4	O	1	1.201509( 3)	2	125.928( 10)	3	190.865( 16)	0
5	5	O	3	1.453750( 4)	1	110.016( 11)	2	45.000( 17)	0
6	6	H	5	0.969369( 5)	3	99.356( 12)	1	90.000( 18)	0
7	7	H	2	1.090170( 6)	1	105.962( 13)	3	90.000( 19)	0
8	8	H	2	1.085634( 7)	1	109.218( 14)	7	116.464( 20)	0
9	9	H	2	1.082715( 8)	1	112.836( 15)	7	-119.331( 21)	0

=====  
-304.19393806 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 105

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                Z-MATRIX (ANGSTROMS AND DEGREES)
  CD  Cent  Atom  N1   Length/X    N2   Alpha/Y    N3   Beta/Z    J
-----
  1   1  C
  2   2  C    1  1.497167( 1)
  3   3  O    1  1.397464( 2)  2  115.990( 9)
  4   4  O    1  1.201588( 3)  2  126.540( 10)  3  190.723( 16)  0
  5   5  O    3  1.454701( 4)  1  109.726( 11)  2  45.000( 17)  0
  6   6  H    5  0.969386( 5)  3  99.304( 12)  1  90.000( 18)  0
  7   7  H    2  1.084289( 6)  1  108.704( 13)  3  180.000( 19)  0
  8   8  H    2  1.085115( 7)  1  111.962( 14)  7  122.744( 20)  0
  9   9  H    2  1.089285( 8)  1  107.484( 15)  7 -119.274( 21)  0
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-304.19427585 Energy CCSD(T)-F12/CVTA-F12

=====  
 Geometry (MP2/AVTZ) 106

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                Z-MATRIX (ANGSTROMS AND DEGREES)
  CD  Cent  Atom  N1   Length/X    N2   Alpha/Y    N3   Beta/Z    J
-----
  1   1  C
  2   2  C    1  1.499320( 1)
  3   3  O    1  1.396454( 2)  2  115.722( 9)
  4   4  O    1  1.201331( 3)  2  126.564( 10)  3  189.311( 16)  0
  5   5  O    3  1.455537( 4)  1  108.174( 11)  2  45.000( 17)  0
  6   6  H    5  0.969428( 5)  3  99.228( 12)  1  90.000( 18)  0
  7   7  H    2  1.088383( 6)  1  110.467( 13)  3  270.000( 19)  0
  8   8  H    2  1.085489( 7)  1  110.378( 14)  7  119.396( 20)  0
  9   9  H    2  1.085235( 8)  1  107.686( 15)  7 -118.718( 21)  0
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-304.19432017 Energy CCSD(T)-F12/CVTA-F12

=====  
 Geometry (MP2/AVTZ) 107

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-----
                Z-MATRIX (ANGSTROMS AND DEGREES)
  CD  Cent  Atom  N1   Length/X    N2   Alpha/Y    N3   Beta/Z    J
-----
  1   1  C
  2   2  C    1  1.499950( 1)
  3   3  O    1  1.391400( 2)  2  116.231( 9)
  4   4  O    1  1.201074( 3)  2  125.864( 10)  3  190.614( 16)  0
  5   5  O    3  1.465245( 4)  1  107.128( 11)  2  45.000( 17)  0
  6   6  H    5  0.968546( 5)  3  97.149( 12)  1  135.000( 18)  0
  7   7  H    2  1.083248( 6)  1  112.404( 13)  3  0.000( 19)  0
  8   8  H    2  1.087522( 7)  1  106.546( 14)  7  121.518( 20)  0
  9   9  H    2  1.088053( 8)  1  109.534( 15)  7 -121.995( 21)  0
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-304.19425925 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 108

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 Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.497698( 1)					
3	3	O	1	1.391927( 2)	2	116.330( 9)			
4	4	O	1	1.201377( 3)	2	125.896( 10)	3	191.857( 16)	0
5	5	O	3	1.463990( 4)	1	108.404( 11)	2	45.000( 17)	0
6	6	H	5	0.968506( 5)	3	97.217( 12)	1	135.000( 18)	0
7	7	H	2	1.090033( 6)	1	105.974( 13)	3	90.000( 19)	0
8	8	H	2	1.085614( 7)	1	109.164( 14)	7	116.477( 20)	0
9	9	H	2	1.083116( 8)	1	112.978( 15)	7	-119.535( 21)	0

-304.19452957 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 109

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.496443( 1)					
3	3	O	1	1.392973( 2)	2	115.611( 9)			
4	4	O	1	1.201446( 3)	2	126.623( 10)	3	191.719( 16)	0
5	5	O	3	1.464462( 4)	1	108.163( 11)	2	45.000( 17)	0
6	6	H	5	0.968353( 5)	3	97.222( 12)	1	135.000( 18)	0
7	7	H	2	1.084258( 6)	1	108.786( 13)	3	180.000( 19)	0
8	8	H	2	1.085746( 7)	1	111.695( 14)	7	122.497( 20)	0
9	9	H	2	1.089137( 8)	1	107.524( 15)	7	-119.372( 21)	0

