

Supporting Information for:

Cooperative and Competitive Effects Associated with $\text{Fe}(\text{CO})_3$ Binding to Annelated Benzenes

XIAOGUANG BAO, DAVID A. HROVAT, AND WESTON THATCHER BORDEN*

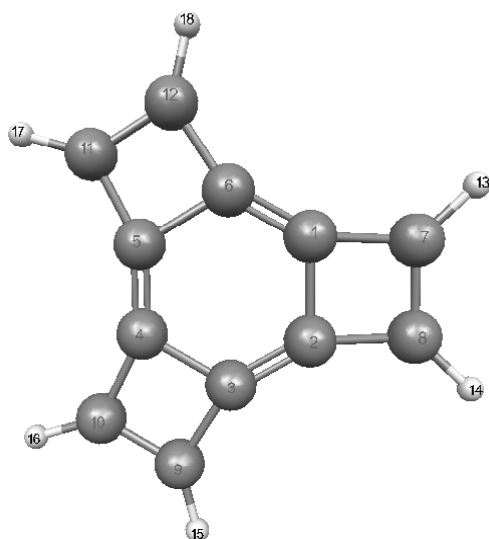
Department of Chemistry and the Center for Advanced, Scientific Computing
and Modeling, University of North Texas, 1155 Union Circle, #305070,
Denton, Texas 76203-5070

* Corresponding author E-mail: borden@unt.edu

This Supporting Information contains fully optimized geometries and energies of **3**, **5**, **6**, **7a/7b**, **8a/8b**, **9a**, **10a**, **11a**, and **12** (*trans*, *gauche*, and TS).

(3) B3LYP/6-31G(d) D_{3h} Geometry

Nuclear repulsion energy	575.78689610	Hartrees
B3LYP/6-31G(d) energy	-460.63040964	Hartrees
Zero-point energy correction	0.131527	Hartrees
Thermal correction to Enthalpy	0.140713	Hartrees
Thermal correction to Gibbs Free Energy	0.100282	Hartrees



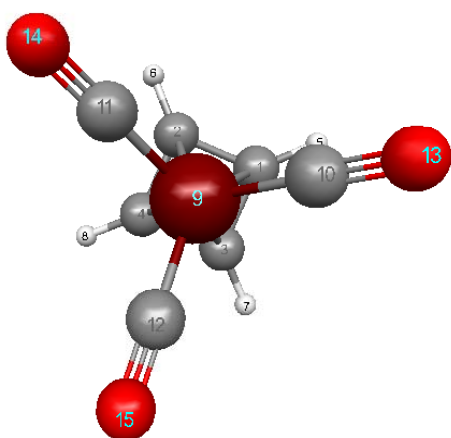
	X	Y	Z
C1	0.668825	1.260989	0.000000
C2	1.426461	-0.051275	0.000000
C3	0.757636	-1.209714	0.000000
C4	-0.757636	-1.209714	0.000000
C5	-1.426461	-0.051275	0.000000
C6	-0.668825	1.260989	0.000000
C7	1.977960	1.935681	0.000000
C8	2.665329	0.745123	0.000000
C9	0.687369	-2.680804	0.000000
C10	-0.687369	-2.680804	0.000000
C11	-2.665329	0.745123	0.000000
C12	-1.977960	1.935681	0.000000
H13	2.287957	2.974679	0.000000
H14	3.720126	0.494089	0.000000
H15	1.432169	-3.468768	0.000000
H16	-1.432169	-3.468768	0.000000
H17	-3.720126	0.494089	0.000000
H18	-2.287957	2.974679	0.000000

(1-2)	1.515	(1-6)	1.338	(1-7)	1.473	(2-3)	1.338	(2-8)	1.473
(3-4)	1.515	(3-9)	1.473	(4-5)	1.338	(4-10)	1.473	(5-6)	1.515
(5-11)	1.473	(6-12)	1.473	(7-8)	1.375	(7-13)	1.084	(8-14)	1.084
(9-10)	1.375	(9-15)	1.084	(10-16)	1.084	(11-12)	1.375	(11-17)	1.084
(12-18)	1.084								
(2-1-6)	120.0	(2-1-7)	87.3	(6-1-7)	152.7	(1-2-3)	120.0		
(1-2-8)	87.3	(3-2-8)	152.7	(2-3-4)	120.0	(2-3-9)	152.7		
(4-3-9)	87.3	(3-4-5)	120.0	(3-4-10)	87.3	(5-4-10)	152.7		
(4-5-6)	120.0	(4-5-11)	152.7	(6-5-11)	87.3	(1-6-5)	120.0		
(1-6-12)	152.7	(5-6-12)	87.3	(1-7-8)	92.7	(1-7-13)	133.9		
(8-7-13)	133.4	(2-8-7)	92.7	(2-8-14)	133.9	(7-8-14)	133.4		
(3-9-10)	92.7	(3-9-15)	133.9	(10-9-15)	133.4	(4-10-9)	92.7		
(4-10-16)	133.9	(9-10-16)	133.4	(5-11-12)	92.7	(5-11-17)	133.9		
(12-11-17)	133.4	(6-12-11)	92.7	(6-12-18)	133.9	(11-12-18)	133.4		
(6-1-2-3)		0.0	(6-1-2-8)	180.0	(7-1-2-3)	180.0			
(7-1-2-8)		0.0	(2-1-6-5)	0.0	(2-1-6-12)	180.0			
(7-1-6-5)	180.0	(7-1-6-12)	0.0	(2-1-7-8)	0.0				
(2-1-7-13)	180.0	(6-1-7-8)	180.0	(6-1-7-13)	0.0				
(1-2-3-4)	0.0	(1-2-3-9)	180.0	(8-2-3-4)	180.0				
(8-2-3-9)	0.0	(1-2-8-7)	0.0	(1-2-8-14)	180.0				
(3-2-8-7)	180.0	(3-2-8-14)	0.0	(2-3-4-5)	0.0				
(2-3-4-10)	180.0	(9-3-4-5)	180.0	(9-3-4-10)	0.0				
(2-3-9-10)	180.0	(2-3-9-15)	0.0	(4-3-9-10)	0.0				
(4-3-9-15)	180.0	(3-4-5-6)	0.0	(3-4-5-11)	180.0				
(10-4-5-6)	180.0	(10-4-5-11)	0.0	(3-4-10-9)	0.0				
(3-4-10-16)	180.0	(5-4-10-9)	180.0	(5-4-10-16)	0.0				
(4-5-6-1)	0.0	(4-5-6-12)	180.0	(11-5-6-1)	180.0				
(11-5-6-12)	0.0	(4-5-11-12)	180.0	(4-5-11-17)	0.0				
(6-5-11-12)	0.0	(6-5-11-17)	180.0	(1-6-12-11)	180.0				
(1-6-12-18)	0.0	(5-6-12-11)	0.0	(5-6-12-18)	180.0				
(1-7-8-2)	0.0	(1-7-8-14)	180.0	(13-7-8-2)	180.0				
(13-7-8-14)	0.0	(3-9-10-4)	0.0	(3-9-10-16)	180.0				
(15-9-10-4)	180.0	(15-9-10-16)	0.0	(5-11-12-6)	0.0				

(5-11-12-18)	180.0	(17-11-12-6)	180.0	(17-11-12-18)	0.0
Frequencies (cm ⁻¹):					
145.4	217.8	217.8	305.8	343.7	343.7
374.3	374.3	514.3	514.3	611.8	655.2
700.3	700.3	754.2	780.1	780.1	798.8
889.8	889.8	894.2	913.8	959.4	988.1
988.1	1020.1	1020.1	1072.9	1098.7	1098.7
1124.9	1186.5	1186.5	1309.7	1309.7	1359.5
1476.7	1503.0	1503.0	1782.3	1790.3	1790.3
3227.4	3228.5	3228.5	3253.4	3253.4	3254.7

(5) B3LYP/6-31G(d)+LANL2DZ C₁ Geometry

Nuclear repulsion energy	683.62691247	Hartrees
B3LYP/6-31G(d)+LANL2DZ energy	-618.23450042	Hartrees
Zero-point energy correction	0.091084	Hartrees
Thermal correction to Enthalpy	0.102946	Hartrees
Thermal correction to Gibbs Free Energy	0.052240	Hartrees



	X	Y	Z
C1	-1.783357	-0.619809	-0.846460
C2	-1.780397	0.806764	-0.643689
C3	-1.756058	-0.838390	0.585217
C4	-1.750275	0.609807	0.798506
H5	-1.848426	-1.263206	-1.713390
H6	-1.865604	1.665623	-1.294867
H7	-1.872850	-1.703194	1.222684
H8	-1.890200	1.253534	1.654961
Fe9	0.010547	-0.001012	-0.006261
C10	0.909688	-1.112706	-1.072154
C11	0.872538	1.501830	-0.419262
C12	0.841140	-0.375470	1.520697
O13	1.479098	-1.843194	-1.758744
O14	1.409159	2.489668	-0.674511
O15	1.347142	-0.616298	2.527787

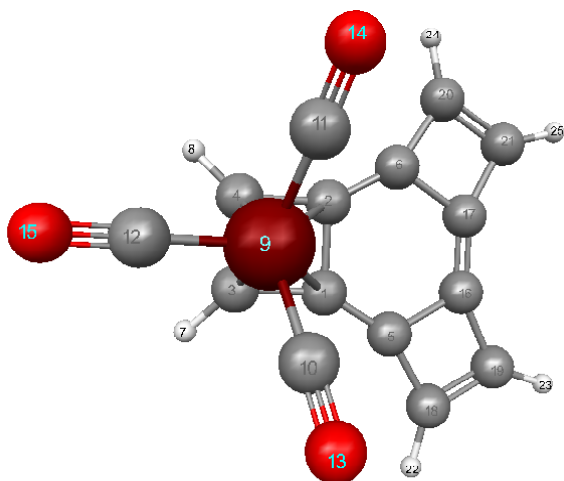
(1-2)	1.441	(1-3)	1.449	(1-5)	1.082	(1-9)	2.075	(2-4)	1.456
(2-6)	1.081	(2-9)	2.066	(3-4)	1.464	(3-7)	1.081	(3-9)	2.043
(4-8)	1.080	(4-9)	2.030	(9-10)	1.783	(9-11)	1.781	(9-12)	1.778
(10-13)	1.153	(11-14)	1.153	(12-15)	1.153				
(2-1-3)	90.6	(2-1-5)	134.6	(2-1-9)	69.3	(3-1-5)	134.7		
(3-1-9)	68.2	(5-1-9)	123.6	(1-2-4)	90.3	(1-2-6)	134.6		
(1-2-9)	70.0	(4-2-6)	134.9	(4-2-9)	67.9	(6-2-9)	124.4		
(1-3-4)	89.7	(1-3-7)	134.6	(1-3-9)	70.6	(4-3-7)	134.9		
(4-3-9)	68.5	(7-3-9)	126.3	(2-4-3)	89.4	(2-4-8)	134.6		
(2-4-9)	70.5	(3-4-8)	134.8	(3-4-9)	69.4	(8-4-9)	127.3		
(1-9-2)	40.7	(1-9-3)	41.2	(1-9-4)	60.0	(1-9-10)	90.5		
(1-9-11)	125.2	(1-9-12)	133.5	(2-9-3)	60.0	(2-9-4)	41.6		
(2-9-10)	119.8	(2-9-11)	91.0	(2-9-12)	138.8	(3-9-4)	42.1		
(3-9-10)	110.7	(3-9-11)	146.3	(3-9-12)	94.0	(4-9-10)	149.5		
(4-9-11)	104.9	(4-9-12)	97.4	(10-9-11)	98.2	(10-9-12)	98.4		
(11-9-12)	98.7	(9-10-13)	179.2	(9-11-14)	178.6	(9-12-15)	178.2		
(3-1-2-4)	0.1	(3-1-2-6)	-174.6	(3-1-2-9)	66.4				
(5-1-2-4)	176.5	(5-1-2-6)	1.7	(5-1-2-9)	-117.3				
(9-1-2-4)	-66.3	(9-1-2-6)	119.0	(2-1-3-4)	-0.1				
(2-1-3-7)	170.3	(2-1-3-9)	-67.3	(5-1-3-4)	-176.4				
(5-1-3-7)	-6.0	(5-1-3-9)	116.3	(9-1-3-4)	67.2				
(9-1-3-7)	-122.3	(2-1-9-3)	99.4	(2-1-9-4)	49.3				
(2-1-9-10)	-138.7	(2-1-9-11)	-38.3	(2-1-9-12)	119.2				
(3-1-9-2)	-99.4	(3-1-9-4)	-50.1	(3-1-9-10)	121.9				
(3-1-9-11)	-137.7	(3-1-9-12)	19.8	(5-1-9-2)	130.5				
(5-1-9-3)	-130.1	(5-1-9-4)	179.8	(5-1-9-10)	-8.2				
(5-1-9-11)	92.2	(5-1-9-12)	-110.3	(1-2-4-3)	-0.1				

(1-2-4-8)	-168.2	(1-2-4-9)	68.2	(6-2-4-3)	174.6
(6-2-4-8)	6.5	(6-2-4-9)	-117.1	(9-2-4-3)	-68.3
(9-2-4-8)	123.6	(1-2-9-3)	-48.6	(1-2-9-4)	-98.9
(1-2-9-10)	49.4	(1-2-9-11)	149.5	(1-2-9-12)	-106.0
(4-2-9-1)	98.9	(4-2-9-3)	50.3	(4-2-9-10)	148.3
(4-2-9-11)	-111.6	(4-2-9-12)	-7.1	(6-2-9-1)	-131.0
(6-2-9-3)	-179.6	(6-2-9-4)	130.2	(6-2-9-10)	-81.5
(6-2-9-11)	18.6	(6-2-9-12)	123.0	(1-3-4-2)	0.1
(1-3-4-8)	168.2	(1-3-4-9)	-69.2	(7-3-4-2)	-170.3
(7-3-4-8)	-2.2	(7-3-4-9)	120.4	(9-3-4-2)	69.3
(9-3-4-8)	-122.6	(1-3-9-2)	48.0	(1-3-9-4)	97.6
(1-3-9-10)	-65.2	(1-3-9-11)	82.2	(1-3-9-12)	-165.8
(4-3-9-1)	-97.6	(4-3-9-2)	-49.6	(4-3-9-10)	-162.8
(4-3-9-11)	-15.5	(4-3-9-12)	96.6	(7-3-9-1)	131.7
(7-3-9-2)	179.7	(7-3-9-4)	-130.7	(7-3-9-10)	66.4
(7-3-9-11)	-146.2	(7-3-9-12)	-34.1	(2-4-9-1)	-48.1
(2-4-9-3)	-97.0	(2-4-9-10)	-64.0	(2-4-9-11)	74.2
(2-4-9-12)	175.3	(3-4-9-1)	48.9	(3-4-9-2)	97.0
(3-4-9-10)	32.9	(3-4-9-11)	171.2	(3-4-9-12)	-87.8
(8-4-9-1)	-179.9	(8-4-9-2)	-131.8	(8-4-9-3)	131.3
(8-4-9-10)	164.2	(8-4-9-11)	-57.6	(8-4-9-12)	43.5
(1-9-10-13)	-41.0	(2-9-10-13)	-70.7	(3-9-10-13)	-4.3
(4-9-10-13)	-27.2	(11-9-10-13)	-166.7	(12-9-10-13)	93.2
(1-9-11-14)	68.0	(2-9-11-14)	44.1	(3-9-11-14)	15.0
(4-9-11-14)	4.4	(10-9-11-14)	164.4	(12-9-11-14)	-95.7
(1-9-12-15)	-41.5	(2-9-12-15)	18.4	(3-9-12-15)	-28.6
(4-9-12-15)	13.6	(10-9-12-15)	-140.2	(11-9-12-15)	120.0

Frequencies (cm⁻¹): 10.6 87.9 90.8 106.4 133.8 135.0 352.0 368.1
 411.7 414.0 467.5 475.9 513.6 519.1 523.7 590.2 607.4 608.9
 626.4 759.4 764.1 832.7 841.6 946.7 957.5 964.2 984.4 1197.6
 1220.5 1273.5 1374.9 1379.2 2085.9 2089.4 2136.8 3264.1 3282.7 3283.9

(6) B3LYP/6-31G(d)+LANL2DZ C_s Geometry

Nuclear repulsion energy	1437.85359241 Hartrees
B3LYP/6-31G(d)+LANL2DZ energy	-924.08860278 Hartrees
Zero-point energy correction	0.157643 Hartrees
Thermal correction to Enthalpy	0.174387 Hartrees
Thermal correction to Gibbs Free Energy	0.113700 Hartrees



	X	Y	Z
C1	0.998911	0.646830	0.753332
C2	0.998911	0.646830	-0.753332
C3	1.663622	-0.677942	0.737361
C4	1.663622	-0.677942	-0.737361
C5	0.429324	1.677239	1.424512
C6	0.429324	1.677239	-1.424512
H7	2.304550	-1.158967	1.465555
H8	2.304550	-1.158967	-1.465555
Fe9	-0.047267	-1.411781	0.000000
C10	-1.120369	-1.569803	1.456160
C11	-1.120369	-1.569803	-1.456160
C12	0.476510	-3.077531	0.000000
O13	-1.776472	-1.680189	2.395714
O14	-1.776472	-1.680189	-2.395714
O15	0.857174	-4.166926	0.000000
C16	-0.182257	2.814365	0.670403
C17	-0.182257	2.814365	-0.670403
C18	0.089290	2.392246	2.670762