-304.19497505 Energy CCSD(T)-F12/CVTA-F12

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=====

Geometry (MP2/AVTZ) 110

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498677( 1)					
3	3	O	1	1.392247( 2)	2	115.420( 9)			
4	4	O	1	1.201155( 3)	2	126.612( 10)	3	190.403( 16)	0
5	5	O	3	1.465854( 4)	1	106.734( 11)	2	45.000( 17)	0
6	6	H	5	0.968334( 5)	3	97.201( 12)	1	135.000( 18)	0
7	7	H	2	1.088652( 6)	1	110.149( 13)	3	270.000( 19)	0
8	8	H	2	1.085636( 7)	1	110.408( 14)	7	119.417( 20)	0
9	9	H	2	1.085082( 8)	1	107.775( 15)	7	-118.690( 21)	0

-304.19476498 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 111

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							

```

2  2 C   1  1.500298(  1)
3  3 O   1  1.388670(  2)  2 116.615(  9)
4  4 O   1  1.201401(  3)  2 125.709( 10)  3 190.750( 16)  0
5  5 O   3  1.466789(  4)  1 107.054( 11)  2  45.000( 17)  0
6  6 H   5  0.968367(  5)  3  97.167( 12)  1 180.000( 18)  0
7  7 H   2  1.082856(  6)  1 112.392( 13)  3   0.000( 19)  0
8  8 H   2  1.087408(  7)  1 106.458( 14)  7 121.746( 20)  0
9  9 H   2  1.088219(  8)  1 109.505( 15)  7 -121.878( 21)  0

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-304.19339710 Energy CCSD(T)-F12/CVTA-F12  
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=====  
Geometry (MP2/AVTZ) 112  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498307( 1)					
3	3	O	1	1.388950( 2)	2	116.699( 9)			
4	4	O	1	1.201636( 3)	2	125.705( 10)	3	191.919( 16)	0
5	5	O	3	1.466592( 4)	1	108.112( 11)	2	45.000( 17)	0
6	6	H	5	0.968398( 5)	3	97.130( 12)	1	180.000( 18)	0
7	7	H	2	1.090021( 6)	1	105.937( 13)	3	90.000( 19)	0
8	8	H	2	1.085572( 7)	1	109.017( 14)	7	116.336( 20)	0
9	9	H	2	1.082873( 8)	1	113.099( 15)	7	-119.638( 21)	0

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-304.19365073 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 113  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.497158( 1)					
3	3	O	1	1.389685( 2)	2	115.896( 9)			
4	4	O	1	1.201652( 3)	2	126.450( 10)	3	191.672( 16)	0
5	5	O	3	1.467206( 4)	1	107.573( 11)	2	45.000( 17)	0
6	6	H	5	0.968302( 5)	3	97.160( 12)	1	180.000( 18)	0
7	7	H	2	1.084247( 6)	1	108.567( 13)	3	180.000( 19)	0
8	8	H	2	1.085821( 7)	1	111.866( 14)	7	122.216( 20)	0
9	9	H	2	1.088948( 8)	1	107.642( 15)	7	-119.512( 21)	0

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-304.19426150 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 114  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498957( 1)					
3	3	O	1	1.389232( 2)	2	115.664( 9)			
4	4	O	1	1.201403( 3)	2	126.493( 10)	3	190.426( 16)	0

5	5	O	3	1.467685( 4)	1	106.294( 11)	2	45.000( 17)	0
6	6	H	5	0.968241( 5)	3	97.268( 12)	1	180.000( 18)	0
7	7	H	2	1.088986( 6)	1	110.253( 13)	3	270.000( 19)	0
8	8	H	2	1.085198( 7)	1	110.496( 14)	7	119.564( 20)	0
9	9	H	2	1.085115( 8)	1	107.568( 15)	7	-118.465( 21)	0

-304.19411741 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 115

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.500449( 1)					
3	3	O	1	1.391794( 2)	2	117.281( 9)			
4	4	O	1	1.201210( 3)	2	125.389( 10)	3	190.154( 16)	0
5	5	O	3	1.456669( 4)	1	108.199( 11)	2	45.000( 17)	0
6	6	H	5	0.968758( 5)	3	99.159( 12)	1	225.000( 18)	0
7	7	H	2	1.082394( 6)	1	112.801( 13)	3	0.000( 19)	0
8	8	H	2	1.087409( 7)	1	106.493( 14)	7	122.112( 20)	0
9	9	H	2	1.088214( 8)	1	109.393( 15)	7	-121.565( 21)	0

-304.19393438 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 116

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498712( 1)					
3	3	O	1	1.392191( 2)	2	117.293( 9)			
4	4	O	1	1.201420( 3)	2	125.501( 10)	3	191.440( 16)	0
5	5	O	3	1.456345( 4)	1	109.312( 11)	2	45.000( 17)	0
6	6	H	5	0.968642( 5)	3	99.056( 12)	1	225.000( 18)	0
7	7	H	2	1.090048( 6)	1	106.150( 13)	3	90.000( 19)	0
8	8	H	2	1.085675( 7)	1	108.842( 14)	7	116.202( 20)	0
9	9	H	2	1.082430( 8)	1	113.146( 15)	7	-120.249( 21)	0

-304.19408335 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 117

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.497891( 1)					
3	3	O	1	1.392880( 2)	2	116.437( 9)			
4	4	O	1	1.201403( 3)	2	126.244( 10)	3	191.133( 16)	0
5	5	O	3	1.457488( 4)	1	108.705( 11)	2	45.000( 17)	0
6	6	H	5	0.968571( 5)	3	99.134( 12)	1	225.000( 18)	0
7	7	H	2	1.084316( 6)	1	108.414( 13)	3	180.000( 19)	0

8 8 H 2 1.085254( 7) 1 111.908( 14) 7 122.054( 20) 0  
9 9 H 2 1.089290( 8) 1 107.840( 15) 7 -119.233( 21) 0

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-304.19477131 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 118  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.499445( 1)  
3 3 O 1 1.392097( 2) 2 116.232( 9)  
4 4 O 1 1.201148( 3) 2 126.235( 10) 3 189.777( 16) 0  
5 5 O 3 1.457711( 4) 1 107.293( 11) 2 45.000( 17) 0  
6 6 H 5 0.968670( 5) 3 99.215( 12) 1 225.000( 18) 0  
7 7 H 2 1.088462( 6) 1 110.373( 13) 3 270.000( 19) 0  
8 8 H 2 1.085383( 7) 1 110.828( 14) 7 119.879( 20) 0  
9 9 H 2 1.085279( 8) 1 107.427( 15) 7 -118.505( 21) 0  
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-304.19479560 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 119  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.502344( 1)  
3 3 O 1 1.391426( 2) 2 118.007( 9)  
4 4 O 1 1.200967( 3) 2 124.471( 10) 3 190.122( 16) 0  
5 5 O 3 1.449878( 4) 1 110.167( 11) 2 45.000( 17) 0  
6 6 H 5 0.969643( 5) 3 101.573( 12) 1 270.000( 18) 0  
7 7 H 2 1.083625( 6) 1 114.219( 13) 3 0.000( 19) 0  
8 8 H 2 1.087228( 7) 1 106.498( 14) 7 121.836( 20) 0  
9 9 H 2 1.088020( 8) 1 109.218( 15) 7 -121.805( 21) 0  
-----

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-304.19162271 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 120  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.500428( 1)  
3 3 O 1 1.392697( 2) 2 117.748( 9)  
4 4 O 1 1.201052( 3) 2 124.829( 10) 3 191.655( 16) 0  
5 5 O 3 1.449533( 4) 1 111.184( 11) 2 45.000( 17) 0  
6 6 H 5 0.969702( 5) 3 101.426( 12) 1 270.000( 18) 0  
7 7 H 2 1.089795( 6) 1 106.493( 13) 3 90.000( 19) 0  
8 8 H 2 1.085899( 7) 1 108.548( 14) 7 115.998( 20) 0  
9 9 H 2 1.083362( 8) 1 114.086( 15) 7 -121.486( 21) 0  
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-304.19195334 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 121

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.499402( 1)					
3	3	O	1	1.393729( 2)	2	116.498( 9)			
4	4	O	1	1.200892( 3)	2	125.917( 10)	3	191.242( 16)	0
5	5	O	3	1.450528( 4)	1	110.469( 11)	2	45.000( 17)	0
6	6	H	5	0.970067( 5)	3	101.413( 12)	1	270.000( 18)	0
7	7	H	2	1.084298( 6)	1	108.473( 13)	3	180.000( 19)	0
8	8	H	2	1.086384( 7)	1	111.904( 14)	7	121.118( 20)	0
9	9	H	2	1.089901( 8)	1	108.214( 15)	7	-119.164( 21)	0

-304.19300712 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 122

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.501518( 1)					
3	3	O	1	1.391762( 2)	2	116.511( 9)			
4	4	O	1	1.200822( 3)	2	125.698( 10)	3	189.734( 16)	0
5	5	O	3	1.450917( 4)	1	109.154( 11)	2	45.000( 17)	0
6	6	H	5	0.970098( 5)	3	101.509( 12)	1	270.000( 18)	0
7	7	H	2	1.088487( 6)	1	110.481( 13)	3	270.000( 19)	0
8	8	H	2	1.087068( 7)	1	111.447( 14)	7	121.104( 20)	0
9	9	H	2	1.085253( 8)	1	107.366( 15)	7	-118.269( 21)	0

-304.19290723 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 123

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.506642( 1)					
3	3	O	1	1.383409( 2)	2	118.382( 9)			
4	4	O	1	1.201664( 3)	2	123.577( 10)	3	190.678( 16)	0
5	5	O	3	1.451750( 4)	1	113.066( 11)	2	45.000( 17)	0
6	6	H	5	0.969787( 5)	3	103.266( 12)	1	315.000( 18)	0
7	7	H	2	1.087101( 6)	1	115.500( 13)	3	0.000( 19)	0
8	8	H	2	1.086918( 7)	1	106.173( 14)	7	120.393( 20)	0
9	9	H	2	1.088024( 8)	1	109.488( 15)	7	-123.243( 21)	0

-304.18534763 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 124

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Z-MATRIX (ANGSTROMS AND DEGREES)  
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.505799( 1)					
3	3	O	1	1.384454( 2)	2	118.781( 9)			
4	4	O	1	1.201781( 3)	2	123.312( 10)	3	192.636( 16)	0
5	5	O	3	1.451896( 4)	1	114.140( 11)	2	45.000( 17)	0
6	6	H	5	0.968812( 5)	3	103.262( 12)	1	315.000( 18)	0
7	7	H	2	1.089450( 6)	1	106.139( 13)	3	90.000( 19)	0
8	8	H	2	1.085635( 7)	1	108.244( 14)	7	116.072( 20)	0
9	9	H	2	1.086242( 8)	1	116.717( 15)	7	-121.151( 21)	0

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-304.18501552 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 125

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Z-MATRIX (ANGSTROMS AND DEGREES)  
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.504243( 1)					
3	3	O	1	1.386562( 2)	2	117.118( 9)			
4	4	O	1	1.201557( 3)	2	124.842( 10)	3	192.233( 16)	0
5	5	O	3	1.453243( 4)	1	113.507( 11)	2	45.000( 17)	0
6	6	H	5	0.969572( 5)	3	103.274( 12)	1	315.000( 18)	0
7	7	H	2	1.084410( 6)	1	108.007( 13)	3	180.000( 19)	0
8	8	H	2	1.089402( 7)	1	113.320( 14)	7	119.109( 20)	0
9	9	H	2	1.089243( 8)	1	108.559( 15)	7	-119.628( 21)	0