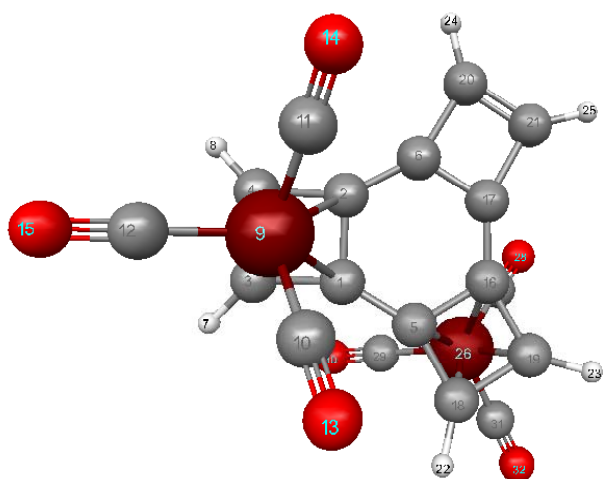
					C19	-0.480574	3.436491	1.987749	
					C20	0.089290	2.392246	-2.670762	
					C21	-0.480574	3.436491	-1.987749	
					H22	0.233036	2.177223	3.723158	
					H23	-0.957238	4.360145	2.294028	
					H24	0.233036	2.177223	-3.723158	
					H25	-0.957238	4.360145	-2.294028	
(1-2)	1.507	(1-3)	1.482	(1-5)	1.355	(1-9)	2.429	(2-4)	1.482
(2-6)	1.355	(2-9)	2.429	(3-4)	1.475	(3-7)	1.083	(3-9)	2.002
(4-8)	1.083	(4-9)	2.002	(5-16)	1.495	(5-18)	1.476	(6-17)	1.495
(6-20)	1.476	(9-10)	1.816	(9-11)	1.816	(9-12)	1.746	(10-13)	1.151
(11-14)	1.151	(12-15)	1.154	(16-17)	1.341	(16-19)	1.487	(17-21)	1.487
(18-19)	1.372	(18-22)	1.084	(19-23)	1.084	(20-21)	1.372	(20-24)	1.084
(21-25)	1.084								
(2-1-3)	89.4	(2-1-5)	119.7	(2-1-9)	71.9	(3-1-5)	150.8		
(3-1-9)	55.4	(5-1-9)	128.1	(1-2-4)	89.4	(1-2-6)	119.7		
(1-2-9)	71.9	(4-2-6)	150.8	(4-2-9)	55.4	(6-2-9)	128.1		
(1-3-4)	90.6	(1-3-7)	130.9	(1-3-9)	87.0	(4-3-7)	132.3		
(4-3-9)	68.4	(7-3-9)	126.2	(2-4-3)	90.6	(2-4-8)	130.9		
(2-4-9)	87.0	(3-4-8)	132.3	(3-4-9)	68.4	(8-4-9)	126.2		
(1-5-16)	120.0	(1-5-18)	152.0	(16-5-18)	87.9	(2-6-17)	120.0		
(2-6-20)	152.0	(17-6-20)	87.9	(1-9-2)	36.1	(1-9-3)	37.5		
(1-9-4)	55.6	(1-9-10)	94.6	(1-9-11)	125.2	(1-9-12)	132.8		
(2-9-3)	55.6	(2-9-4)	37.5	(2-9-10)	125.2	(2-9-11)	94.6		
(2-9-12)	132.8	(3-9-4)	43.2	(3-9-10)	104.0	(3-9-11)	146.3		
(3-9-12)	95.4	(4-9-10)	146.3	(4-9-11)	104.0	(4-9-12)	95.4		
(10-9-11)	106.6	(10-9-12)	95.4	(11-9-12)	95.4	(9-10-13)	178.5		
(9-11-14)	178.5	(9-12-15)	178.2	(5-16-17)	120.3	(5-16-19)	87.3		
(17-16-19)	152.4	(6-17-16)	120.3	(6-17-21)	87.3	(16-17-21)	152.4		
(5-18-19)	92.5	(5-18-22)	133.9	(19-18-22)	133.6	(16-19-18)	92.3		
(16-19-23)	134.0	(18-19-23)	133.7	(6-20-21)	92.5	(6-20-24)	133.9		
(21-20-24)	133.6	(17-21-20)	92.3	(17-21-25)	134.0	(20-21-25)	133.7		
(3-1-2-4)	0.0	(3-1-2-6)	177.7	(3-1-2-9)	53.6				
(5-1-2-4)	-177.7	(5-1-2-6)	0.0	(5-1-2-9)	-124.1				
(9-1-2-4)	-53.6	(9-1-2-6)	124.1	(2-1-3-4)	0.0				
(2-1-3-7)	154.1	(2-1-3-9)	-68.3	(5-1-3-4)	175.9				
(5-1-3-7)	-30.0	(5-1-3-9)	107.6	(9-1-3-4)	68.3				
(9-1-3-7)	-137.6	(2-1-5-16)	-0.7	(2-1-5-18)	-176.0				
(3-1-5-16)	-176.0	(3-1-5-18)	8.7	(9-1-5-16)	-90.3				
(9-1-5-18)	94.4	(2-1-9-3)	102.2	(2-1-9-4)	46.2				
(2-1-9-10)	-150.7	(2-1-9-11)	-36.6	(2-1-9-12)	107.6				
(3-1-9-2)	-102.2	(3-1-9-4)	-56.0	(3-1-9-10)	107.1				
(3-1-9-11)	-138.8	(3-1-9-12)	5.4	(5-1-9-2)	114.0				
(5-1-9-3)	-143.8	(5-1-9-4)	160.2	(5-1-9-10)	-36.8				
(5-1-9-11)	77.3	(5-1-9-12)	-138.5	(1-2-4-3)	0.0				
(1-2-4-8)	-154.1	(1-2-4-9)	68.3	(6-2-4-3)	-175.9				
(6-2-4-8)	30.0	(6-2-4-9)	-107.6	(9-2-4-3)	-68.3				
(9-2-4-8)	137.6	(1-2-6-17)	0.7	(1-2-6-20)	176.0				
(4-2-6-17)	176.0	(4-2-6-20)	-8.7	(9-2-6-17)	90.3				
(9-2-6-20)	-94.4	(1-2-9-3)	-46.2	(1-2-9-4)	-102.2				
(1-2-9-10)	36.6	(1-2-9-11)	150.7	(1-2-9-12)	-107.6				
(4-2-9-1)	102.2	(4-2-9-3)	56.0	(4-2-9-10)	138.8				
(4-2-9-11)	-107.1	(4-2-9-12)	-5.4	(6-2-9-1)	-114.0				
(6-2-9-3)	-160.2	(6-2-9-4)	143.8	(6-2-9-10)	-77.3				
(6-2-9-11)	36.8	(6-2-9-12)	138.5	(1-3-4-2)	0.0				
(1-3-4-8)	153.5	(1-3-4-9)	-86.6	(7-3-4-2)	-153.5				
(7-3-4-8)	0.0	(7-3-4-9)	119.9	(9-3-4-2)	86.6				
(9-3-4-8)	-119.9	(1-3-9-2)	44.3	(1-3-9-4)	91.8				
(1-3-9-10)	-79.1	(1-3-9-11)	75.8	(1-3-9-12)	-176.0				
(4-3-9-1)	-91.8	(4-3-9-2)	-47.6	(4-3-9-10)	-170.9				

(4-3-9-11)	-16.0	(4-3-9-12)	92.1	(7-3-9-1)	140.8
(7-3-9-2)	-174.9	(7-3-9-4)	-127.3	(7-3-9-10)	61.7
(7-3-9-11)	-143.4	(7-3-9-12)	-35.2	(2-4-9-1)	-44.3
(2-4-9-3)	-91.8	(2-4-9-10)	-75.8	(2-4-9-11)	79.1
(2-4-9-12)	176.0	(3-4-9-1)	47.6	(3-4-9-2)	91.8
(3-4-9-10)	16.0	(3-4-9-11)	170.9	(3-4-9-12)	-92.1
(8-4-9-1)	174.9	(8-4-9-2)	-140.8	(8-4-9-3)	127.3
(8-4-9-10)	143.4	(8-4-9-11)	-61.7	(8-4-9-12)	35.2
(1-5-16-17)	0.7	(1-5-16-19)	-178.1	(18-5-16-17)	178.5
(18-5-16-19)	-0.3	(1-5-18-19)	176.3	(1-5-18-22)	-3.7
(16-5-18-19)	0.3	(16-5-18-22)	-179.7	(2-6-17-16)	-0.7
(2-6-17-21)	178.1	(20-6-17-16)	-178.5	(20-6-17-21)	0.3
(2-6-20-21)	-176.3	(2-6-20-24)	3.7	(17-6-20-21)	-0.3
(17-6-20-24)	179.7	(1-9-10-13)	-77.2	(2-9-10-13)	-97.9
(3-9-10-13)	-40.3	(4-9-10-13)	-51.5	(11-9-10-13)	153.9
(12-9-10-13)	56.6	(1-9-11-14)	97.9	(2-9-11-14)	77.2
(3-9-11-14)	51.5	(4-9-11-14)	40.3	(10-9-11-14)	-153.9
(12-9-11-14)	-56.6	(1-9-12-15)	-25.0	(2-9-12-15)	25.0
(3-9-12-15)	-21.7	(4-9-12-15)	21.7	(10-9-12-15)	-126.3
(11-9-12-15)	126.3	(5-16-17-6)	0.0	(5-16-17-21)	-177.3
(19-16-17-6)	177.3	(19-16-17-21)	0.0	(5-16-19-18)	0.3
(5-16-19-23)	179.9	(17-16-19-18)	-177.4	(17-16-19-23)	2.2
(6-17-21-20)	-0.3	(6-17-21-25)	-179.9	(16-17-21-20)	177.4
(16-17-21-25)	-2.2	(5-18-19-16)	-0.3	(5-18-19-23)	180.0
(22-18-19-16)	179.7	(22-18-19-23)	0.1	(6-20-21-17)	0.3
(6-20-21-25)	180.0	(24-20-21-17)	-179.7	(24-20-21-25)	-0.1

Frequencies (cm ⁻¹):	-3.7	45.1	48.4	70.9	74.3	98.5	107.4	122.0		
	171.8	214.1	252.4	335.5	338.8	342.5	383.7	400.1	423.3	449.0
	456.5	463.9	472.5	488.1	508.2	524.8	532.9	563.5	590.5	616.1
	620.9	648.4	669.4	696.6	745.3	765.1	775.1	820.8	829.2	856.5
	888.1	888.2	916.7	965.5	990.0	994.0	1026.4	1057.5	1125.1	1126.3
	1160.0	1167.1	1202.0	1272.9	1286.4	1304.4	1338.2	1487.2	1518.5	1688.7
	1696.9	1775.5	2079.8	2085.3	2129.8	3238.3	3239.3	3241.3	3255.8	3264.5

(7a) B3LYP/6-31G(d)+LANL2DZ C₂ Geometry

Nuclear repulsion energy	2599.00099260	Hartrees
B3LYP/6-31G(d)+LANL2DZ energy	-1387.57932060	Hartrees
Zero-point energy correction	0.183979	Hartrees
Thermal correction to Enthalpy	0.209969	Hartrees
Thermal correction to Gibbs Free Energy	0.125674	Hartrees



	X	Y	Z
C1	-0.011748	0.710547	-0.443013
C2	-0.011748	1.420209	0.836184
C3	0.038501	1.978849	-1.166308
C4	-0.000833	2.706265	0.119565
C5	0.011748	-0.710547	-0.443013
C6	-0.015319	0.696876	2.033757
H7	0.329014	2.247412	-2.172011
H8	0.277830	3.708707	0.412974
Fe9	-1.809055	2.001350	-0.374804
C10	-2.789888	0.812497	-1.302612
C11	-2.842668	2.242184	1.079910
C12	-2.328717	3.444165	-1.243761
O13	-3.393756	0.047171	-1.915751
O14	-3.497008	2.432304	2.008526
O15	-2.639384	4.395533	-1.816141
C16	0.011748	-1.420209	0.836184

(9-1-5-26)	-175.6	(2-1-9-3)	100.6	(2-1-9-4)	47.6
(2-1-9-10)	-145.7	(2-1-9-11)	-40.4	(2-1-9-12)	111.8
(3-1-9-2)	-100.6	(3-1-9-4)	-53.0	(3-1-9-10)	113.7
(3-1-9-11)	-141.1	(3-1-9-12)	11.2	(5-1-9-2)	113.2
(5-1-9-3)	-146.2	(5-1-9-4)	160.8	(5-1-9-10)	-32.5
(5-1-9-11)	72.7	(5-1-9-12)	-135.1	(1-2-4-3)	-1.5
(1-2-4-8)	-159.8	(1-2-4-9)	66.8	(6-2-4-3)	178.0
(6-2-4-8)	19.7	(6-2-4-9)	-113.7	(9-2-4-3)	-68.3
(9-2-4-8)	133.4	(1-2-6-17)	1.6	(1-2-6-20)	179.6
(4-2-6-17)	-177.8	(4-2-6-20)	0.1	(9-2-6-17)	87.5
(9-2-6-20)	-94.6	(1-2-9-3)	-48.1	(1-2-9-4)	-101.6
(1-2-9-10)	42.2	(1-2-9-11)	147.7	(1-2-9-12)	-109.0
(4-2-9-1)	101.6	(4-2-9-3)	53.5	(4-2-9-10)	143.8
(4-2-9-11)	-110.7	(4-2-9-12)	-7.3	(6-2-9-1)	-112.8
(6-2-9-3)	-160.9	(6-2-9-4)	145.6	(6-2-9-10)	-70.6
(6-2-9-11)	34.9	(6-2-9-12)	138.3	(1-3-4-2)	1.5
(1-3-4-8)	159.7	(1-3-4-9)	-76.6	(7-3-4-2)	-160.1
(7-3-4-8)	-1.9	(7-3-4-9)	121.8	(9-3-4-2)	78.1
(9-3-4-8)	-123.7	(1-3-9-2)	45.8	(1-3-9-4)	94.8
(1-3-9-10)	-72.9	(1-3-9-11)	76.6	(1-3-9-12)	-172.0
(4-3-9-1)	-94.8	(4-3-9-2)	-49.1	(4-3-9-10)	-167.8
(4-3-9-11)	-18.2	(4-3-9-12)	93.1	(7-3-9-1)	135.7
(7-3-9-2)	-178.5	(7-3-9-4)	-129.5	(7-3-9-10)	62.8
(7-3-9-11)	-147.7	(7-3-9-12)	-36.3	(2-4-9-1)	-45.3
(2-4-9-3)	-94.0	(2-4-9-10)	-71.3	(2-4-9-11)	76.0
(2-4-9-12)	174.8	(3-4-9-1)	48.7	(3-4-9-2)	94.0
(3-4-9-10)	22.8	(3-4-9-11)	170.1	(3-4-9-12)	-91.1
(8-4-9-1)	177.8	(8-4-9-2)	-136.9	(8-4-9-3)	129.1
(8-4-9-10)	151.9	(8-4-9-11)	-60.9	(8-4-9-12)	38.0
(1-5-16-17)	-1.3	(1-5-16-19)	178.5	(1-5-16-26)	-122.4
(18-5-16-17)	-178.2	(18-5-16-19)	1.5	(18-5-16-26)	60.6
(26-5-16-17)	121.2	(26-5-16-19)	-59.1	(1-5-18-19)	-176.2
(1-5-18-22)	-14.3	(1-5-18-26)	116.2	(16-5-18-19)	-1.5
(16-5-18-22)	160.3	(16-5-18-26)	-69.2	(26-5-18-19)	67.6
(26-5-18-22)	-130.6	(1-5-26-16)	113.2	(1-5-26-18)	-146.2
(1-5-26-19)	160.8	(1-5-26-27)	72.7	(1-5-26-29)	-32.5
(1-5-26-31)	-135.1	(16-5-26-18)	100.6	(16-5-26-19)	47.6
(16-5-26-27)	-40.4	(16-5-26-29)	-145.7	(16-5-26-31)	111.8
(18-5-26-16)	-100.6	(18-5-26-19)	-53.0	(18-5-26-27)	-141.1
(18-5-26-29)	113.7	(18-5-26-31)	11.2	(2-6-17-16)	-1.9
(2-6-17-21)	179.2	(20-6-17-16)	179.2	(20-6-17-21)	0.2
(2-6-20-21)	-178.5	(2-6-20-24)	1.8	(17-6-20-21)	-0.3
(17-6-20-24)	180.0	(1-9-10-13)	-43.3	(2-9-10-13)	-67.9
(3-9-10-13)	-5.3	(4-9-10-13)	-21.4	(11-9-10-13)	-169.3
(12-9-10-13)	92.2	(1-9-11-14)	121.5	(2-9-11-14)	97.7
(3-9-11-14)	71.9	(4-9-11-14)	59.0	(10-9-11-14)	-137.7
(12-9-11-14)	-38.9	(1-9-12-15)	-28.3	(2-9-12-15)	27.1
(3-9-12-15)	-21.1	(4-9-12-15)	22.3	(10-9-12-15)	-128.9
(11-9-12-15)	129.0	(5-16-17-6)	1.6	(5-16-17-21)	179.6
(19-16-17-6)	-177.8	(19-16-17-21)	0.1	(26-16-17-6)	87.5
(26-16-17-21)	-94.6	(5-16-19-18)	-1.5	(5-16-19-23)	-159.8
(5-16-19-26)	66.8	(17-16-19-18)	178.0	(17-16-19-23)	19.7
(17-16-19-26)	-113.7	(26-16-19-18)	-68.3	(26-16-19-23)	133.4
(5-16-26-18)	-48.1	(5-16-26-19)	-101.6	(5-16-26-27)	147.7
(5-16-26-29)	42.2	(5-16-26-31)	-109.0	(17-16-26-5)	-112.8
(17-16-26-18)	-160.9	(17-16-26-19)	145.6	(17-16-26-27)	34.9
(17-16-26-29)	-70.6	(17-16-26-31)	138.3	(19-16-26-5)	101.6
(19-16-26-18)	53.5	(19-16-26-27)	-110.7	(19-16-26-29)	143.8
(19-16-26-31)	-7.3	(6-17-21-20)	-0.3	(6-17-21-25)	180.0
(16-17-21-20)	-178.5	(16-17-21-25)	1.8	(5-18-19-16)	1.5
(5-18-19-23)	159.7	(5-18-19-26)	-76.6	(22-18-19-16)	-160.1
(22-18-19-23)	-1.9	(22-18-19-26)	121.8	(26-18-19-16)	78.1

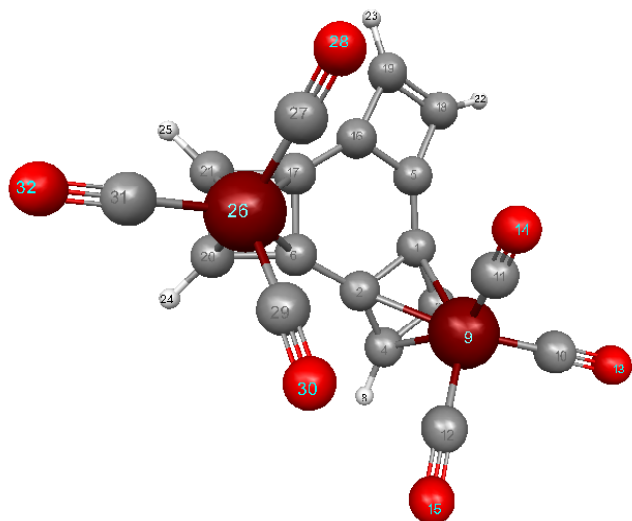
(26-18-19-23)	-123.7	(5-18-26-16)	45.8	(5-18-26-19)	94.8
(5-18-26-27)	76.6	(5-18-26-29)	-72.9	(5-18-26-31)	-172.0
(19-18-26-5)	-94.8	(19-18-26-16)	-49.1	(19-18-26-27)	-18.2
(19-18-26-29)	-167.8	(19-18-26-31)	93.1	(22-18-26-5)	135.7
(22-18-26-16)	-178.5	(22-18-26-19)	-129.5	(22-18-26-27)	-147.7
(22-18-26-29)	62.8	(22-18-26-31)	-36.3	(16-19-26-5)	-45.3
(16-19-26-18)	-94.0	(16-19-26-27)	76.0	(16-19-26-29)	-71.3
(16-19-26-31)	174.8	(18-19-26-5)	48.7	(18-19-26-16)	94.0
(18-19-26-27)	170.1	(18-19-26-29)	22.8	(18-19-26-31)	-91.1
(23-19-26-5)	177.8	(23-19-26-16)	-136.9	(23-19-26-18)	129.1
(23-19-26-27)	-60.9	(23-19-26-29)	151.9	(23-19-26-31)	38.0
(6-20-21-17)	0.2	(6-20-21-25)	180.0	(24-20-21-17)	180.0
(24-20-21-25)	-0.3	(5-26-27-28)	121.5	(16-26-27-28)	97.7
(18-26-27-28)	71.9	(19-26-27-28)	59.0	(29-26-27-28)	-137.7
(31-26-27-28)	-38.9	(5-26-29-30)	-43.3	(16-26-29-30)	-67.9
(18-26-29-30)	-5.3	(19-26-29-30)	-21.4	(27-26-29-30)	-169.3
(31-26-29-30)	92.2	(5-26-31-32)	-28.3	(16-26-31-32)	27.1
(18-26-31-32)	-21.1	(19-26-31-32)	22.3	(27-26-31-32)	129.0
(29-26-31-32)	-128.9				

Frequencies (cm⁻¹):

5.4	17.7	39.1	41.9	56.4	64.2	78.0	79.4		
84.6	86.7	101.6	103.9	119.2	132.1	135.4	142.6	186.7	238.1
298.8	316.8	333.3	369.6	387.8	395.5	412.3	412.6	440.8	448.6
448.7	459.3	464.1	466.1	487.3	497.2	502.4	502.7	512.1	512.4
529.6	542.2	574.2	580.5	588.9	591.7	596.3	601.3	609.4	620.3
628.4	639.9	675.3	711.1	773.6	775.1	792.9	795.3	866.4	896.0
941.1	951.8	955.7	1018.1	1057.0	1091.1	1124.2	1151.4	1164.2	1195.2
1232.5	1257.0	1272.2	1307.3	1329.9	1395.4	1540.5	1560.3	1584.1	1616.4
2085.1	2085.2	2086.7	2087.1	2120.4	2136.0	3250.4	3270.2	3270.2	3280.7
3284.9	3285.4								