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-304.18634724 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 126

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Z-MATRIX (ANGSTROMS AND DEGREES)  
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.505818( 1)					
3	3	O	1	1.384631( 2)	2	116.553( 9)			
4	4	O	1	1.201411( 3)	2	125.095( 10)	3	190.667( 16)	0
5	5	O	3	1.453648( 4)	1	112.047( 11)	2	45.000( 17)	0
6	6	H	5	0.970849( 5)	3	103.320( 12)	1	315.000( 18)	0
7	7	H	2	1.090077( 6)	1	111.146( 13)	3	270.000( 19)	0
8	8	H	2	1.089304( 7)	1	111.235( 14)	7	122.313( 20)	0
9	9	H	2	1.084893( 8)	1	107.311( 15)	7	-117.885( 21)	0

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-304.18692288 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 127

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Z-MATRIX (ANGSTROMS AND DEGREES)  
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.507972( 1)					
3	3	O	1	1.370364( 2)	2	122.067( 9)			
4	4	O	1	1.204040( 3)	2	122.412( 10)	3	180.000( 16)	0
5	5	O	3	1.450846( 4)	1	118.230( 11)	2	0.000( 17)	0
6	6	H	5	0.967115( 5)	3	103.760( 12)	1	0.000( 18)	0
7	7	H	2	1.086269( 6)	1	118.770( 13)	3	0.000( 19)	0
8	8	H	2	1.087462( 7)	1	106.748( 14)	7	122.400( 20)	0
9	9	H	2	1.087462( 8)	1	106.748( 15)	7	-122.400( 21)	0

-304.18580562 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 128

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.505945( 1)					
3	3	O	1	1.370635( 2)	2	120.145( 9)			
4	4	O	1	1.203901( 3)	2	123.954( 10)	3	181.172( 16)	0
5	5	O	3	1.451550( 4)	1	117.388( 11)	2	0.000( 17)	0
6	6	H	5	0.968039( 5)	3	103.926( 12)	1	0.000( 18)	0
7	7	H	2	1.089514( 6)	1	109.117( 13)	3	90.000( 19)	0
8	8	H	2	1.085987( 7)	1	106.007( 14)	7	115.368( 20)	0
9	9	H	2	1.088185( 8)	1	115.817( 15)	7	-125.252( 21)	0

-304.18795146 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 129

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503077( 1)					
3	3	O	1	1.371946( 2)	2	118.501( 9)			
4	4	O	1	1.203512( 3)	2	125.317( 10)	3	180.000( 16)	0
5	5	O	3	1.452420( 4)	1	116.767( 11)	2	0.000( 17)	0
6	6	H	5	0.968450( 5)	3	104.167( 12)	1	0.000( 18)	0
7	7	H	2	1.084206( 6)	1	107.336( 13)	3	180.000( 19)	0
8	8	H	2	1.090835( 7)	1	111.228( 14)	7	118.888( 20)	0
9	9	H	2	1.090835( 8)	1	111.228( 15)	7	-118.888( 21)	0

-304.18994045 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 130

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							

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2  2 C   1  1.504016(  1)
3  3 O   1  1.378625(  2)  2 120.853(  9)
4  4 O   1  1.202985(  3)  2 123.819( 10)  3 179.722( 16)  0
5  5 O   3  1.449563(  4)  1 116.386( 11)  2  0.000( 17)  0
6  6 H   5  0.968656(  5)  3 102.734( 12)  1  45.000( 18)  0
7  7 H   2  1.083265(  6)  1 116.338( 13)  3  0.000( 19)  0
8  8 H   2  1.088006(  7)  1 106.708( 14)  7 121.010( 20)  0
9  9 H   2  1.087641(  8)  1 107.433( 15)  7 -123.861( 21)  0

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-304.19053125 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 131  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503099( 1)					
3	3	O	1	1.377174( 2)	2	120.127( 9)			
4	4	O	1	1.203224( 3)	2	124.322( 10)	3	180.931( 16)	0
5	5	O	3	1.449034( 4)	1	115.838( 11)	2	0.000( 17)	0
6	6	H	5	0.968129( 5)	3	102.836( 12)	1	45.000( 18)	0
7	7	H	2	1.089437( 6)	1	108.065( 13)	3	90.000( 19)	0
8	8	H	2	1.085585( 7)	1	106.528( 14)	7	115.860( 20)	0
9	9	H	2	1.085164( 8)	1	116.318( 15)	7	-122.153( 21)	0

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-304.19140824 Energy CCSD(T)-F12/CVTA-F12  
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=====  
Geometry (MP2/AVTZ) 132  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.500323( 1)					
3	3	O	1	1.378166( 2)	2	118.141( 9)			
4	4	O	1	1.202903( 3)	2	125.884( 10)	3	179.828( 16)	0
5	5	O	3	1.449579( 4)	1	114.839( 11)	2	0.000( 17)	0
6	6	H	5	0.968927( 5)	3	102.956( 12)	1	45.000( 18)	0
7	7	H	2	1.084283( 6)	1	107.392( 13)	3	180.000( 19)	0
8	8	H	2	1.091261( 7)	1	111.545( 14)	7	118.034( 20)	0
9	9	H	2	1.087599( 8)	1	110.660( 15)	7	-121.278( 21)	0

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-304.19383933 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 133  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.501622( 1)					
3	3	O	1	1.379182( 2)	2	118.866( 9)			
4	4	O	1	1.202847( 3)	2	125.373( 10)	3	178.954( 16)	0

5	5	O	3	1.450047( 4)	1	115.305( 11)	2	0.000( 17)	0
6	6	H	5	0.969424( 5)	3	102.887( 12)	1	45.000( 18)	0