(7b) B3LYP/6-31G(d)+LANL2DZ C₁ Geometry

Nuclear repulsion energy	2673.15051807	Hartrees
B3LYP/6-31G(d)+LANL2DZ energy	-1387.57494266	Hartrees
Zero-point energy correction	0.184073	Hartrees
Thermal correction to Enthalpy	0.209903	Hartrees
Thermal correction to Gibbs Free Energy	0.127739	Hartrees



	X	Y	Z
C1	1.488262	1.413837	-0.733369
C2	0.748840	0.256888	-1.302157
C3	2.688713	0.975798	-1.438180
C4	1.958873	-0.121546	-2.035613
C5	0.774436	2.471556	-0.142367
C6	-0.686522	0.309541	-1.325148
H7	3.674849	1.392660	-1.587590
H8	2.184301	-0.841308	-2.810239
Fe9	2.248803	-0.448657	-0.023192
C10	3.913361	-0.317090	0.590807
C11	1.443542	-0.396856	1.570799
C12	2.199692	-2.213957	-0.278518
O13	4.995919	-0.241321	0.981126
O14	0.893695	-0.344086	2.580349
O15	2.213788	-3.351569	-0.455813
C16	-0.610432	2.488947	-0.127987
C17	-1.361718	1.471034	-0.741266
C18	0.783139	3.902492	0.450157
C19	-0.560844	3.921327	0.464324

C20	-1.926432	-0.081236	-1.989741
C21	-2.622020	1.051298	-1.352549
H22	1.561914	4.597928	0.735837
H23	-1.311452	4.641497	0.764724
H24	-2.158556	-0.738616	-2.815642
H25	-3.556816	1.557787	-1.546439
Fe26	-2.268506	-0.419494	-0.027016
C27	-2.463021	0.234113	1.634139
O28	-2.614401	0.662280	2.692806
C29	-1.414245	-1.946150	0.342412
O30	-0.866127	-2.939549	0.546090
C31	-3.892206	-1.099979	-0.189502
O32	-4.954183	-1.530522	-0.321145

(1-2)	1.486	(1-3)	1.459	(1-5)	1.406	(1-9)	2.133	(2-4)	1.465
(2-6)	1.437	(2-9)	2.094	(3-4)	1.447	(3-7)	1.081	(3-9)	2.055
(4-8)	1.081	(4-9)	2.059	(5-16)	1.385	(5-18)	1.549	(6-17)	1.465
(6-20)	1.460	(6-26)	2.172	(9-10)	1.779	(9-11)	1.787	(9-12)	1.784
(10-13)	1.153	(11-14)	1.151	(12-15)	1.151	(16-17)	1.406	(16-19)	1.551
(17-21)	1.462	(17-26)	2.215	(18-19)	1.344	(18-22)	1.082	(19-23)	1.083
(20-21)	1.474	(20-24)	1.081	(20-26)	2.021	(21-25)	1.081	(21-26)	2.011
(26-27)	1.796	(26-29)	1.788	(26-31)	1.768	(27-28)	1.152	(29-30)	1.153
(31-32)	1.153								
(2-1-3)	89.5	(2-1-5)	119.6	(2-1-9)	68.0	(3-1-5)	147.8		
(3-1-9)	66.8	(5-1-9)	134.2	(1-2-4)	89.0	(1-2-6)	118.3		
(1-2-9)	70.9	(4-2-6)	145.8	(4-2-9)	68.1	(6-2-9)	137.6		
(1-3-4)	90.7	(1-3-7)	134.5	(1-3-9)	72.5	(4-3-7)	134.1		
(4-3-9)	69.6	(7-3-9)	123.9	(2-4-3)	90.8	(2-4-8)	134.7		
(2-4-9)	70.6	(3-4-8)	134.1	(3-4-9)	69.3	(8-4-9)	124.4		
(1-5-16)	121.4	(1-5-18)	148.5	(16-5-18)	89.4	(2-6-17)	118.9		
(2-6-20)	147.8	(2-6-26)	134.9	(17-6-20)	90.1	(17-6-26)	72.1		
(20-6-26)	64.1	(1-9-2)	41.2	(1-9-3)	40.7	(1-9-4)	59.1		
(1-9-10)	112.6	(1-9-11)	96.4	(1-9-12)	143.7	(2-9-3)	60.0		
(2-9-4)	41.3	(2-9-10)	148.9	(2-9-11)	102.3	(2-9-12)	103.1		
(3-9-4)	41.2	(3-9-10)	89.2	(3-9-11)	133.7	(3-9-12)	126.4		
(4-9-10)	117.2	(4-9-11)	143.5	(4-9-12)	90.8	(10-9-11)	96.4		
(10-9-12)	98.5	(11-9-12)	98.3	(9-10-13)	179.4	(9-11-14)	178.0		
(9-12-15)	177.6	(5-16-17)	121.4	(5-16-19)	89.1	(17-16-19)	148.5		
(6-17-16)	120.1	(6-17-21)	90.2	(6-17-26)	68.9	(16-17-21)	148.3		
(16-17-26)	134.1	(21-17-26)	62.4	(5-18-19)	90.7	(5-18-22)	134.3		
(19-18-22)	135.0	(16-19-18)	90.9	(16-19-23)	134.3	(18-19-23)	134.9		
(6-20-21)	89.9	(6-20-24)	133.9	(6-20-26)	75.3	(21-20-24)	134.1		
(21-20-26)	68.2	(24-20-26)	127.2	(17-21-20)	89.7	(17-21-25)	133.3		
(17-21-26)	77.5	(20-21-25)	133.7	(20-21-26)	68.9	(25-21-26)	127.8		
(6-26-17)	39.0	(6-26-20)	40.6	(6-26-21)	59.3	(6-26-27)	120.6		
(6-26-29)	93.6	(6-26-31)	138.0	(17-26-20)	58.3	(17-26-21)	40.1		
(17-26-27)	91.8	(17-26-29)	126.9	(17-26-31)	132.4	(20-26-21)	42.9		
(20-26-27)	148.9	(20-26-29)	105.2	(20-26-31)	97.5	(21-26-27)	108.9		
(21-26-29)	147.6	(21-26-31)	93.4	(27-26-29)	99.9	(27-26-31)	97.2		
(29-26-31)	97.4	(26-27-28)	178.6	(26-29-30)	178.2	(26-31-32)	178.6		
(3-1-2-4)	-2.1	(3-1-2-6)	-160.5	(3-1-2-9)	65.1				
(5-1-2-4)	163.4	(5-1-2-6)	5.0	(5-1-2-9)	-129.5				
(9-1-2-4)	-67.1	(9-1-2-6)	134.5	(2-1-3-4)	2.1				
(2-1-3-7)	173.1	(2-1-3-9)	-66.2	(5-1-3-4)	-153.7				
(5-1-3-7)	17.3	(5-1-3-9)	138.0	(9-1-3-4)	68.3				
(9-1-3-7)	-120.7	(2-1-5-16)	-2.8	(2-1-5-18)	-170.1				
(3-1-5-16)	149.1	(3-1-5-18)	-18.2	(9-1-5-16)	-90.0				
(9-1-5-18)	102.7	(2-1-9-3)	99.4	(2-1-9-4)	49.8				
(2-1-9-10)	159.0	(2-1-9-11)	-101.4	(2-1-9-12)	12.0				
(3-1-9-2)	-99.4	(3-1-9-4)	-49.6	(3-1-9-10)	59.6				
(3-1-9-11)	159.3	(3-1-9-12)	-87.3	(5-1-9-2)	110.5				

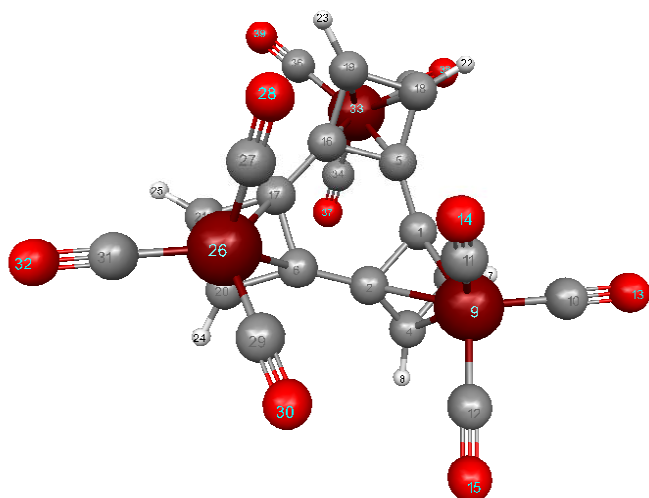
(5-1-9-3)	-150.2	(5-1-9-4)	160.3	(5-1-9-10)	-90.6
(5-1-9-11)	9.1	(5-1-9-12)	122.5	(1-2-4-3)	2.1
(1-2-4-8)	-170.6	(1-2-4-9)	69.7	(6-2-4-3)	146.9
(6-2-4-8)	-25.8	(6-2-4-9)	-145.4	(9-2-4-3)	-67.6
(9-2-4-8)	119.6	(1-2-6-17)	-2.4	(1-2-6-20)	149.3
(1-2-6-26)	-95.5	(4-2-6-17)	-141.6	(4-2-6-20)	10.1
(4-2-6-26)	125.4	(9-2-6-17)	89.7	(9-2-6-20)	-118.5
(9-2-6-26)	-3.3	(1-2-9-3)	-48.0	(1-2-9-4)	-96.8
(1-2-9-10)	-39.9	(1-2-9-11)	85.6	(1-2-9-12)	-172.7
(4-2-9-1)	96.8	(4-2-9-3)	48.8	(4-2-9-10)	56.9
(4-2-9-11)	-177.5	(4-2-9-12)	-75.9	(6-2-9-1)	-111.4
(6-2-9-3)	-159.5	(6-2-9-4)	151.8	(6-2-9-10)	-151.3
(6-2-9-11)	-25.8	(6-2-9-12)	75.9	(1-3-4-2)	-2.1
(1-3-4-8)	170.7	(1-3-4-9)	-71.0	(7-3-4-2)	-173.3
(7-3-4-8)	-0.5	(7-3-4-9)	117.9	(9-3-4-2)	68.9
(9-3-4-8)	-118.3	(1-3-9-2)	48.6	(1-3-9-4)	97.5
(1-3-9-10)	-127.2	(1-3-9-11)	-29.1	(1-3-9-12)	132.8
(4-3-9-1)	-97.5	(4-3-9-2)	-48.9	(4-3-9-10)	135.3
(4-3-9-11)	-126.6	(4-3-9-12)	35.3	(7-3-9-1)	132.4
(7-3-9-2)	-179.0	(7-3-9-4)	-130.1	(7-3-9-10)	5.2
(7-3-9-11)	103.3	(7-3-9-12)	-94.8	(2-4-9-1)	-49.6
(2-4-9-3)	-98.6	(2-4-9-10)	-150.9	(2-4-9-11)	4.0
(2-4-9-12)	109.1	(3-4-9-1)	48.9	(3-4-9-2)	98.6
(3-4-9-10)	-52.3	(3-4-9-11)	102.6	(3-4-9-12)	-152.3
(8-4-9-1)	178.9	(8-4-9-2)	-131.5	(8-4-9-3)	130.0
(8-4-9-10)	77.6	(8-4-9-11)	-127.4	(8-4-9-12)	-22.4
(1-5-16-17)	-2.1	(1-5-16-19)	-173.4	(18-5-16-17)	171.3
(18-5-16-19)	0.0	(1-5-18-19)	169.2	(1-5-18-22)	-10.9
(16-5-18-19)	0.0	(16-5-18-22)	179.9	(2-6-17-16)	-2.3
(2-6-17-21)	167.9	(2-6-17-26)	-132.0	(20-6-17-16)	-167.6
(20-6-17-21)	2.5	(20-6-17-26)	62.7	(26-6-17-16)	129.7
(26-6-17-21)	-60.2	(2-6-20-21)	-158.0	(2-6-20-24)	6.7
(2-6-20-26)	134.6	(17-6-20-21)	-2.5	(17-6-20-24)	162.2
(17-6-20-26)	-69.9	(26-6-20-21)	67.5	(26-6-20-24)	-127.9
(2-6-26-17)	113.2	(2-6-26-20)	-147.6	(2-6-26-21)	160.5
(2-6-26-27)	65.5	(2-6-26-29)	-38.2	(2-6-26-31)	-143.4
(17-6-26-20)	99.2	(17-6-26-21)	47.2	(17-6-26-27)	-47.8
(17-6-26-29)	-151.4	(17-6-26-31)	103.4	(20-6-26-17)	-99.2
(20-6-26-21)	-52.0	(20-6-26-27)	-146.9	(20-6-26-29)	109.4
(20-6-26-31)	4.2	(1-9-10-13)	-126.7	(2-9-10-13)	-99.5
(3-9-10-13)	-92.4	(4-9-10-13)	-61.0	(11-9-10-13)	133.7
(12-9-10-13)	34.3	(1-9-11-14)	33.2	(2-9-11-14)	-8.1
(3-9-11-14)	51.8	(4-9-11-14)	-10.8	(10-9-11-14)	146.9
(12-9-11-14)	-113.5	(1-9-12-15)	114.4	(2-9-12-15)	122.5
(3-9-12-15)	60.4	(4-9-12-15)	82.7	(10-9-12-15)	-35.0
(11-9-12-15)	-132.8	(5-16-17-6)	4.7	(5-16-17-21)	-156.3
(5-16-17-26)	93.7	(19-16-17-6)	167.9	(19-16-17-21)	6.9
(19-16-17-26)	-103.1	(5-16-19-18)	0.0	(5-16-19-23)	179.9
(17-16-19-18)	-165.8	(17-16-19-23)	14.2	(6-17-21-20)	-2.5
(6-17-21-25)	-163.2	(6-17-21-26)	66.0	(16-17-21-20)	161.1
(16-17-21-25)	0.4	(16-17-21-26)	-130.4	(26-17-21-20)	-68.4
(26-17-21-25)	130.8	(6-17-26-20)	-49.0	(6-17-26-21)	-101.8
(6-17-26-27)	140.4	(6-17-26-29)	36.6	(6-17-26-31)	-118.1
(16-17-26-6)	-112.0	(16-17-26-20)	-161.0	(16-17-26-21)	146.1
(16-17-26-27)	28.4	(16-17-26-29)	-75.4	(16-17-26-31)	129.9
(21-17-26-6)	101.8	(21-17-26-20)	52.9	(21-17-26-27)	-117.8
(21-17-26-29)	138.5	(21-17-26-31)	-16.2	(5-18-19-16)	0.0
(5-18-19-23)	-179.9	(22-18-19-16)	-179.9	(22-18-19-23)	0.2
(6-20-21-17)	2.5	(6-20-21-25)	163.1	(6-20-21-26)	-74.2
(24-20-21-17)	-162.1	(24-20-21-25)	-1.5	(24-20-21-26)	121.2
(26-20-21-17)	76.7	(26-20-21-25)	-122.7	(6-20-26-17)	46.9
(6-20-26-21)	95.9	(6-20-26-27)	65.2	(6-20-26-29)	-77.3

(6-20-26-31)	-177.2	(21-20-26-6)	-95.9	(21-20-26-17)	-49.0
(21-20-26-27)	-30.7	(21-20-26-29)	-173.2	(21-20-26-31)	86.9
(24-20-26-6)	134.4	(24-20-26-17)	-178.7	(24-20-26-21)	-129.6
(24-20-26-27)	-160.3	(24-20-26-29)	57.1	(24-20-26-31)	-42.7
(17-21-26-6)	-45.8	(17-21-26-20)	-94.6	(17-21-26-27)	69.2
(17-21-26-29)	-82.3	(17-21-26-31)	168.1	(20-21-26-6)	48.8
(20-21-26-17)	94.6	(20-21-26-27)	163.8	(20-21-26-29)	12.2
(20-21-26-31)	-97.4	(25-21-26-6)	178.4	(25-21-26-17)	-135.8
(25-21-26-20)	129.6	(25-21-26-27)	-66.6	(25-21-26-29)	141.9
(25-21-26-31)	32.3	(6-26-27-28)	119.9	(17-26-27-28)	92.1
(20-26-27-28)	76.6	(21-26-27-28)	55.1	(29-26-27-28)	-139.9
(31-26-27-28)	-41.1	(6-26-29-30)	-64.1	(17-26-29-30)	-86.2
(20-26-29-30)	-24.7	(21-26-29-30)	-33.3	(27-26-29-30)	173.9
(31-26-29-30)	75.2	(6-26-31-32)	-25.1	(17-26-31-32)	31.0
(20-26-31-32)	-22.3	(21-26-31-32)	20.6	(27-26-31-32)	130.2
(29-26-31-32)	-128.8				

Frequencies (cm ⁻¹):	15.8	32.6	45.0	53.8	64.0	72.5	82.4	86.1		
	93.4	96.9	107.8	109.8	127.4	129.3	137.1	183.9	200.7	218.9
	246.7	310.8	340.7	359.4	374.6	384.4	406.1	411.2	421.1	444.7
	451.9	453.7	462.2	467.5	497.6	500.9	503.5	509.1	512.8	515.1
	524.4	537.9	566.5	582.4	592.2	596.3	601.3	601.6	612.8	616.8
	627.0	640.6	658.8	696.2	763.0	784.9	804.3	816.8	860.0	889.4
	935.5	954.4	969.6	1016.3	1056.6	1088.3	1121.8	1142.5	1167.9	1179.0
	1241.2	1253.7	1287.9	1323.1	1333.0	1417.9	1528.1	1549.3	1575.7	1621.1
	2073.4	2079.6	2087.0	2096.7	2108.6	2139.9	3248.3	3271.7	3271.8	3279.4
	3286.4	3288.5								

(8a) B3LYP/6-31G(d)+LANL2DZ C₁ Geometry

Nuclear repulsion energy	4118.93384044 Hartrees
B3LYP/6-31G(d)+LANL2DZ energy	-1851.11551388 Hartrees
Zero-point energy correction	0.213182 Hartrees
Thermal correction to Enthalpy	0.246603 Hartrees
Thermal correction to Gibbs Free Energy	0.146181 Hartrees



	X	Y	Z
C1	0.322718	-1.477465	-0.294388
C2	-0.671778	-0.732115	-1.107494
C3	0.158130	-2.620628	-1.184589
C4	-0.810798	-1.902967	-1.965995
C5	1.261349	-0.734462	0.519285
C6	-0.659640	0.717171	-1.127241
H7	0.622806	-3.594234	-1.265329
H8	-1.367175	-2.122989	-2.867299
Fe9	-1.540730	-2.270368	-0.042923
C10	-1.404911	-3.908102	0.653061
C11	-1.915718	-1.417706	1.472330
C12	-3.208250	-2.414559	-0.675333
O13	-1.308559	-4.961604	1.109931
O14	-2.130202	-0.855929	2.454078
O15	-4.277288	-2.501198	-1.092854
C16	1.270756	0.748342	0.485667
C17	0.337107	1.460410	-0.358255
C18	2.058368	-0.692446	1.732367
C19	2.068703	0.747675	1.709368
C20	-0.917519	1.909999	-1.933736
C21	0.088518	2.639591	-1.161683
H22	2.445388	-1.438232	2.413615
H23	2.439035	1.511174	2.379218

H24	-1.452092	2.102919	-2.852755
H25	0.564490	3.605513	-1.254258
Fe26	-1.584245	2.255933	-0.041472
C27	-1.305546	2.280118	1.722546
O28	-1.094350	2.306656	2.855055
C29	-3.171571	1.448143	-0.071110
O30	-4.189672	0.910949	-0.125471
C31	-2.157938	3.932676	-0.208059
O32	-2.520718	5.018576	-0.340424
Fe33	3.132076	0.016830	0.085843
C34	2.986463	-0.169446	-1.679054
C35	4.381000	-1.232104	0.353738
C36	4.200558	1.446266	0.107730
O37	2.856992	-0.288472	-2.817165
O38	5.177572	-2.046764	0.524380
O39	4.874087	2.380689	0.116750