7	7	H	2	1.091177( 6)	1	109.172( 13)	3	270.000( 19)	0
8	8	H	2	1.084823( 7)	1	113.367( 14)	7	123.523( 20)	0
9	9	H	2	1.085761( 8)	1	106.668( 15)	7	-115.265( 21)	0

-304.19289240 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 134

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.499685( 1)					
3	3	O	1	1.386883( 2)	2	120.001( 9)			
4	4	O	1	1.202471( 3)	2	125.111( 10)	3	180.138( 16)	0
5	5	O	3	1.447588( 4)	1	114.073( 11)	2	0.000( 17)	0
6	6	H	5	0.969572( 5)	3	100.415( 12)	1	90.000( 18)	0
7	7	H	2	1.081059( 6)	1	114.234( 13)	3	0.000( 19)	0
8	8	H	2	1.087933( 7)	1	107.049( 14)	7	121.824( 20)	0
9	9	H	2	1.088089( 8)	1	107.413( 15)	7	-123.022( 21)	0

-304.19720489 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 135

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498468( 1)					
3	3	O	1	1.385209( 2)	2	119.221( 9)			
4	4	O	1	1.202668( 3)	2	125.575( 10)	3	181.082( 16)	0
5	5	O	3	1.447578( 4)	1	113.287( 11)	2	0.000( 17)	0
6	6	H	5	0.969459( 5)	3	100.442( 12)	1	90.000( 18)	0
7	7	H	2	1.089675( 6)	1	108.012( 13)	3	90.000( 19)	0
8	8	H	2	1.085756( 7)	1	106.930( 14)	7	116.028( 20)	0
9	9	H	2	1.082239( 8)	1	114.155( 15)	7	-120.783( 21)	0

-304.19820278 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 136

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.496865( 1)					
3	3	O	1	1.384814( 2)	2	117.878( 9)			
4	4	O	1	1.202487( 3)	2	126.565( 10)	3	180.299( 16)	0
5	5	O	3	1.447721( 4)	1	112.381( 11)	2	0.000( 17)	0
6	6	H	5	0.969392( 5)	3	100.528( 12)	1	90.000( 18)	0
7	7	H	2	1.084469( 6)	1	107.452( 13)	3	180.000( 19)	0

8 8 H 2 1.087869( 7) 1 111.028( 14) 7 119.903( 20) 0  
9 9 H 2 1.087083( 8) 1 110.330( 15) 7 -121.048( 21) 0

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-304.19992990 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 137  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.498215( 1)  
3 3 O 1 1.385743( 2) 2 118.786( 9)  
4 4 O 1 1.202595( 3) 2 125.948( 10) 3 179.472( 16) 0  
5 5 O 3 1.447631( 4) 1 113.079( 11) 2 0.000( 17) 0  
6 6 H 5 0.969411( 5) 3 100.516( 12) 1 90.000( 18) 0  
7 7 H 2 1.090364( 6) 1 108.661( 13) 3 270.000( 19) 0  
8 8 H 2 1.082649( 7) 1 113.003( 14) 7 121.632( 20) 0  
9 9 H 2 1.085763( 8) 1 106.835( 15) 7 -115.751( 21) 0  
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-304.19883256 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 138  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.498658( 1)  
3 3 O 1 1.382449( 2) 2 119.830( 9)  
4 4 O 1 1.203130( 3) 2 125.296( 10) 3 180.566( 16) 0  
5 5 O 3 1.454763( 4) 1 112.519( 11) 2 0.000( 17) 0  
6 6 H 5 0.968689( 5) 3 98.069( 12) 1 135.000( 18) 0  
7 7 H 2 1.080691( 6) 1 114.112( 13) 3 0.000( 19) 0  
8 8 H 2 1.087879( 7) 1 107.115( 14) 7 122.468( 20) 0  
9 9 H 2 1.088093( 8) 1 107.218( 15) 7 -122.379( 21) 0  
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-304.19892531 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 139  
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Z-MATRIX (ANGSTROMS AND DEGREES)  
CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J  
-----  
1 1 C  
2 2 C 1 1.496828( 1)  
3 3 O 1 1.381698( 2) 2 118.883( 9)  
4 4 O 1 1.203362( 3) 2 125.977( 10) 3 181.421( 16) 0  
5 5 O 3 1.454706( 4) 1 111.816( 11) 2 0.000( 17) 0  
6 6 H 5 0.968545( 5) 3 98.140( 12) 1 135.000( 18) 0  
7 7 H 2 1.089826( 6) 1 108.120( 13) 3 90.000( 19) 0  
8 8 H 2 1.085753( 7) 1 106.964( 14) 7 116.006( 20) 0  
9 9 H 2 1.082009( 8) 1 113.259( 15) 7 -120.925( 21) 0  
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-304.20015503 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 140

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.495245( 1)					
3	3	O	1	1.381114( 2)	2	117.605( 9)			
4	4	O	1	1.203088( 3)	2	126.871( 10)	3	180.767( 16)	0
5	5	O	3	1.455080( 4)	1	110.741( 11)	2	0.000( 17)	0
6	6	H	5	0.968550( 5)	3	98.158( 12)	1	135.000( 18)	0
7	7	H	2	1.084361( 6)	1	107.561( 13)	3	180.000( 19)	0
8	8	H	2	1.086950( 7)	1	110.461( 14)	7	120.663( 20)	0
9	9	H	2	1.087645( 8)	1	110.275( 15)	7	-120.790( 21)	0

-304.20177089 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 141

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.497264( 1)					
3	3	O	1	1.381040( 2)	2	118.699( 9)			
4	4	O	1	1.203266( 3)	2	126.040( 10)	3	179.903( 16)	0
5	5	O	3	1.455250( 4)	1	111.437( 11)	2	0.000( 17)	0
6	6	H	5	0.968630( 5)	3	98.152( 12)	1	135.000( 18)	0
7	7	H	2	1.089664( 6)	1	108.414( 13)	3	270.000( 19)	0