(1-2)	1.485	(1-3)	1.458	(1-5)	1.447	(1-9)	2.041	(2-4)	1.459
(2-6)	1.449	(2-9)	2.063	(3-4)	1.437	(3-7)	1.082	(3-9)	2.077
(4-8)	1.082	(4-9)	2.089	(5-16)	1.483	(5-18)	1.452	(5-33)	2.062
(6-17)	1.462	(6-20)	1.463	(6-26)	2.098	(9-10)	1.785	(9-11)	1.779
(9-12)	1.789	(10-13)	1.152	(11-14)	1.151	(12-15)	1.151	(16-17)	1.446
(16-19)	1.461	(16-33)	2.039	(17-21)	1.448	(17-26)	2.104	(18-19)	1.440
(18-22)	1.082	(18-33)	2.090	(19-23)	1.081	(19-33)	2.074	(20-21)	1.463
(20-24)	1.081	(20-26)	2.036	(21-25)	1.081	(21-26)	2.049	(26-27)	1.786
(26-29)	1.781	(26-31)	1.780	(27-28)	1.152	(29-30)	1.152	(31-32)	1.153
(33-34)	1.781	(33-35)	1.786	(33-36)	1.785	(34-37)	1.152	(35-38)	1.152
(36-39)	1.152								
(2-1-3)	89.1	(2-1-5)	119.0	(2-1-9)	69.6	(3-1-5)	145.0		
(3-1-9)	70.6	(5-1-9)	136.2	(1-2-4)	89.0	(1-2-6)	120.2		
(1-2-9)	68.0	(4-2-6)	142.7	(4-2-9)	70.4	(6-2-9)	139.1		
(1-3-4)	90.9	(1-3-7)	134.6	(1-3-9)	67.9	(4-3-7)	134.3		
(4-3-9)	70.3	(7-3-9)	123.0	(2-4-3)	90.9	(2-4-8)	134.6		
(2-4-9)	68.5	(3-4-8)	134.3	(3-4-9)	69.3	(8-4-9)	123.5		
(1-5-16)	120.3	(1-5-18)	147.2	(1-5-33)	131.1	(16-5-18)	89.2		
(16-5-33)	68.0	(18-5-33)	70.6	(2-6-17)	120.5	(2-6-20)	145.2		
(2-6-26)	136.3	(17-6-20)	89.7	(17-6-26)	69.8	(20-6-26)	67.0		
(1-9-2)	42.4	(1-9-3)	41.5	(1-9-4)	60.0	(1-9-10)	109.6		
(1-9-11)	96.4	(1-9-12)	147.0	(2-9-3)	59.8	(2-9-4)	41.1		
(2-9-10)	148.6	(2-9-11)	99.8	(2-9-12)	105.7	(3-9-4)	40.3		
(3-9-10)	89.8	(3-9-11)	136.2	(3-9-12)	123.7	(4-9-10)	119.6		
(4-9-11)	140.7	(4-9-12)	90.8	(10-9-11)	97.1	(10-9-12)	97.7		
(11-9-12)	98.2	(9-10-13)	179.4	(9-11-14)	178.5	(9-12-15)	179.4		
(5-16-17)	120.1	(5-16-19)	89.1	(5-16-33)	69.6	(17-16-19)	147.3		
(17-16-33)	130.7	(19-16-33)	70.5	(6-17-16)	119.8	(6-17-21)	90.3		
(6-17-26)	69.4	(16-17-21)	146.7	(16-17-26)	133.5	(21-17-26)	67.6		
(5-18-19)	91.1	(5-18-22)	134.6	(5-18-33)	68.5	(19-18-22)	134.2		
(19-18-33)	69.2	(22-18-33)	123.1	(16-19-18)	90.6	(16-19-23)	134.9		
(16-19-33)	67.9	(18-19-23)	134.3	(18-19-33)	70.4	(23-19-33)	123.9		
(6-20-21)	89.7	(6-20-24)	134.6	(6-20-26)	71.6	(21-20-24)	134.4		
(21-20-26)	69.5	(24-20-26)	126.7	(17-21-20)	90.3	(17-21-25)	134.4		
(17-21-26)	71.6	(20-21-25)	134.7	(20-21-26)	68.5	(25-21-26)	125.0		
(6-26-17)	40.7	(6-26-20)	41.4	(6-26-21)	59.6	(6-26-27)	116.9		
(6-26-29)	93.0	(6-26-31)	141.7	(17-26-20)	59.8	(17-26-21)	40.8		
(17-26-27)	90.6	(17-26-29)	129.8	(17-26-31)	129.5	(20-26-21)	42.0		
(20-26-27)	150.4	(20-26-29)	101.5	(20-26-31)	100.3	(21-26-27)	114.2		
(21-26-29)	143.4	(21-26-31)	92.0	(27-26-29)	99.3	(27-26-31)	97.5		
(29-26-31)	98.0	(26-27-28)	178.3	(26-29-30)	178.1	(26-31-32)	178.7		
(5-33-16)	42.4	(5-33-18)	40.9	(5-33-19)	59.9	(5-33-34)	95.5		
(5-33-35)	110.4	(5-33-36)	146.3	(16-33-18)	59.9	(16-33-19)	41.6		
(16-33-34)	99.0	(16-33-35)	149.2	(16-33-36)	104.9	(18-33-19)	40.5		

(18-33-34)	134.7	(18-33-35)	90.2	(18-33-36)	124.7	(19-33-34)	140.4
(19-33-35)	119.2	(19-33-36)	90.9	(34-33-35)	97.6	(34-33-36)	98.3
(35-33-36)	98.0	(33-34-37)	178.2	(33-35-38)	179.4	(33-36-39)	179.0
(3-1-2-4)	0.4	(3-1-2-6)	-155.3	(3-1-2-9)	69.6		
(5-1-2-4)	158.3	(5-1-2-6)	2.7	(5-1-2-9)	-132.4		
(9-1-2-4)	-69.2	(9-1-2-6)	135.1	(2-1-3-4)	-0.4		
(2-1-3-7)	176.2	(2-1-3-9)	-68.6	(5-1-3-4)	-145.5		
(5-1-3-7)	31.1	(5-1-3-9)	146.2	(9-1-3-4)	68.3		
(9-1-3-7)	-115.2	(2-1-5-16)	-3.0	(2-1-5-18)	148.3		
(2-1-5-33)	-89.2	(3-1-5-16)	136.2	(3-1-5-18)	-72.5		
(3-1-5-33)	50.0	(9-1-5-16)	-93.1	(9-1-5-18)	58.2		
(9-1-5-33)	-179.3	(2-1-9-3)	96.5	(2-1-9-4)	48.9		
(2-1-9-10)	162.5	(2-1-9-11)	-97.6	(2-1-9-12)	18.3		
(3-1-9-2)	-96.5	(3-1-9-4)	-47.5	(3-1-9-10)	66.0		
(3-1-9-11)	165.9	(3-1-9-12)	-78.2	(5-1-9-2)	111.0		
(5-1-9-3)	-152.5	(5-1-9-4)	159.9	(5-1-9-10)	-86.5		
(5-1-9-11)	13.4	(5-1-9-12)	129.3	(1-2-4-3)	-0.4		
(1-2-4-8)	-176.8	(1-2-4-9)	66.9	(6-2-4-3)	143.6		
(6-2-4-8)	-32.7	(6-2-4-9)	-149.1	(9-2-4-3)	-67.3		
(9-2-4-8)	116.3	(1-2-6-17)	0.6	(1-2-6-20)	147.5		
(1-2-6-26)	-91.5	(4-2-6-17)	-136.6	(4-2-6-20)	10.3		
(4-2-6-26)	131.3	(9-2-6-17)	91.2	(9-2-6-20)	-121.9		
(9-2-6-26)	-0.9	(1-2-9-3)	-49.6	(1-2-9-4)	-97.2		
(1-2-9-10)	-33.0	(1-2-9-11)	88.7	(1-2-9-12)	-169.8		
(4-2-9-1)	97.2	(4-2-9-3)	47.6	(4-2-9-10)	64.2		
(4-2-9-11)	-174.1	(4-2-9-12)	-72.6	(6-2-9-1)	-111.3		
(6-2-9-3)	-160.9	(6-2-9-4)	151.6	(6-2-9-10)	-144.3		
(6-2-9-11)	-22.6	(6-2-9-12)	78.9	(1-3-4-2)	0.4		
(1-3-4-8)	176.8	(1-3-4-9)	-66.1	(7-3-4-2)	-176.2		
(7-3-4-8)	0.2	(7-3-4-9)	117.3	(9-3-4-2)	66.5		
(9-3-4-8)	-117.1	(1-3-9-2)	50.9	(1-3-9-4)	99.4		
(1-3-9-10)	-120.6	(1-3-9-11)	-20.5	(1-3-9-12)	140.2		
(4-3-9-1)	-99.4	(4-3-9-2)	-48.6	(4-3-9-10)	140.0		
(4-3-9-11)	-119.9	(4-3-9-12)	40.7	(7-3-9-1)	129.9		
(7-3-9-2)	-179.3	(7-3-9-4)	-130.7	(7-3-9-10)	9.3		
(7-3-9-11)	109.4	(7-3-9-12)	-90.0	(2-4-9-1)	-50.7		
(2-4-9-3)	-99.7	(2-4-9-10)	-147.4	(2-4-9-11)	9.1		
(2-4-9-12)	113.2	(3-4-9-1)	49.0	(3-4-9-2)	99.7		
(3-4-9-10)	-47.7	(3-4-9-11)	108.8	(3-4-9-12)	-147.1		
(8-4-9-1)	179.2	(8-4-9-2)	-130.1	(8-4-9-3)	130.2		
(8-4-9-10)	82.5	(8-4-9-11)	-121.0	(8-4-9-12)	-16.9		
(1-5-16-17)	0.2	(1-5-16-19)	164.8	(1-5-16-33)	-125.8		
(18-5-16-17)	-164.7	(18-5-16-19)	-0.2	(18-5-16-33)	69.3		
(33-5-16-17)	126.0	(33-5-16-19)	-69.5	(1-5-18-19)	-155.4		
(1-5-18-22)	21.7	(1-5-18-33)	137.6	(16-5-18-19)	0.2		
(16-5-18-22)	177.2	(16-5-18-33)	-66.9	(33-5-18-19)	67.0		
(33-5-18-22)	-115.9	(1-5-33-16)	111.7	(1-5-33-18)	-151.0		
(1-5-33-19)	161.4	(1-5-33-34)	14.3	(1-5-33-35)	-85.9		
(1-5-33-36)	128.4	(16-5-33-18)	97.3	(16-5-33-19)	49.7		
(16-5-33-34)	-97.4	(16-5-33-35)	162.4	(16-5-33-36)	16.7		
(18-5-33-16)	-97.3	(18-5-33-19)	-47.6	(18-5-33-34)	165.3		
(18-5-33-35)	65.0	(18-5-33-36)	-80.6	(2-6-17-16)	-3.4		
(2-6-17-21)	161.5	(2-6-17-26)	-132.6	(20-6-17-16)	-165.3		
(20-6-17-21)	-0.3	(20-6-17-26)	65.5	(26-6-17-16)	129.2		
(26-6-17-21)	-65.9	(2-6-20-21)	-151.6	(2-6-20-24)	16.1		
(2-6-20-26)	139.9	(17-6-20-21)	0.3	(17-6-20-24)	168.0		
(17-6-20-26)	-68.1	(26-6-20-21)	68.5	(26-6-20-24)	-123.8		
(2-6-26-17)	113.4	(2-6-26-20)	-147.9	(2-6-26-21)	161.8		
(2-6-26-27)	58.1	(2-6-26-29)	-43.8	(2-6-26-31)	-150.6		
(17-6-26-20)	98.7	(17-6-26-21)	48.4	(17-6-26-27)	-55.3		
(17-6-26-29)	-157.3	(17-6-26-31)	96.0	(20-6-26-17)	-98.7		
(20-6-26-21)	-50.3	(20-6-26-27)	-153.9	(20-6-26-29)	104.1		

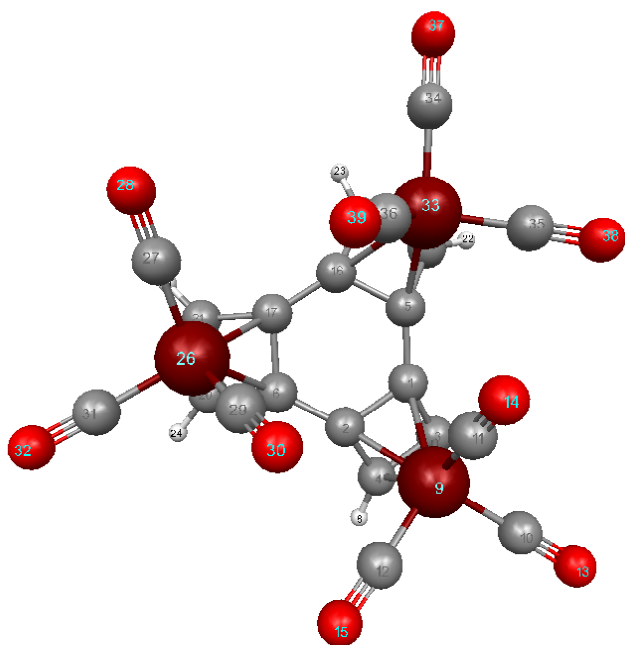
(20-6-26-31)	-2.7	(1-9-10-13)	41.8	(2-9-10-13)	64.8
(3-9-10-13)	79.1	(4-9-10-13)	107.7	(11-9-10-13)	-57.6
(12-9-10-13)	-156.9	(1-9-11-14)	-7.9	(2-9-11-14)	-50.7
(3-9-11-14)	5.6	(4-9-11-14)	-56.7	(10-9-11-14)	102.8
(12-9-11-14)	-158.3	(1-9-12-15)	7.8	(2-9-12-15)	20.5
(3-9-12-15)	-43.4	(4-9-12-15)	-18.4	(10-9-12-15)	-138.4
(11-9-12-15)	123.2	(5-16-17-6)	3.0	(5-16-17-21)	-148.8
(5-16-17-26)	92.2	(19-16-17-6)	-147.4	(19-16-17-21)	60.8
(19-16-17-26)	-58.2	(33-16-17-6)	91.1	(33-16-17-21)	-60.6
(33-16-17-26)	-179.7	(5-16-19-18)	0.2	(5-16-19-23)	-174.8
(5-16-19-33)	68.7	(17-16-19-18)	154.9	(17-16-19-23)	-20.1
(17-16-19-33)	-136.7	(33-16-19-18)	-68.5	(33-16-19-23)	116.5
(5-16-33-18)	-48.7	(5-16-33-19)	-96.5	(5-16-33-34)	88.3
(5-16-33-35)	-33.7	(5-16-33-36)	-170.5	(17-16-33-5)	-112.7
(17-16-33-18)	-161.4	(17-16-33-19)	150.8	(17-16-33-34)	-24.4
(17-16-33-35)	-146.5	(17-16-33-36)	76.8	(19-16-33-5)	96.5
(19-16-33-18)	47.8	(19-16-33-34)	-175.2	(19-16-33-35)	62.8
(19-16-33-36)	-74.0	(6-17-21-20)	0.3	(6-17-21-25)	-171.1
(6-17-21-26)	67.5	(16-17-21-20)	156.1	(16-17-21-25)	-15.3
(16-17-21-26)	-136.7	(26-17-21-20)	-67.2	(26-17-21-25)	121.4
(6-17-26-20)	-49.2	(6-17-26-21)	-99.2	(6-17-26-27)	132.9
(6-17-26-29)	30.2	(6-17-26-31)	-126.9	(16-17-26-6)	-112.1
(16-17-26-20)	-161.2	(16-17-26-21)	148.7	(16-17-26-27)	20.8
(16-17-26-29)	-81.9	(16-17-26-31)	121.0	(21-17-26-6)	99.2
(21-17-26-20)	50.1	(21-17-26-27)	-127.9	(21-17-26-29)	129.4
(21-17-26-31)	-27.7	(5-18-19-16)	-0.2	(5-18-19-23)	174.9
(5-18-19-33)	-66.5	(22-18-19-16)	-177.3	(22-18-19-23)	-2.2
(22-18-19-33)	116.5	(33-18-19-16)	66.3	(33-18-19-23)	-118.7
(5-18-33-16)	50.6	(5-18-33-19)	99.9	(5-18-33-34)	-20.8
(5-18-33-35)	-121.8	(5-18-33-36)	138.3	(19-18-33-5)	-99.9
(19-18-33-16)	-49.3	(19-18-33-34)	-120.7	(19-18-33-35)	138.3
(19-18-33-36)	38.4	(22-18-33-5)	130.1	(22-18-33-16)	-179.2
(22-18-33-19)	-129.9	(22-18-33-34)	109.3	(22-18-33-35)	8.4
(22-18-33-36)	-91.6	(16-19-33-5)	-50.7	(16-19-33-18)	-99.0
(16-19-33-34)	7.5	(16-19-33-35)	-148.6	(16-19-33-36)	111.7
(18-19-33-5)	48.2	(18-19-33-16)	99.0	(18-19-33-34)	106.4
(18-19-33-35)	-49.6	(18-19-33-36)	-149.3	(23-19-33-5)	179.1
(23-19-33-16)	-130.2	(23-19-33-18)	130.8	(23-19-33-34)	-122.7
(23-19-33-35)	81.2	(23-19-33-36)	-18.5	(6-20-21-17)	-0.3
(6-20-21-25)	171.1	(6-20-21-26)	-70.4	(24-20-21-17)	-168.1
(24-20-21-25)	3.3	(24-20-21-26)	121.9	(26-20-21-17)	70.1
(26-20-21-25)	-118.5	(6-20-26-17)	48.3	(6-20-26-21)	96.8
(6-20-26-27)	52.4	(6-20-26-29)	-81.3	(6-20-26-31)	178.3
(21-20-26-6)	-96.8	(21-20-26-17)	-48.5	(21-20-26-27)	-44.4
(21-20-26-29)	-178.1	(21-20-26-31)	81.5	(24-20-26-6)	132.4
(24-20-26-17)	-179.3	(24-20-26-21)	-130.8	(24-20-26-27)	-175.2
(24-20-26-29)	51.1	(24-20-26-31)	-49.3	(17-21-26-6)	-48.3
(17-21-26-20)	-97.8	(17-21-26-27)	59.9	(17-21-26-29)	-94.7
(17-21-26-31)	159.0	(20-21-26-6)	49.6	(20-21-26-17)	97.8
(20-21-26-27)	157.7	(20-21-26-29)	3.1	(20-21-26-31)	-103.2
(25-21-26-6)	179.9	(25-21-26-17)	-131.8	(25-21-26-20)	130.3
(25-21-26-27)	-72.0	(25-21-26-29)	133.4	(25-21-26-31)	27.2
(6-26-27-28)	73.6	(17-26-27-28)	41.2	(20-26-27-28)	37.6
(21-26-27-28)	6.7	(29-26-27-28)	171.7	(31-26-27-28)	-88.9
(6-26-29-30)	-32.9	(17-26-29-30)	-52.1	(20-26-29-30)	8.0
(21-26-29-30)	5.8	(27-26-29-30)	-150.8	(31-26-29-30)	110.2
(6-26-31-32)	-1.8	(17-26-31-32)	55.5	(20-26-31-32)	-3.6
(21-26-31-32)	37.9	(27-26-31-32)	152.6	(29-26-31-32)	-106.9
(5-33-34-37)	24.5	(16-33-34-37)	-18.1	(18-33-34-37)	38.0
(19-33-34-37)	-23.1	(35-33-34-37)	135.9	(36-33-34-37)	-124.8
(5-33-35-38)	25.9	(16-33-35-38)	49.5	(18-33-35-38)	62.4
(19-33-35-38)	92.0	(34-33-35-38)	-72.9	(36-33-35-38)	-172.4

(5-33-36-39)	-37.8	(16-33-36-39)	-26.2	(18-33-36-39)	-89.6
(19-33-36-39)	-65.9	(34-33-36-39)	75.5	(35-33-36-39)	174.5