8	8	H	2	1.082503( 7)	1	113.220( 14)	7	121.217( 20)	0
9	9	H	2	1.085807( 8)	1	106.828( 15)	7	-116.078( 21)	0

-304.20045093 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 142

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498738( 1)					
3	3	O	1	1.377321( 2)	2	119.605( 9)			
4	4	O	1	1.203665( 3)	2	125.287( 10)	3	180.000( 16)	0
5	5	O	3	1.461335( 4)	1	111.514( 11)	2	0.000( 17)	0
6	6	H	5	0.968862( 5)	3	96.883( 12)	1	180.000( 18)	0
7	7	H	2	1.081001( 6)	1	114.304( 13)	3	0.000( 19)	0
8	8	H	2	1.087956( 7)	1	107.147( 14)	7	122.399( 20)	0
9	9	H	2	1.087956( 8)	1	107.147( 15)	7	-122.399( 21)	0

-304.19884550 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 143

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                Z-MATRIX (ANGSTROMS AND DEGREES)
CD  Cent  Atom  N1   Length/X   N2   Alpha/Y   N3   Beta/Z   J
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.496844( 1)					
3	3	O	1	1.376935( 2)	2	118.480( 9)			
4	4	O	1	1.203721( 3)	2	126.139( 10)	3	180.695( 16)	0
5	5	O	3	1.461602( 4)	1	110.650( 11)	2	0.000( 17)	0
6	6	H	5	0.968680( 5)	3	96.880( 12)	1	180.000( 18)	0
7	7	H	2	1.089665( 6)	1	108.255( 13)	3	90.000( 19)	0
8	8	H	2	1.085644( 7)	1	106.958( 14)	7	116.154( 20)	0
9	9	H	2	1.082769( 8)	1	113.140( 15)	7	-121.101( 21)	0

-304.20022249 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 144

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                Z-MATRIX (ANGSTROMS AND DEGREES)
CD  Cent  Atom  N1   Length/X   N2   Alpha/Y   N3   Beta/Z   J
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.494796( 1)					
3	3	O	1	1.377081( 2)	2	117.311( 9)			
4	4	O	1	1.203584( 3)	2	127.019( 10)	3	180.000( 16)	0
5	5	O	3	1.461606( 4)	1	109.824( 11)	2	0.000( 17)	0
6	6	H	5	0.968529( 5)	3	97.008( 12)	1	180.000( 18)	0
7	7	H	2	1.084210( 6)	1	107.703( 13)	3	180.000( 19)	0
8	8	H	2	1.087522( 7)	1	110.217( 14)	7	120.772( 20)	0
9	9	H	2	1.087522( 8)	1	110.217( 15)	7	-120.772( 21)	0

-304.20166241 Energy CCSD(T)-F12/CVTA-F12

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 Geometry (MP2/AVTZ) 145

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                Z-MATRIX (ANGSTROMS AND DEGREES)
CD  Cent  Atom  N1   Length/X   N2   Alpha/Y   N3   Beta/Z   J
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CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498658( 1)					
3	3	O	1	1.382449( 2)	2	119.830( 9)			
4	4	O	1	1.203130( 3)	2	125.296( 10)	3	179.434( 16)	0
5	5	O	3	1.454763( 4)	1	112.519( 11)	2	0.000( 17)	0
6	6	H	5	0.968689( 5)	3	98.069( 12)	1	225.000( 18)	0
7	7	H	2	1.080691( 6)	1	114.112( 13)	3	0.000( 19)	0
8	8	H	2	1.088093( 7)	1	107.218( 14)	7	122.379( 20)	0
9	9	H	2	1.087879( 8)	1	107.115( 15)	7	-122.468( 21)	0

-304.19892531 Energy CCSD(T)-F12/CVTA-F12

=====  
 Geometry (MP2/AVTZ) 146

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 Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.497264( 1)					
3	3	O	1	1.381040( 2)	2	118.699( 9)			
4	4	O	1	1.203266( 3)	2	126.040( 10)	3	180.097( 16)	0
5	5	O	3	1.455250( 4)	1	111.437( 11)	2	0.000( 17)	0
6	6	H	5	0.968630( 5)	3	98.152( 12)	1	225.000( 18)	0
7	7	H	2	1.089664( 6)	1	108.414( 13)	3	90.000( 19)	0
8	8	H	2	1.085807( 7)	1	106.828( 14)	7	116.078( 20)	0
9	9	H	2	1.082503( 8)	1	113.220( 15)	7	-121.217( 21)	0

-304.20045093 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 147

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.495245( 1)					
3	3	O	1	1.381114( 2)	2	117.605( 9)			
4	4	O	1	1.203088( 3)	2	126.871( 10)	3	179.233( 16)	0
5	5	O	3	1.455080( 4)	1	110.741( 11)	2	0.000( 17)	0
6	6	H	5	0.968550( 5)	3	98.158( 12)	1	225.000( 18)	0
7	7	H	2	1.084361( 6)	1	107.561( 13)	3	180.000( 19)	0
8	8	H	2	1.087645( 7)	1	110.275( 14)	7	120.790( 20)	0
9	9	H	2	1.086950( 8)	1	110.461( 15)	7	-120.663( 21)	0

-304.20177089 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 148

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.496828( 1)					
3	3	O	1	1.381698( 2)	2	118.883( 9)			
4	4	O	1	1.203362( 3)	2	125.977( 10)	3	178.579( 16)	0
5	5	O	3	1.454706( 4)	1	111.816( 11)	2	0.000( 17)	0
6	6	H	5	0.968545( 5)	3	98.140( 12)	1	225.000( 18)	0
7	7	H	2	1.089826( 6)	1	108.120( 13)	3	270.000( 19)	0
8	8	H	2	1.082009( 7)	1	113.259( 14)	7	120.925( 20)	0
9	9	H	2	1.085753( 8)	1	106.964( 15)	7	-116.006( 21)	0

-304.20015502 Energy CCSD(T)-F12/CVTA-F12

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Geometry (MP2/AVTZ) 149

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							

```

2  2 C   1  1.499685(  1)
3  3 O   1  1.386883(  2)  2 120.001(  9)
4  4 O   1  1.202471(  3)  2 125.111( 10)  3 179.862( 16)  0
5  5 O   3  1.447588(  4)  1 114.073( 11)  2  0.000( 17)  0
6  6 H   5  0.969572(  5)  3 100.415( 12)  1 270.000( 18)  0
7  7 H   2  1.081059(  6)  1 114.234( 13)  3  0.000( 19)  0
8  8 H   2  1.088089(  7)  1 107.413( 14)  7 123.022( 20)  0
9  9 H   2  1.087933(  8)  1 107.049( 15)  7 -121.824( 21)  0

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-304.19720489 Energy CCSD(T)-F12/CVTA-F12  
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Geometry (MP2/AVTZ) 150  
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Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498215( 1)					
3	3	O	1	1.385743( 2)	2	118.786( 9)			
4	4	O	1	1.202595( 3)	2	125.948( 10)	3	180.528( 16)	0
5	5	O	3	1.447631( 4)	1	113.079( 11)	2	0.000( 17)	0
6	6	H	5	0.969411( 5)	3	100.516( 12)	1	270.000( 18)	0
7	7	H	2	1.090364( 6)	1	108.661( 13)	3	90.000( 19)	0
8	8	H	2	1.085763( 7)	1	106.835( 14)	7	115.751( 20)	0
9	9	H	2	1.082649( 8)	1	113.003( 15)	7	-121.632( 21)	0