Frequencies (cm ⁻¹):	14.1	21.0	30.0	39.9	41.3	51.1	52.5	73.0
	77.1	84.0	84.6	87.5	92.2	93.2	95.5	107.3
	110.8	113.5	136.4	142.8	148.1	152.9	169.7	209.3
	242.3	321.1	331.4	340.2	346.2	352.9	368.4	373.2
	391.5	405.2	413.6	419.8	438.0	447.9	458.5	463.5
	464.0	467.2	471.3	472.3	502.1	504.3	507.0	510.4
	513.7	516.5	520.0	524.0	529.6	543.8	550.8	591.3
	595.1	600.1	602.7	604.6	606.2	609.7	613.9	622.2
	626.6	631.1	651.0	665.8	680.6	764.7	788.2	812.8
	820.7	831.5	834.6	931.7	965.4	980.7	1009.9	1017.2
	1021.0	1106.5	1133.4	1158.2	1174.6	1176.8	1191.4	1298.0
	1304.9	1315.3	1338.9	1347.1	1365.3	1534.7	1552.2	1567.7
	2078.9	2081.2	2088.8	2091.1	2092.0	2098.6	2117.8	2128.1
	2145.1	3264.3	3270.0	3275.4	3282.4	3288.9	3291.2	

(8b) B3LYP/6-31G(d)+LANL2DZ C₁ Geometry

Nuclear repulsion energy	4174.99205069	Hartrees
B3LYP/6-31G(d)+LANL2DZ energy	-1851.11174037	Hartrees
Zero-point energy correction	0.213169	Hartrees
Thermal correction to Enthalpy	0.246418	Hartrees
Thermal correction to Gibbs Free Energy	0.147634	Hartrees



	X	Y	Z
C1	0.968746	-1.083572	1.328794
C2	1.433639	0.320964	1.280365
C3	2.215215	-1.473134	1.938093
C4	2.691942	-0.104086	1.918489
C5	-0.437893	-1.401715	1.279811
C6	0.454868	1.380297	1.329336
H7	2.603874	-2.404247	2.328948
H8	3.525756	0.412424	2.372425
Fe9	2.604634	-0.784430	0.007515
C10	3.886817	-2.010342	-0.172666
C11	1.678001	-1.265168	-1.443477
C12	3.494251	0.597209	-0.679910
O13	4.725837	-2.793926	-0.271103
O14	1.090290	-1.582064	-2.380974
O15	4.064207	1.509948	-1.089396
C16	-1.422060	-0.296650	1.329847
C17	-0.994168	1.080590	1.281354
C18	-1.434677	-2.278929	1.918731
C19	-2.381852	-1.181677	1.939834
C20	0.169248	2.654596	1.938601
C21	-1.254687	2.382905	1.919748
H22	-1.404171	-3.260038	2.371055
H23	-3.382412	-1.052805	2.331108
H24	0.781857	3.456960	2.328152
H25	-2.118920	2.847330	2.373064
Fe26	-0.622941	2.646726	0.008118
C27	-2.265209	2.729672	-0.676850
O28	-3.340755	2.768882	-1.085860
C29	0.253271	2.081433	-1.443750
O30	0.819479	1.728550	-2.381635
C31	-0.198143	4.369015	-0.174801
O32	0.063803	5.486478	-0.275915
Fe33	-1.981562	-1.862342	0.008116
C34	-3.686321	-2.353027	-0.173076
C35	-1.235786	-3.327248	-0.677734

					C36	-1.930578	-0.821578	-1.444595	
					O37	-4.785736	-2.683040	-0.272897	
					O38	-0.734892	-4.279617	-1.087257	
					O39	-1.906875	-0.154680	-2.382349	
(1-2)	1.480	(1-3)	1.441	(1-5)	1.443	(1-9)	2.124	(2-4)	1.473
(2-6)	1.443	(2-9)	2.053	(3-4)	1.450	(3-7)	1.082	(3-9)	2.086
(4-8)	1.081	(4-9)	2.030	(5-16)	1.481	(5-18)	1.474	(5-33)	2.052
(6-17)	1.480	(6-20)	1.441	(6-26)	2.124	(9-10)	1.783	(9-11)	1.787
(9-12)	1.781	(10-13)	1.152	(11-14)	1.151	(12-15)	1.151	(16-17)	1.443
(16-19)	1.441	(16-33)	2.124	(17-21)	1.474	(17-26)	2.052	(18-19)	1.450
(18-22)	1.081	(18-33)	2.031	(19-23)	1.082	(19-33)	2.087	(20-21)	1.450
(20-24)	1.082	(20-26)	2.087	(21-25)	1.081	(21-26)	2.031	(26-27)	1.781
(26-29)	1.788	(26-31)	1.783	(27-28)	1.151	(29-30)	1.151	(31-32)	1.152
(33-34)	1.783	(33-35)	1.781	(33-36)	1.788	(34-37)	1.152	(35-38)	1.151
(36-39)	1.151								
(2-1-3)	89.9	(2-1-5)	120.9	(2-1-9)	66.7	(3-1-5)	142.9		
(3-1-9)	68.6	(5-1-9)	139.5	(1-2-4)	88.9	(1-2-6)	118.8		
(1-2-9)	71.8	(4-2-6)	140.9	(4-2-9)	68.0	(6-2-9)	143.4		
(1-3-4)	91.3	(1-3-7)	134.1	(1-3-9)	71.4	(4-3-7)	134.4		
(4-3-9)	67.3	(7-3-9)	123.5	(2-4-3)	89.9	(2-4-8)	134.7		
(2-4-9)	69.7	(3-4-8)	134.4	(3-4-9)	71.5	(8-4-9)	126.1		
(1-5-16)	118.8	(1-5-18)	140.9	(1-5-33)	143.5	(16-5-18)	88.9		
(16-5-33)	71.9	(18-5-33)	68.1	(2-6-17)	120.9	(2-6-20)	142.9		
(2-6-26)	139.5	(17-6-20)	89.9	(17-6-26)	66.7	(20-6-26)	68.6		
(1-9-2)	41.5	(1-9-3)	40.0	(1-9-4)	59.7	(1-9-10)	121.3		
(1-9-11)	93.9	(1-9-12)	137.2	(2-9-3)	59.8	(2-9-4)	42.3		
(2-9-10)	147.5	(2-9-11)	110.6	(2-9-12)	96.1	(3-9-4)	41.2		
(3-9-10)	90.0	(3-9-11)	124.4	(3-9-12)	134.9	(4-9-10)	107.1		
(4-9-11)	151.2	(4-9-12)	94.7	(10-9-11)	96.1	(10-9-12)	97.8		
(11-9-12)	98.9	(9-10-13)	178.9	(9-11-14)	179.4	(9-12-15)	178.0		
(5-16-17)	120.9	(5-16-19)	89.9	(5-16-33)	66.7	(17-16-19)	142.9		
(17-16-33)	139.5	(19-16-33)	68.6	(6-17-16)	118.8	(6-17-21)	88.9		
(6-17-26)	71.9	(16-17-21)	140.9	(16-17-26)	143.4	(21-17-26)	68.1		
(5-18-19)	89.9	(5-18-22)	134.7	(5-18-33)	69.6	(19-18-22)	134.4		
(19-18-33)	71.5	(22-18-33)	126.0	(16-19-18)	91.3	(16-19-23)	134.1		
(16-19-33)	71.4	(18-19-23)	134.4	(18-19-33)	67.3	(23-19-33)	123.4		
(6-20-21)	91.3	(6-20-24)	134.1	(6-20-26)	71.4	(21-20-24)	134.4		
(21-20-26)	67.3	(24-20-26)	123.4	(17-21-20)	89.9	(17-21-25)	134.7		
(17-21-26)	69.6	(20-21-25)	134.4	(20-21-26)	71.5	(25-21-26)	126.0		
(6-26-17)	41.5	(6-26-20)	40.0	(6-26-21)	59.7	(6-26-27)	137.3		
(6-26-29)	93.9	(6-26-31)	121.3	(17-26-20)	59.8	(17-26-21)	42.3		
(17-26-27)	96.2	(17-26-29)	110.6	(17-26-31)	147.5	(20-26-21)	41.2		
(20-26-27)	134.9	(20-26-29)	124.5	(20-26-31)	90.0	(21-26-27)	94.7		
(21-26-29)	151.2	(21-26-31)	107.2	(27-26-29)	98.9	(27-26-31)	97.8		
(29-26-31)	96.0	(26-27-28)	178.0	(26-29-30)	179.4	(26-31-32)	178.9		
(5-33-16)	41.5	(5-33-18)	42.3	(5-33-19)	59.8	(5-33-34)	147.5		
(5-33-35)	96.2	(5-33-36)	110.6	(16-33-18)	59.7	(16-33-19)	40.0		
(16-33-34)	121.2	(16-33-35)	137.4	(16-33-36)	94.0	(18-33-19)	41.2		
(18-33-34)	107.3	(18-33-35)	94.6	(18-33-36)	151.2	(19-33-34)	90.0		
(19-33-35)	134.8	(19-33-36)	124.6	(34-33-35)	97.7	(34-33-36)	96.0		
(35-33-36)	98.9	(33-34-37)	178.9	(33-35-38)	178.1	(33-36-39)	179.5		
(3-1-2-4)	-0.6	(3-1-2-6)	-151.7	(3-1-2-9)	66.6				
(5-1-2-4)	157.8	(5-1-2-6)	6.7	(5-1-2-9)	-135.0				
(9-1-2-4)	-67.2	(9-1-2-6)	141.7	(2-1-3-4)	0.6				
(2-1-3-7)	176.2	(2-1-3-9)	-64.9	(5-1-3-4)	-147.7				
(5-1-3-7)	27.8	(5-1-3-9)	146.8	(9-1-3-4)	65.5				
(9-1-3-7)	-118.9	(2-1-5-16)	-6.6	(2-1-5-18)	-136.5				
(2-1-5-33)	91.8	(3-1-5-16)	135.7	(3-1-5-18)	5.8				
(3-1-5-33)	-126.0	(9-1-5-16)	-96.2	(9-1-5-18)	134.0				
(9-1-5-33)	2.2	(2-1-9-3)	99.6	(2-1-9-4)	50.8				

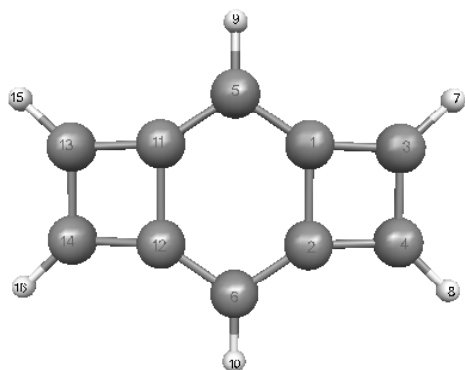
(2-1-9-10)	143.3	(2-1-9-11)	-117.2	(2-1-9-12)	-9.6
(3-1-9-2)	-99.6	(3-1-9-4)	-48.8	(3-1-9-10)	43.7
(3-1-9-11)	143.2	(3-1-9-12)	-109.3	(5-1-9-2)	110.9
(5-1-9-3)	-149.4	(5-1-9-4)	161.8	(5-1-9-10)	-105.7
(5-1-9-11)	-6.2	(5-1-9-12)	101.3	(1-2-4-3)	0.6
(1-2-4-8)	-168.1	(1-2-4-9)	70.9	(6-2-4-3)	138.4
(6-2-4-8)	-30.2	(6-2-4-9)	-151.3	(9-2-4-3)	-70.2
(9-2-4-8)	121.1	(1-2-6-17)	-6.5	(1-2-6-20)	135.7
(1-2-6-26)	-96.0	(4-2-6-17)	-136.5	(4-2-6-20)	5.8
(4-2-6-26)	134.0	(9-2-6-17)	91.8	(9-2-6-20)	-125.9
(9-2-6-26)	2.3	(1-2-9-3)	-47.2	(1-2-9-4)	-96.3
(1-2-9-10)	-71.7	(1-2-9-11)	71.5	(1-2-9-12)	173.4
(4-2-9-1)	96.3	(4-2-9-3)	49.1	(4-2-9-10)	24.6
(4-2-9-11)	167.8	(4-2-9-12)	-90.3	(6-2-9-1)	-114.2
(6-2-9-3)	-161.4	(6-2-9-4)	149.5	(6-2-9-10)	174.1
(6-2-9-11)	-42.7	(6-2-9-12)	59.2	(1-3-4-2)	-0.6
(1-3-4-8)	168.1	(1-3-4-9)	-69.2	(7-3-4-2)	-176.2
(7-3-4-8)	-7.4	(7-3-4-9)	115.3	(9-3-4-2)	68.5
(9-3-4-8)	-122.7	(1-3-9-2)	49.0	(1-3-9-4)	99.6
(1-3-9-10)	-143.9	(1-3-9-11)	-46.5	(1-3-9-12)	115.1
(4-3-9-1)	-99.6	(4-3-9-2)	-50.6	(4-3-9-10)	116.5
(4-3-9-11)	-146.1	(4-3-9-12)	15.4	(7-3-9-1)	131.1
(7-3-9-2)	-179.8	(7-3-9-4)	-129.2	(7-3-9-10)	-12.7
(7-3-9-11)	84.7	(7-3-9-12)	-113.8	(2-4-9-1)	-49.7
(2-4-9-3)	-97.0	(2-4-9-10)	-166.4	(2-4-9-11)	-24.2
(2-4-9-12)	93.9	(3-4-9-1)	47.3	(3-4-9-2)	97.0
(3-4-9-10)	-69.5	(3-4-9-11)	72.8	(3-4-9-12)	-169.1
(8-4-9-1)	179.2	(8-4-9-2)	-131.1	(8-4-9-3)	131.9
(8-4-9-10)	62.5	(8-4-9-11)	-155.3	(8-4-9-12)	-37.2
(1-5-16-17)	6.7	(1-5-16-19)	-151.6	(1-5-16-33)	141.7
(18-5-16-17)	157.7	(18-5-16-19)	-0.6	(18-5-16-33)	-67.2
(33-5-16-17)	-135.0	(33-5-16-19)	66.6	(1-5-18-19)	138.3
(1-5-18-22)	-30.4	(1-5-18-33)	-151.4	(16-5-18-19)	0.6
(16-5-18-22)	-168.2	(16-5-18-33)	70.9	(33-5-18-19)	-70.3
(33-5-18-22)	121.0	(1-5-33-16)	-114.2	(1-5-33-18)	149.5
(1-5-33-19)	-161.4	(1-5-33-34)	174.5	(1-5-33-35)	59.4
(1-5-33-36)	-42.5	(16-5-33-18)	-96.3	(16-5-33-19)	-47.2
(16-5-33-34)	-71.3	(16-5-33-35)	173.7	(16-5-33-36)	71.7
(18-5-33-16)	96.3	(18-5-33-19)	49.1	(18-5-33-34)	25.0
(18-5-33-35)	-90.1	(18-5-33-36)	168.0	(2-6-17-16)	6.6
(2-6-17-21)	157.7	(2-6-17-26)	-135.0	(20-6-17-16)	-151.7
(20-6-17-21)	-0.6	(20-6-17-26)	66.6	(26-6-17-16)	141.6
(26-6-17-21)	-67.2	(2-6-20-21)	-147.7	(2-6-20-24)	27.9
(2-6-20-26)	146.8	(17-6-20-21)	0.6	(17-6-20-24)	176.3
(17-6-20-26)	-64.9	(26-6-20-21)	65.5	(26-6-20-24)	-118.9
(2-6-26-17)	110.9	(2-6-26-20)	-149.4	(2-6-26-21)	161.8
(2-6-26-27)	101.5	(2-6-26-29)	-6.1	(2-6-26-31)	-105.6
(17-6-26-20)	99.6	(17-6-26-21)	50.8	(17-6-26-27)	-9.5
(17-6-26-29)	-117.0	(17-6-26-31)	143.5	(20-6-26-17)	-99.6
(20-6-26-21)	-48.8	(20-6-26-27)	-109.1	(20-6-26-29)	143.3
(20-6-26-31)	43.8	(1-9-10-13)	-84.6	(2-9-10-13)	-37.2
(3-9-10-13)	-58.2	(4-9-10-13)	-20.1	(11-9-10-13)	177.1
(12-9-10-13)	77.2	(1-9-11-14)	-130.9	(2-9-11-14)	-170.0
(3-9-11-14)	-103.1	(4-9-11-14)	-152.8	(10-9-11-14)	-8.8
(12-9-11-14)	90.0	(1-9-12-15)	35.6	(2-9-12-15)	29.2
(3-9-12-15)	-23.5	(4-9-12-15)	-13.3	(10-9-12-15)	-121.4
(11-9-12-15)	141.2	(5-16-17-6)	-6.6	(5-16-17-21)	-136.6
(5-16-17-26)	91.8	(19-16-17-6)	135.7	(19-16-17-21)	5.7
(19-16-17-26)	-126.0	(33-16-17-6)	-96.1	(33-16-17-21)	133.9
(33-16-17-26)	2.3	(5-16-19-18)	0.6	(5-16-19-23)	176.3
(5-16-19-33)	-64.9	(17-16-19-18)	-147.7	(17-16-19-23)	27.9
(17-16-19-33)	146.8	(33-16-19-18)	65.5	(33-16-19-23)	-118.9

(5-16-33-18)	50.8	(5-16-33-19)	99.6	(5-16-33-34)	143.5					
(5-16-33-35)	-9.3	(5-16-33-36)	-117.0	(17-16-33-5)	110.9					
(17-16-33-18)	161.7	(17-16-33-19)	-149.4	(17-16-33-34)	-105.5					
(17-16-33-35)	101.6	(17-16-33-36)	-6.1	(19-16-33-5)	-99.6					
(19-16-33-18)	-48.8	(19-16-33-34)	43.9	(19-16-33-35)	-109.0					
(19-16-33-36)	143.4	(6-17-21-20)	0.6	(6-17-21-25)	-168.2					
(6-17-21-26)	70.9	(16-17-21-20)	138.4	(16-17-21-25)	-30.3					
(16-17-21-26)	-151.3	(26-17-21-20)	-70.2	(26-17-21-25)	121.0					
(6-17-26-20)	-47.1	(6-17-26-21)	-96.3	(6-17-26-27)	173.6					
(6-17-26-29)	71.7	(6-17-26-31)	-71.4	(16-17-26-6)	-114.2					
(16-17-26-20)	-161.4	(16-17-26-21)	149.5	(16-17-26-27)	59.3					
(16-17-26-29)	-42.6	(16-17-26-31)	174.4	(21-17-26-6)	96.3					
(21-17-26-20)	49.1	(21-17-26-27)	-90.2	(21-17-26-29)	167.9					
(21-17-26-31)	24.9	(5-18-19-16)	-0.6	(5-18-19-23)	-176.2					
(5-18-19-33)	68.5	(22-18-19-16)	168.2	(22-18-19-23)	-7.4					
(22-18-19-33)	-122.6	(33-18-19-16)	-69.1	(33-18-19-23)	115.2					
(5-18-33-16)	-49.7	(5-18-33-19)	-97.0	(5-18-33-34)	-166.3					
(5-18-33-35)	94.1	(5-18-33-36)	-23.8	(19-18-33-5)	97.0					
(19-18-33-16)	47.3	(19-18-33-34)	-69.3	(19-18-33-35)	-168.9					
(19-18-33-36)	73.2	(22-18-33-5)	-131.1	(22-18-33-16)	179.2					
(22-18-33-19)	131.9	(22-18-33-34)	62.7	(22-18-33-35)	-36.9					
(22-18-33-36)	-154.8	(16-19-33-5)	49.1	(16-19-33-18)	99.7					
(16-19-33-34)	-143.6	(16-19-33-35)	115.4	(16-19-33-36)	-46.3					
(18-19-33-5)	-50.6	(18-19-33-16)	-99.7	(18-19-33-34)	116.7					
(18-19-33-35)	15.7	(18-19-33-36)	-145.9	(23-19-33-5)	-179.8					
(23-19-33-16)	131.1	(23-19-33-18)	-129.2	(23-19-33-34)	-12.5					
(23-19-33-35)	-113.5	(23-19-33-36)	84.8	(6-20-21-17)	-0.6					
(6-20-21-25)	168.2	(6-20-21-26)	-69.2	(24-20-21-17)	-176.3					
(24-20-21-25)	-7.4	(24-20-21-26)	115.2	(26-20-21-17)	68.5					
(26-20-21-25)	-122.7	(6-20-26-17)	49.0	(6-20-26-21)	99.6					
(6-20-26-27)	115.3	(6-20-26-29)	-46.3	(6-20-26-31)	-143.7					
(21-20-26-6)	-99.6	(21-20-26-17)	-50.6	(21-20-26-27)	15.6					
(21-20-26-29)	-146.0	(21-20-26-31)	116.7	(24-20-26-6)	131.1					
(24-20-26-17)	-179.9	(24-20-26-21)	-129.3	(24-20-26-27)	-113.6					
(24-20-26-29)	84.8	(24-20-26-31)	-12.6	(17-21-26-6)	-49.7					
(17-21-26-20)	-97.0	(17-21-26-27)	94.0	(17-21-26-29)	-23.9					
(17-21-26-31)	-166.3	(20-21-26-6)	47.3	(20-21-26-17)	97.0					
(20-21-26-27)	-169.0	(20-21-26-29)	73.0	(20-21-26-31)	-69.3					
(25-21-26-6)	179.2	(25-21-26-17)	-131.1	(25-21-26-20)	131.9					
(25-21-26-27)	-37.0	(25-21-26-29)	-155.0	(25-21-26-31)	62.6					
(6-26-27-28)	34.6	(17-26-27-28)	28.3	(20-26-27-28)	-24.5					
(21-26-27-28)	-14.2	(29-26-27-28)	140.3	(31-26-27-28)	-122.3					
(6-26-29-30)	-130.0	(17-26-29-30)	-169.0	(20-26-29-30)	-102.2					
(21-26-29-30)	-152.1	(27-26-29-30)	90.9	(31-26-29-30)	-7.9					
(6-26-31-32)	-85.8	(17-26-31-32)	-38.5	(20-26-31-32)	-59.3					
(21-26-31-32)	-21.3	(27-26-31-32)	76.1	(29-26-31-32)	175.9					
(5-33-34-37)	-37.8	(16-33-34-37)	-84.9	(18-33-34-37)	-20.4					
(19-33-34-37)	-58.5	(35-33-34-37)	76.9	(36-33-34-37)	176.7					
(5-33-35-38)	29.5	(16-33-35-38)	35.7	(18-33-35-38)	-13.0					
(19-33-35-38)	-23.3	(34-33-35-38)	-121.1	(36-33-35-38)	141.5					
(5-33-36-39)	-168.3	(16-33-36-39)	-129.2	(18-33-36-39)	-151.4					
(19-33-36-39)	-101.4	(34-33-36-39)	-7.2	(35-33-36-39)	91.6					
Frequencies (cm ⁻¹):	16.2	21.1	43.4	46.1	46.4	57.1	70.3	83.7		
	84.1	85.6	88.4	89.5	95.2	95.3	101.7	112.8	113.5	114.5
	135.4	135.7	143.5	182.6	209.1	209.8	238.7	239.8	247.3	350.3
	350.5	379.2	386.0	386.3	392.5	403.8	404.0	425.2	450.7	451.1
	460.5	465.5	465.8	468.0	469.0	469.1	500.9	506.6	506.8	509.0
	509.2	511.7	515.1	530.6	530.8	554.3	554.4	594.9	600.4	600.7
	601.9	606.8	607.5	617.4	619.8	620.2	628.6	648.0	659.5	660.4
	705.1	769.9	771.7	781.4	826.8	827.8	832.7	924.5	969.4	969.7

1010.6 1018.6 1018.9 1093.7 1136.3 1157.9 1158.2 1181.1 1181.5 1305.2
 1305.3 1311.5 1331.7 1331.9 1363.2 1539.1 1539.9 1540.7 2081.5 2081.6
 2086.2 2094.6 2094.8 2098.3 2121.7 2121.8 2151.3 3265.1 3265.5 3265.9
 3285.6 3285.9 3286.3

(9a) B3LYP/6-31G(d) D_{2h} Geometry

Nuclear repulsion energy 436.31508718 Hartrees
 B3LYP/6-31G(d) energy -384.46618151 Hartrees
 Zero-point energy correction 0.119156 Hartrees
 Thermal correction to Enthalpy 0.127230 Hartrees
 Thermal correction to Gibbs Free Energy 0.089163 Hartrees



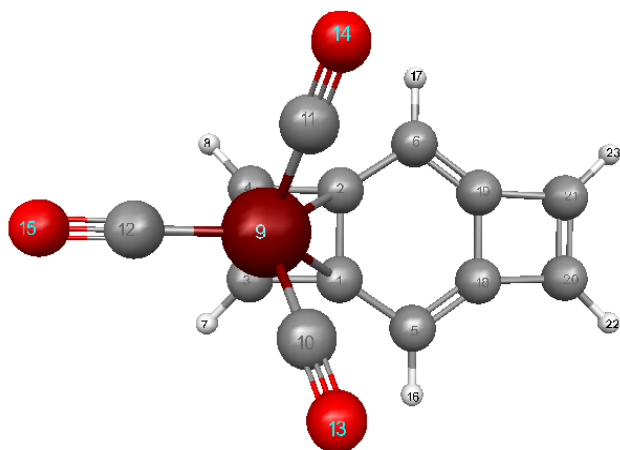
	X	Y	Z
C1	0.000000	1.150441	0.782092
C2	0.000000	1.150441	-0.782092
C3	0.000000	2.541059	0.729104
C4	0.000000	2.541059	-0.729104
C5	0.000000	0.000000	1.559929
C6	0.000000	0.000000	-1.559929
H7	0.000000	3.327203	1.476054
H8	0.000000	3.327203	-1.476054
H9	0.000000	0.000000	2.647423
H10	0.000000	0.000000	-2.647423
C11	0.000000	-1.150441	0.782092
C12	0.000000	-1.150441	-0.782092
C13	0.000000	-2.541059	0.729104
C14	0.000000	-2.541059	-0.729104
H15	0.000000	-3.327203	1.476054
H16	0.000000	-3.327203	-1.476054

(1-2)	1.564	(1-3)	1.392	(1-5)	1.389	(2-4)	1.392	(2-6)	1.389
(3-4)	1.458	(3-7)	1.084	(4-8)	1.084	(5-9)	1.087	(5-11)	1.389
(6-10)	1.087	(6-12)	1.389	(11-12)	1.564	(11-13)	1.392	(12-14)	1.392
(13-14)	1.458	(13-15)	1.084	(14-16)	1.084				
(2-1-3)	87.8	(2-1-5)	124.1	(3-1-5)	148.1	(1-2-4)	87.8		
(1-2-6)	124.1	(4-2-6)	148.1	(1-3-4)	92.2	(1-3-7)	134.3		
(4-3-7)	133.5	(2-4-3)	92.2	(2-4-8)	134.3	(3-4-8)	133.5		
(1-5-9)	124.1	(1-5-11)	111.9	(9-5-11)	124.1	(2-6-10)	124.1		
(2-6-12)	111.9	(10-6-12)	124.1	(5-11-12)	124.1	(5-11-13)	148.1		
(12-11-13)	87.8	(6-12-11)	124.1	(6-12-14)	148.1	(11-12-14)	87.8		
(11-13-14)	92.2	(11-13-15)	134.3	(14-13-15)	133.5	(12-14-13)	92.2		
(12-14-16)	134.3	(13-14-16)	133.5						
(3-1-2-4)	0.0	(3-1-2-6)	180.0	(5-1-2-4)	180.0				
(5-1-2-6)	0.0	(2-1-3-4)	0.0	(2-1-3-7)	180.0				
(5-1-3-4)	180.0	(5-1-3-7)	0.0	(2-1-5-9)	180.0				
(2-1-5-11)	0.0	(3-1-5-9)	0.0	(3-1-5-11)	180.0				
(1-2-4-3)	0.0	(1-2-4-8)	180.0	(6-2-4-3)	180.0				
(6-2-4-8)	0.0	(1-2-6-10)	180.0	(1-2-6-12)	0.0				
(4-2-6-10)	0.0	(4-2-6-12)	180.0	(1-3-4-2)	0.0				
(1-3-4-8)	180.0	(7-3-4-2)	180.0	(7-3-4-8)	0.0				
(1-5-11-12)	0.0	(1-5-11-13)	180.0	(9-5-11-12)	180.0				
(9-5-11-13)	0.0	(2-6-12-11)	0.0	(2-6-12-14)	180.0				
(10-6-12-11)	180.0	(10-6-12-14)	0.0	(5-11-12-6)	0.0				
(5-11-12-14)	180.0	(13-11-12-6)	180.0	(13-11-12-14)	0.0				
(5-11-13-14)	180.0	(5-11-13-15)	0.0	(12-11-13-14)	0.0				
(12-11-13-15)	180.0	(6-12-14-13)	180.0	(6-12-14-16)	0.0				
(11-12-14-13)	0.0	(11-12-14-16)	180.0	(11-13-14-12)	0.0				
(11-13-14-16)	180.0	(15-13-14-12)	180.0	(15-13-14-16)	0.0				

Frequencies (cm⁻¹): 148.0 221.9 371.0 378.7 387.8 426.1 443.8 492.0
 608.2 668.7 724.7 725.2 728.4 793.9 795.6 799.9 801.6 825.1
 842.4 884.6 893.6 1013.6 1114.1 1164.9 1168.7 1215.0 1230.8 1271.5
 1283.9 1324.6 1331.1 1348.6 1561.6 1651.1 1663.3 1667.2 3190.4 3190.5
 3227.4 3229.2 3247.4 3247.4

(10a) B3LYP/6-31G(d)+LANL2DZ C_s Geometry

Nuclear repulsion energy 1252.77584015 Hartrees
 B3LYP/6-31G(d)+LANL2DZ energy -847.98798128 Hartrees
 Zero-point energy correction 0.147980 Hartrees
 Thermal correction to Enthalpy 0.163054 Hartrees
 Thermal correction to Gibbs Free Energy 0.106877 Hartrees



	X	Y	Z
C1	1.000539	0.567097	0.723971
C2	1.000539	0.567097	-0.723971
C3	1.786343	-0.662255	0.735872
C4	1.786343	-0.662255	-0.735872
C5	0.525725	1.686132	1.515376
C6	0.525725	1.686132	-1.515376
H7	2.358593	-1.182901	1.490468
H8	2.358593	-1.182901	-1.490468
Fe9	-0.022870	-1.180716	0.000000
C10	-1.179426	-1.114769	1.359267
C11	-1.179426	-1.114769	-1.359267
C12	0.278113	-2.927527	0.000000
O13	-1.905449	-1.070106	2.254696
O14	-1.905449	-1.070106	-2.254696
O15	0.500674	-4.059820	0.000000
H16	0.520991	1.683599	2.600947
H17	0.520991	1.683599	-2.600947
C18	0.118813	2.714683	0.737559
C19	0.118813	2.714683	-0.737559
C20	-0.480340	4.082236	0.681347
C21	-0.480340	4.082236	-0.681347
H22	-0.805638	4.792571	1.432279
H23	-0.805638	4.792571	-1.432279

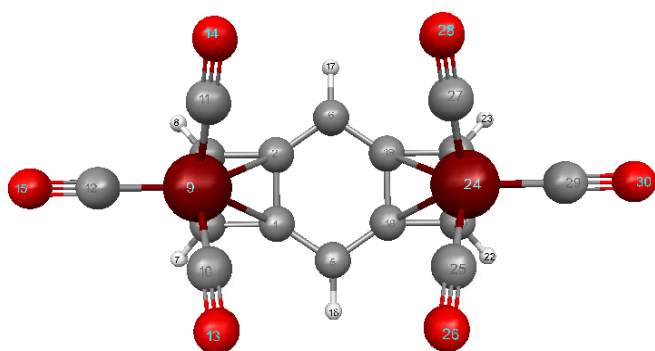
(1-2)	1.448	(1-3)	1.459	(1-5)	1.451	(1-9)	2.151	(2-4)	1.459
(2-6)	1.451	(2-9)	2.151	(3-4)	1.472	(3-7)	1.081	(3-9)	2.021
(4-8)	1.081	(4-9)	2.021	(5-16)	1.086	(5-18)	1.352	(6-17)	1.086
(6-19)	1.352	(9-10)	1.786	(9-11)	1.786	(9-12)	1.773	(10-13)	1.154
(11-14)	1.154	(12-15)	1.154	(18-19)	1.475	(18-20)	1.494	(19-21)	1.494
(20-21)	1.363	(20-22)	1.084	(21-23)	1.084				
(2-1-3)	90.5	(2-1-5)	123.1	(2-1-9)	70.3	(3-1-5)	145.3		
(3-1-9)	64.8	(5-1-9)	130.9	(1-2-4)	90.5	(1-2-6)	123.1		
(1-2-9)	70.3	(4-2-6)	145.3	(4-2-9)	64.8	(6-2-9)	130.9		
(1-3-4)	89.5	(1-3-7)	134.2	(1-3-9)	74.4	(4-3-7)	134.3		
(4-3-9)	68.6	(7-3-9)	127.2	(2-4-3)	89.5	(2-4-8)	134.2		
(2-4-9)	74.4	(3-4-8)	134.3	(3-4-9)	68.6	(8-4-9)	127.2		
(1-5-16)	123.0	(1-5-18)	111.8	(16-5-18)	125.1	(2-6-17)	123.0		
(2-6-19)	111.8	(17-6-19)	125.1	(1-9-2)	39.3	(1-9-3)	40.8		
(1-9-4)	59.2	(1-9-10)	91.3	(1-9-11)	122.3	(1-9-12)	136.1		
(2-9-3)	59.2	(2-9-4)	40.8	(2-9-10)	122.3	(2-9-11)	91.3		
(2-9-12)	136.1	(3-9-4)	42.7	(3-9-10)	107.0	(3-9-11)	147.9		
(3-9-12)	95.8	(4-9-10)	147.9	(4-9-11)	107.0	(4-9-12)	95.8		
(10-9-11)	99.1	(10-9-12)	98.4	(11-9-12)	98.4	(9-10-13)	178.6		
(9-11-14)	178.6	(9-12-15)	178.7	(5-18-19)	125.1	(5-18-20)	147.0		

(19-18-20)	87.8	(6-19-18)	125.1	(6-19-21)	147.0	(18-19-21)	87.8
(18-20-21)	92.2	(18-20-22)	134.0	(21-20-22)	133.9	(19-21-20)	92.2
(19-21-23)	134.0	(20-21-23)	133.9				
(3-1-2-4)	0.0	(3-1-2-6)	-170.4	(3-1-2-9)	62.9		
(5-1-2-4)	170.4	(5-1-2-6)	0.0	(5-1-2-9)	-126.7		
(9-1-2-4)	-62.9	(9-1-2-6)	126.7	(2-1-3-4)	0.0		
(2-1-3-7)	164.9	(2-1-3-9)	-67.9	(5-1-3-4)	-165.8		
(5-1-3-7)	-0.9	(5-1-3-9)	126.3	(9-1-3-4)	67.9		
(9-1-3-7)	-127.2	(2-1-5-16)	179.7	(2-1-5-18)	-1.2		
(3-1-5-16)	-17.3	(3-1-5-18)	161.7	(9-1-5-16)	87.8		
(9-1-5-18)	-93.1	(2-1-9-3)	100.2	(2-1-9-4)	48.5		
(2-1-9-10)	-144.7	(2-1-9-11)	-43.1	(2-1-9-12)	111.8		
(3-1-9-2)	-100.2	(3-1-9-4)	-51.8	(3-1-9-10)	115.0		
(3-1-9-11)	-143.3	(3-1-9-12)	11.5	(5-1-9-2)	117.2		
(5-1-9-3)	-142.6	(5-1-9-4)	165.6	(5-1-9-10)	-27.5		
(5-1-9-11)	74.1	(5-1-9-12)	-131.0	(1-2-4-3)	0.0		
(1-2-4-8)	-164.9	(1-2-4-9)	67.9	(6-2-4-3)	165.8		
(6-2-4-8)	0.9	(6-2-4-9)	-126.3	(9-2-4-3)	-67.9		
(9-2-4-8)	127.2	(1-2-6-17)	-179.7	(1-2-6-19)	1.2		
(4-2-6-17)	17.3	(4-2-6-19)	-161.7	(9-2-6-17)	-87.8		
(9-2-6-19)	93.1	(1-2-9-3)	-48.5	(1-2-9-4)	-100.2		
(1-2-9-10)	43.1	(1-2-9-11)	144.7	(1-2-9-12)	-111.8		
(4-2-9-1)	100.2	(4-2-9-3)	51.8	(4-2-9-10)	143.3		
(4-2-9-11)	-115.0	(4-2-9-12)	-11.5	(6-2-9-1)	-117.2		
(6-2-9-3)	-165.6	(6-2-9-4)	142.6	(6-2-9-10)	-74.1		
(6-2-9-11)	27.5	(6-2-9-12)	131.0	(1-3-4-2)	0.0		
(1-3-4-8)	164.9	(1-3-4-9)	-73.4	(7-3-4-2)	-164.9		
(7-3-4-8)	0.0	(7-3-4-9)	121.7	(9-3-4-2)	73.4		
(9-3-4-8)	-121.7	(1-3-9-2)	46.6	(1-3-9-4)	95.7		
(1-3-9-10)	-71.3	(1-3-9-11)	72.0	(1-3-9-12)	-172.0		
(4-3-9-1)	-95.7	(4-3-9-2)	-49.2	(4-3-9-10)	-167.1		
(4-3-9-11)	-23.8	(4-3-9-12)	92.3	(7-3-9-1)	134.1		
(7-3-9-2)	-179.3	(7-3-9-4)	-130.1	(7-3-9-10)	62.8		
(7-3-9-11)	-153.9	(7-3-9-12)	-37.9	(2-4-9-1)	-46.6		
(2-4-9-3)	-95.7	(2-4-9-10)	-72.0	(2-4-9-11)	71.3		
(2-4-9-12)	172.0	(3-4-9-1)	49.2	(3-4-9-2)	95.7		
(3-4-9-10)	23.8	(3-4-9-11)	167.1	(3-4-9-12)	-92.3		
(8-4-9-1)	179.3	(8-4-9-2)	-134.1	(8-4-9-3)	130.1		
(8-4-9-10)	153.9	(8-4-9-11)	-62.8	(8-4-9-12)	37.9		
(1-5-18-19)	1.3	(1-5-18-20)	177.5	(16-5-18-19)	-179.7		
(16-5-18-20)	-3.5	(2-6-19-18)	-1.3	(2-6-19-21)	-177.5		
(17-6-19-18)	179.7	(17-6-19-21)	3.5	(1-9-10-13)	-50.2		
(2-9-10-13)	-75.8	(3-9-10-13)	-11.9	(4-9-10-13)	-28.5		
(11-9-10-13)	-173.2	(12-9-10-13)	86.8	(1-9-11-14)	75.8		
(2-9-11-14)	50.2	(3-9-11-14)	28.5	(4-9-11-14)	11.9		
(10-9-11-14)	173.2	(12-9-11-14)	-86.8	(1-9-12-15)	-29.0		
(2-9-12-15)	29.0	(3-9-12-15)	-21.5	(4-9-12-15)	21.5		
(10-9-12-15)	-129.7	(11-9-12-15)	129.7	(5-18-19-6)	0.0		
(5-18-19-21)	177.9	(20-18-19-6)	-177.9	(20-18-19-21)	0.0		
(5-18-20-21)	-176.9	(5-18-20-22)	2.2	(19-18-20-21)	0.0		
(19-18-20-22)	179.1	(6-19-21-20)	176.9	(6-19-21-23)	-2.2		
(18-19-21-20)	0.0	(18-19-21-23)	-179.1	(18-20-21-19)	0.0		
(18-20-21-23)	179.1	(22-20-21-19)	-179.1	(22-20-21-23)	0.0		

Frequencies (cm ⁻¹):	-5.6	57.9	84.0	86.6	99.4	102.8	137.7	172.1		
	220.1	296.0	301.5	371.1	388.2	392.6	432.8	446.0	455.1	462.4
	479.4	496.8	511.6	515.4	527.7	600.6	604.1	618.9	629.3	732.5
	746.5	755.1	770.5	775.6	794.7	848.9	857.1	861.1	862.2	920.4
	983.1	1007.5	1048.2	1085.6	1120.1	1193.4	1210.4	1264.6	1279.2	1292.1
	1376.9	1457.5	1512.0	1549.0	1677.1	1704.8	2076.9	2078.3	2123.6	3215.7
	3215.9	3240.7	3267.5	3272.6	3287.8					