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-304.19883256 Energy CCSD(T)-F12/CVTA-F12  
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=====  
Geometry (MP2/AVTZ) 151  
-----

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.496865( 1)					
3	3	O	1	1.384814( 2)	2	117.878( 9)			
4	4	O	1	1.202487( 3)	2	126.565( 10)	3	179.701( 16)	0
5	5	O	3	1.447721( 4)	1	112.381( 11)	2	0.000( 17)	0
6	6	H	5	0.969392( 5)	3	100.528( 12)	1	270.000( 18)	0
7	7	H	2	1.084469( 6)	1	107.452( 13)	3	180.000( 19)	0
8	8	H	2	1.087083( 7)	1	110.330( 14)	7	121.048( 20)	0
9	9	H	2	1.087869( 8)	1	111.028( 15)	7	-119.903( 21)	0

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-304.19992990 Energy CCSD(T)-F12/CVTA-F12  
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=====  
Geometry (MP2/AVTZ) 152  
-----

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.498468( 1)					
3	3	O	1	1.385209( 2)	2	119.221( 9)			
4	4	O	1	1.202668( 3)	2	125.575( 10)	3	178.918( 16)	0



5	5	O	3	1.447578( 4)	1	113.287( 11)	2	0.000( 17)	0
6	6	H	5	0.969459( 5)	3	100.442( 12)	1	270.000( 18)	0
7	7	H	2	1.089675( 6)	1	108.012( 13)	3	270.000( 19)	0
8	8	H	2	1.082240( 7)	1	114.155( 14)	7	120.783( 20)	0
9	9	H	2	1.085756( 8)	1	106.930( 15)	7	-116.028( 21)	0

-304.19820278 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 153

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.504016( 1)					
3	3	O	1	1.378625( 2)	2	120.853( 9)			
4	4	O	1	1.202985( 3)	2	123.819( 10)	3	180.278( 16)	0
5	5	O	3	1.449563( 4)	1	116.386( 11)	2	0.000( 17)	0
6	6	H	5	0.968656( 5)	3	102.734( 12)	1	315.000( 18)	0
7	7	H	2	1.083265( 6)	1	116.338( 13)	3	0.000( 19)	0
8	8	H	2	1.087641( 7)	1	107.433( 14)	7	123.861( 20)	0
9	9	H	2	1.088006( 8)	1	106.708( 15)	7	-121.010( 21)	0

-304.19053125 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 154

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.501622( 1)					
3	3	O	1	1.379182( 2)	2	118.866( 9)			
4	4	O	1	1.202847( 3)	2	125.373( 10)	3	181.046( 16)	0
5	5	O	3	1.450047( 4)	1	115.305( 11)	2	0.000( 17)	0
6	6	H	5	0.969424( 5)	3	102.887( 12)	1	315.000( 18)	0
7	7	H	2	1.091177( 6)	1	109.172( 13)	3	90.000( 19)	0
8	8	H	2	1.085761( 7)	1	106.668( 14)	7	115.265( 20)	0
9	9	H	2	1.084822( 8)	1	113.367( 15)	7	-123.523( 21)	0

-304.19289240 Energy CCSD(T)-F12/CVTA-F12

=====  
Geometry (MP2/AVTZ) 155

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.500323( 1)					
3	3	O	1	1.378166( 2)	2	118.141( 9)			
4	4	O	1	1.202903( 3)	2	125.884( 10)	3	180.172( 16)	0
5	5	O	3	1.449579( 4)	1	114.839( 11)	2	0.000( 17)	0
6	6	H	5	0.968927( 5)	3	102.956( 12)	1	315.000( 18)	0
7	7	H	2	1.084283( 6)	1	107.392( 13)	3	180.000( 19)	0

8	8	H	2	1.087599( 7)	1	110.660( 14)	7	121.278( 20)	0
9	9	H	2	1.091261( 8)	1	111.545( 15)	7	-118.034( 21)	0

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-304.19383933 Energy CCSD(T)-F12/CVTA-F12  
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=====  
Geometry (MP2/AVTZ) 156  
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Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503099( 1)					
3	3	O	1	1.377174( 2)	2	120.127( 9)			
4	4	O	1	1.203224( 3)	2	124.322( 10)	3	179.069( 16)	0
5	5	O	3	1.449034( 4)	1	115.838( 11)	2	0.000( 17)	0
6	6	H	5	0.968129( 5)	3	102.836( 12)	1	315.000( 18)	0
7	7	H	2	1.089437( 6)	1	108.065( 13)	3	270.000( 19)	0
8	8	H	2	1.085164( 7)	1	116.318( 14)	7	122.153( 20)	0
9	9	H	2	1.085585( 8)	1	106.528( 15)	7	-115.860( 21)	0

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