(11a) B3LYP/6-31G(d)+LANL2DZ C_{2v} Geometry

Nuclear repulsion energy	2355.29935392	Hartrees
B3LYP/6-31G(d)+LANL2DZ energy	-1311.47183165	Hartrees
Zero-point energy correction	0.174764	Hartrees
Thermal correction to Enthalpy	0.198932	Hartrees
Thermal correction to Gibbs Free Energy	0.119892	Hartrees



	X	Y	Z
C1	0.729687	1.166096	1.624936
C2	-0.729687	1.166096	1.624936
C3	0.739598	2.639694	1.699697
C4	-0.739598	2.639694	1.699697
C5	1.507453	0.000000	1.622110
C6	-1.507453	0.000000	1.622110
H7	1.478860	3.340044	2.064501
H8	-1.478860	3.340044	2.064501
Fe9	0.000000	2.463389	-0.139258
C10	1.414261	2.051051	-1.187299
C11	-1.414261	2.051051	-1.187299
C12	0.000000	4.184461	-0.480412
O13	2.336346	1.814680	-1.833849
O14	-2.336346	1.814680	-1.833849
O15	0.000000	5.321622	-0.671604
H16	2.589979	0.000000	1.707934
H17	-2.589979	0.000000	1.707934
C18	0.729687	-1.166096	1.624936
C19	-0.729687	-1.166096	1.624936
C20	0.739598	-2.639694	1.699697
C21	-0.739598	-2.639694	1.699697
H22	1.478860	-3.340044	2.064501
H23	-1.478860	-3.340044	2.064501
Fe24	0.000000	-2.463389	-0.139258
C25	1.414261	-2.051051	-1.187299
O26	2.336346	-1.814680	-1.833849
C27	-1.414261	-2.051051	-1.187299
O28	-2.336346	-1.814680	-1.833849
C29	0.000000	-4.184461	-0.480412
O30	0.000000	-5.321622	-0.671604

(1-2)	1.459	(1-3)	1.476	(1-5)	1.402	(1-9)	2.308	(2-4)	1.476
(2-6)	1.402	(2-9)	2.308	(3-4)	1.479	(3-7)	1.082	(3-9)	1.990
(4-8)	1.082	(4-9)	1.990	(5-16)	1.086	(5-18)	1.402	(6-17)	1.086
(6-19)	1.402	(9-10)	1.808	(9-11)	1.808	(9-12)	1.755	(10-13)	1.151
(11-14)	1.151	(12-15)	1.153	(18-19)	1.459	(18-20)	1.476	(18-24)	2.308
(19-21)	1.476	(19-24)	2.308	(20-21)	1.479	(20-22)	1.082	(20-24)	1.990
(21-23)	1.082	(21-24)	1.990	(24-25)	1.808	(24-27)	1.808	(24-29)	1.755
(25-26)	1.151	(27-28)	1.151	(29-30)	1.153				
(2-1-3)	90.4	(2-1-5)	123.7	(2-1-9)	71.6	(3-1-5)	145.8		
(3-1-9)	58.6	(5-1-9)	129.9	(1-2-4)	90.4	(1-2-6)	123.7		
(1-2-9)	71.6	(4-2-6)	145.8	(4-2-9)	58.6	(6-2-9)	129.9		
(1-3-4)	89.6	(1-3-7)	131.9	(1-3-9)	82.1	(4-3-7)	133.1		
(4-3-9)	68.2	(7-3-9)	128.5	(2-4-3)	89.6	(2-4-8)	131.9		
(2-4-9)	82.1	(3-4-8)	133.1	(3-4-9)	68.2	(8-4-9)	128.5		
(1-5-16)	123.6	(1-5-18)	112.6	(16-5-18)	123.6	(2-6-17)	123.6		
(2-6-19)	112.6	(17-6-19)	123.6	(1-9-2)	36.9	(1-9-3)	39.3		
(1-9-4)	57.4	(1-9-10)	93.9	(1-9-11)	124.2	(1-9-12)	134.4		
(2-9-3)	57.4	(2-9-4)	39.3	(2-9-10)	124.2	(2-9-11)	93.9		
(2-9-12)	134.4	(3-9-4)	43.6	(3-9-10)	105.4	(3-9-11)	147.9		

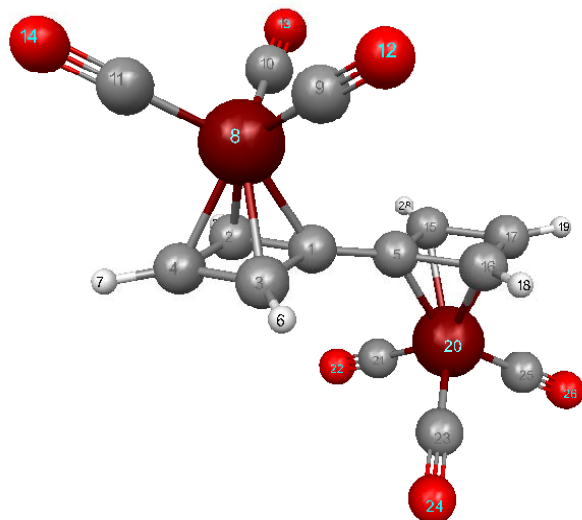
(3-9-12)	95.3	(4-9-10)	147.9	(4-9-11)	105.4	(4-9-12)	95.3
(10-9-11)	102.9	(10-9-12)	96.4	(11-9-12)	96.4	(9-10-13)	178.0
(9-11-14)	178.0	(9-12-15)	178.3	(5-18-19)	123.7	(5-18-20)	145.8
(5-18-24)	129.9	(19-18-20)	90.4	(19-18-24)	71.6	(20-18-24)	58.6
(6-19-18)	123.7	(6-19-21)	145.8	(6-19-24)	129.9	(18-19-21)	90.4
(18-19-24)	71.6	(21-19-24)	58.6	(18-20-21)	89.6	(18-20-22)	131.9
(18-20-24)	82.1	(21-20-22)	133.1	(21-20-24)	68.2	(22-20-24)	128.5
(19-21-20)	89.6	(19-21-23)	131.9	(19-21-24)	82.1	(20-21-23)	133.1
(20-21-24)	68.2	(23-21-24)	128.5	(18-24-19)	36.9	(18-24-20)	39.3
(18-24-21)	57.4	(18-24-25)	93.9	(18-24-27)	124.2	(18-24-29)	134.4
(19-24-20)	57.4	(19-24-21)	39.3	(19-24-25)	124.2	(19-24-27)	93.9
(19-24-29)	134.4	(20-24-21)	43.6	(20-24-25)	105.4	(20-24-27)	147.9
(20-24-29)	95.3	(21-24-25)	147.9	(21-24-27)	105.4	(21-24-29)	95.3
(25-24-27)	102.9	(25-24-29)	96.4	(27-24-29)	96.4	(24-25-26)	178.0
(24-27-28)	178.0	(24-29-30)	178.3				
(3-1-2-4)	0.0	(3-1-2-6)	-177.2	(3-1-2-9)	56.6		
(5-1-2-4)	177.2	(5-1-2-6)	0.0	(5-1-2-9)	-126.2		
(9-1-2-4)	-56.6	(9-1-2-6)	126.2	(2-1-3-4)	0.0		
(2-1-3-7)	155.9	(2-1-3-9)	-68.0	(5-1-3-4)	-175.9		
(5-1-3-7)	-20.0	(5-1-3-9)	116.1	(9-1-3-4)	68.0		
(9-1-3-7)	-136.1	(2-1-5-16)	-174.6	(2-1-5-18)	-0.3		
(3-1-5-16)	0.5	(3-1-5-18)	174.8	(9-1-5-16)	91.9		
(9-1-5-18)	-93.8	(2-1-9-3)	102.2	(2-1-9-4)	47.3		
(2-1-9-10)	-148.1	(2-1-9-11)	-39.6	(2-1-9-12)	109.1		
(3-1-9-2)	-102.2	(3-1-9-4)	-54.9	(3-1-9-10)	109.7		
(3-1-9-11)	-141.8	(3-1-9-12)	6.9	(5-1-9-2)	118.9		
(5-1-9-3)	-138.9	(5-1-9-4)	166.2	(5-1-9-10)	-29.2		
(5-1-9-11)	79.3	(5-1-9-12)	-132.0	(1-2-4-3)	0.0		
(1-2-4-8)	-155.9	(1-2-4-9)	68.0	(6-2-4-3)	175.9		
(6-2-4-8)	20.0	(6-2-4-9)	-116.1	(9-2-4-3)	-68.0		
(9-2-4-8)	136.1	(1-2-6-17)	174.6	(1-2-6-19)	0.3		
(4-2-6-17)	-0.5	(4-2-6-19)	-174.8	(9-2-6-17)	-91.9		
(9-2-6-19)	93.8	(1-2-9-3)	-47.3	(1-2-9-4)	-102.2		
(1-2-9-10)	39.6	(1-2-9-11)	148.1	(1-2-9-12)	-109.1		
(4-2-9-1)	102.2	(4-2-9-3)	54.9	(4-2-9-10)	141.8		
(4-2-9-11)	-109.7	(4-2-9-12)	-6.9	(6-2-9-1)	-118.9		
(6-2-9-3)	-166.2	(6-2-9-4)	138.9	(6-2-9-10)	-79.3		
(6-2-9-11)	29.2	(6-2-9-12)	132.0	(1-3-4-2)	0.0		
(1-3-4-8)	155.4	(1-3-4-9)	-81.6	(7-3-4-2)	-155.4		
(7-3-4-8)	0.0	(7-3-4-9)	123.0	(9-3-4-2)	81.6		
(9-3-4-8)	-123.0	(1-3-9-2)	44.1	(1-3-9-4)	92.8		
(1-3-9-10)	-77.0	(1-3-9-11)	73.9	(1-3-9-12)	-175.1		
(4-3-9-1)	-92.8	(4-3-9-2)	-48.7	(4-3-9-10)	-169.7		
(4-3-9-11)	-18.8	(4-3-9-12)	92.1	(7-3-9-1)	138.7		
(7-3-9-2)	-177.1	(7-3-9-4)	-128.5	(7-3-9-10)	61.8		
(7-3-9-11)	-147.3	(7-3-9-12)	-36.3	(2-4-9-1)	-44.1		
(2-4-9-3)	-92.8	(2-4-9-10)	-73.9	(2-4-9-11)	77.0		
(2-4-9-12)	175.1	(3-4-9-1)	48.7	(3-4-9-2)	92.8		
(3-4-9-10)	18.8	(3-4-9-11)	169.7	(3-4-9-12)	-92.1		
(8-4-9-1)	177.1	(8-4-9-2)	-138.7	(8-4-9-3)	128.5		
(8-4-9-10)	147.3	(8-4-9-11)	-61.8	(8-4-9-12)	36.3		
(1-5-18-19)	0.3	(1-5-18-20)	-174.8	(1-5-18-24)	93.8		
(16-5-18-19)	174.6	(16-5-18-20)	-0.5	(16-5-18-24)	-91.9		
(2-6-19-18)	-0.3	(2-6-19-21)	174.8	(2-6-19-24)	-93.8		
(17-6-19-18)	-174.6	(17-6-19-21)	0.5	(17-6-19-24)	91.9		
(1-9-10-13)	-78.5	(2-9-10-13)	-101.0	(3-9-10-13)	-40.3		
(4-9-10-13)	-53.7	(11-9-10-13)	155.1	(12-9-10-13)	57.0		
(1-9-11-14)	101.0	(2-9-11-14)	78.5	(3-9-11-14)	53.7		
(4-9-11-14)	40.3	(10-9-11-14)	-155.1	(12-9-11-14)	-57.0		
(1-9-12-15)	-26.3	(2-9-12-15)	26.3	(3-9-12-15)	-21.9		
(4-9-12-15)	21.9	(10-9-12-15)	-128.1	(11-9-12-15)	128.1		
(5-18-19-6)	0.0	(5-18-19-21)	-177.2	(5-18-19-24)	126.2		

(20-18-19-6)	177.2	(20-18-19-21)	0.0	(20-18-19-24)	-56.6
(24-18-19-6)	-126.2	(24-18-19-21)	56.6	(5-18-20-21)	175.9
(5-18-20-22)	20.0	(5-18-20-24)	-116.1	(19-18-20-21)	0.0
(19-18-20-22)	-155.9	(19-18-20-24)	68.0	(24-18-20-21)	-68.0
(24-18-20-22)	136.1	(5-18-24-19)	-118.9	(5-18-24-20)	138.9
(5-18-24-21)	-166.2	(5-18-24-25)	29.2	(5-18-24-27)	-79.3
(5-18-24-29)	132.0	(19-18-24-20)	-102.2	(19-18-24-21)	-47.3
(19-18-24-25)	148.1	(19-18-24-27)	39.6	(19-18-24-29)	-109.1
(20-18-24-19)	102.2	(20-18-24-21)	54.9	(20-18-24-25)	-109.7
(20-18-24-27)	141.8	(20-18-24-29)	-6.9	(6-19-21-20)	-175.9
(6-19-21-23)	-20.0	(6-19-21-24)	116.1	(18-19-21-20)	0.0
(18-19-21-23)	155.9	(18-19-21-24)	-68.0	(24-19-21-20)	68.0
(24-19-21-23)	-136.1	(6-19-24-18)	118.9	(6-19-24-20)	166.2
(6-19-24-21)	-138.9	(6-19-24-25)	79.3	(6-19-24-27)	-29.2
(6-19-24-29)	-132.0	(18-19-24-20)	47.3	(18-19-24-21)	102.2
(18-19-24-25)	-39.6	(18-19-24-27)	-148.1	(18-19-24-29)	109.1
(21-19-24-18)	-102.2	(21-19-24-20)	-54.9	(21-19-24-25)	-141.8
(21-19-24-27)	109.7	(21-19-24-29)	6.9	(18-20-21-19)	0.0
(18-20-21-23)	-155.4	(18-20-21-24)	81.6	(22-20-21-19)	155.4
(22-20-21-23)	0.0	(22-20-21-24)	-123.0	(24-20-21-19)	-81.6
(24-20-21-23)	123.0	(18-20-24-19)	-44.1	(18-20-24-21)	-92.8
(18-20-24-25)	77.0	(18-20-24-27)	-73.9	(18-20-24-29)	175.1
(21-20-24-18)	92.8	(21-20-24-19)	48.7	(21-20-24-25)	169.7
(21-20-24-27)	18.8	(21-20-24-29)	-92.1	(22-20-24-18)	-138.7
(22-20-24-19)	177.1	(22-20-24-21)	128.5	(22-20-24-25)	-61.8
(22-20-24-27)	147.3	(22-20-24-29)	36.3	(19-21-24-18)	44.1
(19-21-24-20)	92.8	(19-21-24-25)	73.9	(19-21-24-27)	-77.0
(19-21-24-29)	-175.1	(20-21-24-18)	-48.7	(20-21-24-19)	-92.8
(20-21-24-25)	-18.8	(20-21-24-27)	-169.7	(20-21-24-29)	92.1
(23-21-24-18)	-177.1	(23-21-24-19)	138.7	(23-21-24-20)	-128.5
(23-21-24-25)	-147.3	(23-21-24-27)	61.8	(23-21-24-29)	-36.3
(18-24-25-26)	78.5	(19-24-25-26)	101.0	(20-24-25-26)	40.3
(21-24-25-26)	53.7	(27-24-25-26)	-155.1	(29-24-25-26)	-57.0
(18-24-27-28)	-101.0	(19-24-27-28)	-78.5	(20-24-27-28)	-53.7
(21-24-27-28)	-40.3	(25-24-27-28)	155.1	(29-24-27-28)	57.0
(18-24-29-30)	26.3	(19-24-29-30)	-26.3	(20-24-29-30)	21.9
(21-24-29-30)	-21.9	(25-24-29-30)	128.1	(27-24-29-30)	-128.1

Frequencies (cm ⁻¹):	12.8	32.4	39.2	52.3	55.0	78.1	78.2	85.7		
	87.0	100.8	104.0	110.9	123.3	133.7	147.7	158.9	221.7	353.2
	373.1	378.4	399.3	415.8	419.0	437.7	439.6	444.8	452.3	464.4
	467.7	474.6	479.7	489.3	495.7	511.8	512.8	514.3	536.1	540.7
	579.8	591.7	592.3	593.6	617.1	621.8	673.6	727.4	742.6	780.0
	797.7	798.6	802.1	820.7	852.1	857.3	868.8	881.4	986.4	987.5
	1039.1	1096.2	1133.0	1206.2	1213.3	1238.1	1247.8	1263.9	1301.0	1370.1
	1470.4	1473.8	1578.7	1585.0	2079.9	2082.4	2089.2	2100.5	2116.7	2145.4
	3213.5	3213.8	3258.0	3258.2	3271.9	3272.1				

(12 *trans*) B3LYP/6-31G(d)+LANL2DZ C_{2h} Geometry

Nuclear repulsion energy	2061.17944744	Hartrees
B3LYP/6-31G(d)+LANL2DZ energy	-1235.28512497	Hartrees
Zero-point energy correction	0.162781	Hartrees
Thermal correction to Enthalpy	0.186063	Hartrees
Thermal correction to Gibbs Free Energy	0.108018	Hartrees



	X	Y	Z
C1	0.423076	0.582631	0.000000
C2	1.196431	1.294002	1.027071
C3	1.196431	1.294002	-1.027071
C4	1.950031	1.964692	0.000000
C5	-0.423076	-0.582631	0.000000
H6	1.276643	1.220167	-2.102783
H7	2.777200	2.661201	0.000000
Fe8	-0.042381	2.573949	0.000000
C9	-1.196431	2.654954	-1.351194
C10	-1.196431	2.654954	1.351194
C11	0.469678	4.286608	0.000000
O12	-1.937240	2.672025	-2.234317
O13	-1.937240	2.672025	2.234317
O14	0.799531	5.391040	0.000000
C15	-1.196431	-1.294002	1.027071
C16	-1.196431	-1.294002	-1.027071
C17	-1.950031	-1.964692	0.000000
H18	-1.276643	-1.220167	-2.102783
H19	-2.777200	-2.661201	0.000000
Fe20	0.042381	-2.573949	0.000000
C21	1.196431	-2.654954	1.351194
O22	1.937240	-2.672025	2.234317
C23	1.196431	-2.654954	-1.351194
O24	1.937240	-2.672025	-2.234317
C25	-0.469678	-4.286608	0.000000
O26	-0.799531	-5.391040	0.000000
H27	1.276643	1.220167	2.102783
H28	-1.276643	-1.220167	2.102783

(1-2)	1.469	(1-3)	1.469	(1-5)	1.440	(1-8)	2.045	(2-4)	1.440
(2-8)	2.056	(2-27)	1.081	(3-4)	1.440	(3-6)	1.081	(3-8)	2.056
(4-7)	1.081	(4-8)	2.083	(5-15)	1.469	(5-16)	1.469	(5-20)	2.045
(8-9)	1.779	(8-10)	1.779	(8-11)	1.788	(9-12)	1.153	(10-13)	1.153
(11-14)	1.153	(15-17)	1.440	(15-20)	2.056	(15-28)	1.081	(16-17)	1.440
(16-18)	1.081	(16-20)	2.056	(17-19)	1.081	(17-20)	2.083	(20-21)	1.779
(20-23)	1.779	(20-25)	1.788	(21-22)	1.153	(23-24)	1.153	(25-26)	1.153
(2-1-3)	88.7	(2-1-5)	134.5	(2-1-8)	69.4	(3-1-5)	134.5		
(3-1-8)	69.4	(5-1-8)	130.9	(1-2-4)	90.1	(1-2-8)	68.6		
(1-2-27)	134.5	(4-2-8)	70.7	(4-2-27)	134.6	(8-2-27)	125.7		
(1-3-4)	90.1	(1-3-6)	134.5	(1-3-8)	68.6	(4-3-6)	134.6		
(4-3-8)	70.7	(6-3-8)	125.7	(2-4-3)	91.0	(2-4-7)	134.5		
(2-4-8)	68.6	(3-4-7)	134.5	(3-4-8)	68.6	(7-4-8)	122.9		
(1-5-15)	134.5	(1-5-16)	134.5	(1-5-20)	130.9	(15-5-16)	88.7		
(15-5-20)	69.4	(16-5-20)	69.4	(1-8-2)	42.0	(1-8-3)	42.0		
(1-8-4)	59.8	(1-8-9)	101.1	(1-8-10)	101.1	(1-8-11)	150.2		
(2-8-3)	59.9	(2-8-4)	40.7	(2-8-9)	143.0	(2-8-10)	92.3		
(2-8-11)	115.1	(3-8-4)	40.7	(3-8-9)	92.3	(3-8-10)	143.0		
(3-8-11)	115.1	(4-8-9)	129.3	(4-8-10)	129.3	(4-8-11)	90.4		
(9-8-10)	98.9	(9-8-11)	98.2	(10-8-11)	98.2	(8-9-12)	178.2		
(8-10-13)	178.2	(8-11-14)	180.0	(5-15-17)	90.1	(5-15-20)	68.6		
(5-15-28)	134.5	(17-15-20)	70.7	(17-15-28)	134.6	(20-15-28)	125.7		
(5-16-17)	90.1	(5-16-18)	134.5	(5-16-20)	68.6	(17-16-18)	134.6		
(17-16-20)	70.7	(18-16-20)	125.7	(15-17-16)	91.0	(15-17-19)	134.5		
(15-17-20)	68.6	(16-17-19)	134.5	(16-17-20)	68.6	(19-17-20)	122.9		
(5-20-15)	42.0	(5-20-16)	42.0	(5-20-17)	59.8	(5-20-21)	101.1		
(5-20-23)	101.1	(5-20-25)	150.2	(15-20-16)	59.9	(15-20-17)	40.7		
(15-20-21)	92.3	(15-20-23)	143.0	(15-20-25)	115.1	(16-20-17)	40.7		
(16-20-21)	143.0	(16-20-23)	92.3	(16-20-25)	115.1	(17-20-21)	129.3		
(17-20-23)	129.3	(17-20-25)	90.4	(21-20-23)	98.9	(21-20-25)	98.2		
(23-20-25)	98.2	(20-21-22)	178.2	(20-23-24)	178.2	(20-25-26)	180.0		

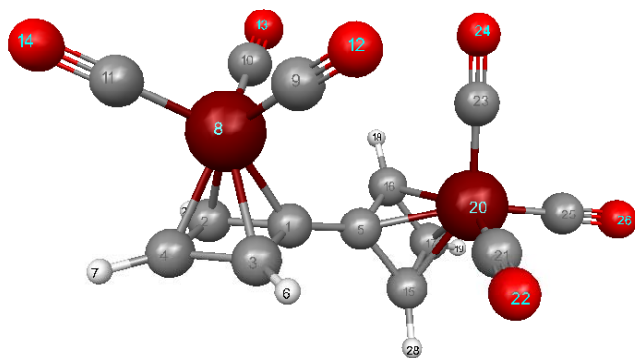
(3-1-2-4)	-0.7	(3-1-2-8)	68.5	(3-1-2-27)	-171.9
(5-1-2-4)	163.2	(5-1-2-8)	-127.6	(5-1-2-27)	-8.0
(8-1-2-4)	-69.1	(8-1-2-27)	119.6	(2-1-3-4)	0.7
(2-1-3-6)	171.9	(2-1-3-8)	-68.5	(5-1-3-4)	-163.2
(5-1-3-6)	8.0	(5-1-3-8)	127.6	(8-1-3-4)	69.1
(8-1-3-6)	-119.6	(2-1-5-15)	22.9	(2-1-5-16)	180.0
(2-1-5-20)	-78.6	(3-1-5-15)	180.0	(3-1-5-16)	-22.9
(3-1-5-20)	78.6	(8-1-5-15)	-78.6	(8-1-5-16)	78.6
(8-1-5-20)	180.0	(2-1-8-3)	96.6	(2-1-8-4)	48.3
(2-1-8-9)	177.6	(2-1-8-10)	-81.0	(2-1-8-11)	48.3
(3-1-8-2)	-96.6	(3-1-8-4)	-48.3	(3-1-8-9)	81.0
(3-1-8-10)	-177.6	(3-1-8-11)	-48.3	(5-1-8-2)	131.7
(5-1-8-3)	-131.7	(5-1-8-4)	180.0	(5-1-8-9)	-50.7
(5-1-8-10)	50.7	(5-1-8-11)	180.0	(1-2-4-3)	0.7
(1-2-4-7)	-177.1	(1-2-4-8)	67.2	(8-2-4-3)	-66.5
(8-2-4-7)	115.7	(27-2-4-3)	171.9	(27-2-4-7)	-5.9
(27-2-4-8)	-121.6	(1-2-8-3)	-50.2	(1-2-8-4)	-98.1
(1-2-8-9)	-3.9	(1-2-8-10)	104.1	(1-2-8-11)	-155.8
(4-2-8-1)	98.1	(4-2-8-3)	47.9	(4-2-8-9)	94.1
(4-2-8-10)	-157.9	(4-2-8-11)	-57.8	(27-2-8-1)	-130.3
(27-2-8-3)	179.6	(27-2-8-4)	131.7	(27-2-8-9)	-134.2
(27-2-8-10)	-26.2	(27-2-8-11)	73.9	(1-3-4-2)	-0.7
(1-3-4-7)	177.1	(1-3-4-8)	-67.2	(6-3-4-2)	-171.9
(6-3-4-7)	5.9	(6-3-4-8)	121.6	(8-3-4-2)	66.5
(8-3-4-7)	-115.7	(1-3-8-2)	50.2	(1-3-8-4)	98.1
(1-3-8-9)	-104.1	(1-3-8-10)	3.9	(1-3-8-11)	155.8
(4-3-8-1)	-98.1	(4-3-8-2)	-47.9	(4-3-8-9)	157.9
(4-3-8-10)	-94.1	(4-3-8-11)	57.8	(6-3-8-1)	130.3
(6-3-8-2)	-179.6	(6-3-8-4)	-131.7	(6-3-8-9)	26.2
(6-3-8-10)	134.2	(6-3-8-11)	-73.9	(2-4-8-1)	-50.0
(2-4-8-3)	-100.0	(2-4-8-9)	-129.1	(2-4-8-10)	29.1
(2-4-8-11)	130.0	(3-4-8-1)	50.0	(3-4-8-2)	100.0
(3-4-8-9)	-29.1	(3-4-8-10)	129.1	(3-4-8-11)	-130.0
(7-4-8-1)	180.0	(7-4-8-2)	-130.0	(7-4-8-3)	130.0
(7-4-8-9)	100.9	(7-4-8-10)	-100.9	(7-4-8-11)	0.0
(1-5-15-17)	163.2	(1-5-15-20)	-127.6	(1-5-15-28)	-8.0
(16-5-15-17)	-0.7	(16-5-15-20)	68.5	(16-5-15-28)	-171.9
(20-5-15-17)	-69.1	(20-5-15-28)	119.6	(1-5-16-17)	-163.2
(1-5-16-18)	8.0	(1-5-16-20)	127.6	(15-5-16-17)	0.7
(15-5-16-18)	171.9	(15-5-16-20)	-68.5	(20-5-16-17)	69.1
(20-5-16-18)	-119.6	(1-5-20-15)	131.7	(1-5-20-16)	-131.7
(1-5-20-17)	180.0	(1-5-20-21)	50.7	(1-5-20-23)	-50.7
(1-5-20-25)	180.0	(15-5-20-16)	96.6	(15-5-20-17)	48.3
(15-5-20-21)	-81.0	(15-5-20-23)	177.6	(15-5-20-25)	48.3
(16-5-20-15)	-96.6	(16-5-20-17)	-48.3	(16-5-20-21)	-177.6
(16-5-20-23)	81.0	(16-5-20-25)	-48.3	(1-8-9-12)	-6.0
(2-8-9-12)	-3.3	(3-8-9-12)	35.4	(4-8-9-12)	53.9
(10-8-9-12)	-109.2	(11-8-9-12)	151.2	(1-8-10-13)	6.0
(2-8-10-13)	-35.4	(3-8-10-13)	3.3	(4-8-10-13)	-53.9
(9-8-10-13)	109.2	(11-8-10-13)	-151.2	(1-8-11-14)	180.0
(2-8-11-14)	-146.5	(3-8-11-14)	146.5	(4-8-11-14)	180.0
(9-8-11-14)	50.1	(10-8-11-14)	-50.1	(5-15-17-16)	0.7
(5-15-17-19)	-177.1	(5-15-17-20)	67.2	(20-15-17-16)	-66.5
(20-15-17-19)	115.7	(28-15-17-16)	171.9	(28-15-17-19)	-5.9
(28-15-17-20)	-121.6	(5-15-20-16)	-50.2	(5-15-20-17)	-98.1
(5-15-20-21)	104.1	(5-15-20-23)	-3.9	(5-15-20-25)	-155.8
(17-15-20-5)	98.1	(17-15-20-16)	47.9	(17-15-20-21)	-157.9
(17-15-20-23)	94.1	(17-15-20-25)	-57.8	(28-15-20-5)	-130.3
(28-15-20-16)	179.6	(28-15-20-17)	131.7	(28-15-20-21)	-26.2
(28-15-20-23)	-134.2	(28-15-20-25)	73.9	(5-16-17-15)	-0.7
(5-16-17-19)	177.1	(5-16-17-20)	-67.2	(18-16-17-15)	-171.9
(18-16-17-19)	5.9	(18-16-17-20)	121.6	(20-16-17-15)	66.5

(20-16-17-19)	-115.7	(5-16-20-15)	50.2	(5-16-20-17)	98.1
(5-16-20-21)	3.9	(5-16-20-23)	-104.1	(5-16-20-25)	155.8
(17-16-20-5)	-98.1	(17-16-20-15)	-47.9	(17-16-20-21)	-94.1
(17-16-20-23)	157.9	(17-16-20-25)	57.8	(18-16-20-5)	130.3
(18-16-20-15)	-179.6	(18-16-20-17)	-131.7	(18-16-20-21)	134.2
(18-16-20-23)	26.2	(18-16-20-25)	-73.9	(15-17-20-5)	-50.0
(15-17-20-16)	-100.0	(15-17-20-21)	29.1	(15-17-20-23)	-129.1
(15-17-20-25)	130.0	(16-17-20-5)	50.0	(16-17-20-15)	100.0
(16-17-20-21)	129.1	(16-17-20-23)	-29.1	(16-17-20-25)	-130.0
(19-17-20-5)	180.0	(19-17-20-15)	-130.0	(19-17-20-16)	130.0
(19-17-20-21)	-100.9	(19-17-20-23)	100.9	(19-17-20-25)	0.0
(5-20-21-22)	6.0	(15-20-21-22)	-35.4	(16-20-21-22)	3.3
(17-20-21-22)	-53.9	(23-20-21-22)	109.2	(25-20-21-22)	-151.2
(5-20-23-24)	-6.0	(15-20-23-24)	-3.3	(16-20-23-24)	35.4
(17-20-23-24)	53.9	(21-20-23-24)	-109.2	(25-20-23-24)	151.2
(5-20-25-26)	180.0	(15-20-25-26)	-146.5	(16-20-25-26)	146.5
(17-20-25-26)	180.0	(21-20-25-26)	-50.1	(23-20-25-26)	50.1

Frequencies (cm ⁻¹):	15.6	19.8	20.7	35.7	64.7	85.9	86.6	88.1		
	91.5	105.2	110.4	132.0	134.7	146.3	150.1	160.9	335.9	348.8
	356.5	358.0	401.3	410.0	413.4	416.5	461.3	463.9	472.5	475.7
	491.6	492.5	510.0	516.8	517.5	517.8	521.4	534.8	597.3	598.3
	602.7	606.3	619.1	623.1	628.2	657.8	761.4	764.3	822.5	824.7
	838.9	839.8	940.0	945.1	972.1	986.3	989.0	1073.0	1105.4	1162.1
	1213.2	1215.9	1280.2	1338.7	1365.2	1369.9	1387.2	1582.5	2085.1	2085.3
	2085.4	2087.5	2122.7	2136.9	3266.4	3266.9	3278.5	3279.6	3291.5	3292.3

(12 *gauche*) B3LYP/6-31G(d)+LANL2DZ C₂ Geometry

Nuclear repulsion energy	2124.16113417	Hartrees
B3LYP/6-31G(d)+LANL2DZ energy	-1235.28285916	Hartrees
Zero-point energy correction	0.162864	Hartrees
Thermal correction to Enthalpy	0.185992	Hartrees
Thermal correction to Gibbs Free Energy	0.109387	Hartrees



	X	Y	Z
C1	-0.228417	0.688636	-1.293465
C2	0.228417	1.903864	-2.000986
C3	-1.525522	1.338102	-1.093042
C4	-1.062676	2.510889	-1.783199
C5	0.228417	-0.688636	-1.293465
H6	-2.472440	1.022924	-0.676354
H7	-1.514983	3.453257	-2.060632
Fe8	-0.015154	2.240618	-0.003213
C9	-0.719544	1.659538	1.529556
C10	1.705865	2.010562	0.374140
C11	-0.115453	3.993090	0.332795
O12	-1.183607	1.261949	2.505982
O13	2.826024	1.837269	0.586897
O14	-0.171618	5.126397	0.534630
C15	-0.228417	-1.903864	-2.000986
C16	1.525522	-1.338102	-1.093042
C17	1.062676	-2.510889	-1.783199
H18	2.472440	-1.022924	-0.676354
H19	1.514983	-3.453257	-2.060632
Fe20	0.015154	-2.240618	-0.003213
C21	-1.705865	-2.010562	0.374140
O22	-2.826024	-1.837269	0.586897
C23	0.719544	-1.659538	1.529556
O24	1.183607	-1.261949	2.505982

					C25	0.115453	-3.993090	0.332795	
					O26	0.171618	-5.126397	0.534630	
					H27	1.097960	2.149836	-2.594329	
					H28	-1.097960	-2.149836	-2.594329	
(1-2)	1.479	(1-3)	1.464	(1-5)	1.451	(1-8)	2.030	(2-4)	1.443
(2-8)	2.041	(2-27)	1.081	(3-4)	1.437	(3-6)	1.081	(3-8)	2.070
(4-7)	1.081	(4-8)	2.083	(5-15)	1.479	(5-16)	1.464	(5-20)	2.030
(8-9)	1.784	(8-10)	1.777	(8-11)	1.787	(9-12)	1.152	(10-13)	1.153
(11-14)	1.153	(15-17)	1.443	(15-20)	2.041	(15-28)	1.081	(16-17)	1.437
(16-18)	1.081	(16-20)	2.070	(17-19)	1.081	(17-20)	2.083	(20-21)	1.777
(20-23)	1.784	(20-25)	1.787	(21-22)	1.153	(23-24)	1.152	(25-26)	1.153
(2-1-3)	88.5	(2-1-5)	133.1	(2-1-8)	69.1	(3-1-5)	134.4		
(3-1-8)	70.5	(5-1-8)	133.8	(1-2-4)	89.8	(1-2-8)	68.3		
(1-2-27)	134.3	(4-2-8)	71.1	(4-2-27)	135.0	(8-2-27)	126.6		
(1-3-4)	90.6	(1-3-6)	134.3	(1-3-8)	67.6	(4-3-6)	134.8		
(4-3-8)	70.2	(6-3-8)	124.3	(2-4-3)	91.0	(2-4-7)	134.6		
(2-4-8)	67.9	(3-4-7)	134.4	(3-4-8)	69.3	(7-4-8)	122.9		
(1-5-15)	133.1	(1-5-16)	134.4	(1-5-20)	133.8	(15-5-16)	88.5		
(15-5-20)	69.1	(16-5-20)	70.5	(1-8-2)	42.6	(1-8-3)	41.8		
(1-8-4)	60.2	(1-8-9)	104.8	(1-8-10)	97.9	(1-8-11)	149.7		
(2-8-3)	60.0	(2-8-4)	41.0	(2-8-9)	146.6	(2-8-10)	94.1		
(2-8-11)	110.6	(3-8-4)	40.5	(3-8-9)	91.3	(3-8-10)	139.7		
(3-8-11)	119.1	(4-8-9)	125.3	(4-8-10)	133.3	(4-8-11)	90.3		
(9-8-10)	99.1	(9-8-11)	97.8	(10-8-11)	98.1	(8-9-12)	178.6		
(8-10-13)	178.0	(8-11-14)	179.1	(5-15-17)	89.8	(5-15-20)	68.3		
(5-15-28)	134.3	(17-15-20)	71.1	(17-15-28)	135.0	(20-15-28)	126.6		
(5-16-17)	90.6	(5-16-18)	134.3	(5-16-20)	67.6	(17-16-18)	134.8		
(17-16-20)	70.2	(18-16-20)	124.3	(15-17-16)	91.0	(15-17-19)	134.6		
(15-17-20)	67.9	(16-17-19)	134.4	(16-17-20)	69.3	(19-17-20)	122.9		
(5-20-15)	42.6	(5-20-16)	41.8	(5-20-17)	60.2	(5-20-21)	97.9		
(5-20-23)	104.8	(5-20-25)	149.7	(15-20-16)	60.0	(15-20-17)	41.0		
(15-20-21)	94.1	(15-20-23)	146.6	(15-20-25)	110.6	(16-20-17)	40.5		
(16-20-21)	139.7	(16-20-23)	91.3	(16-20-25)	119.1	(17-20-21)	133.3		
(17-20-23)	125.3	(17-20-25)	90.3	(21-20-23)	99.1	(21-20-25)	98.1		
(23-20-25)	97.8	(20-21-22)	178.0	(20-23-24)	178.6	(20-25-26)	179.1		
(3-1-2-4)	0.0	(3-1-2-8)		69.7	(3-1-2-27)	-169.8			
(5-1-2-4)	159.2	(5-1-2-8)		-131.2	(5-1-2-27)	-10.6			
(8-1-2-4)	-69.7	(8-1-2-27)		120.5	(2-1-3-4)	0.0			
(2-1-3-6)	175.0	(2-1-3-8)		-68.3	(5-1-3-4)	-158.7			
(5-1-3-6)	16.4	(5-1-3-8)		133.0	(8-1-3-4)	68.3			
(8-1-3-6)	-116.7	(2-1-5-15)		-98.2	(2-1-5-16)	52.0			
(2-1-5-20)	159.1	(3-1-5-15)		52.0	(3-1-5-16)	-157.9			
(3-1-5-20)	-50.8	(8-1-5-15)		159.1	(8-1-5-16)	-50.8			
(8-1-5-20)	56.3	(2-1-8-3)		96.1	(2-1-8-4)	48.5			
(2-1-8-9)	171.0	(2-1-8-10)		-87.4	(2-1-8-11)	34.0			
(3-1-8-2)	-96.1	(3-1-8-4)		-47.6	(3-1-8-9)	74.9			
(3-1-8-10)	176.5	(3-1-8-11)		-62.1	(5-1-8-2)	130.3			
(5-1-8-3)	-133.6	(5-1-8-4)		178.8	(5-1-8-9)	-58.7			
(5-1-8-10)	42.9	(5-1-8-11)		164.3	(1-2-4-3)	0.0			
(1-2-4-7)	-177.9	(1-2-4-8)		67.1	(8-2-4-3)	-67.1			
(8-2-4-7)	115.0	(27-2-4-3)		169.7	(27-2-4-7)	-8.2			
(27-2-4-8)	-123.2	(1-2-8-3)		-50.0	(1-2-8-4)	-97.6			
(1-2-8-9)	-16.0	(1-2-8-10)		97.3	(1-2-8-11)	-162.5			
(4-2-8-1)	97.6	(4-2-8-3)		47.6	(4-2-8-9)	81.7			
(4-2-8-10)	-165.1	(4-2-8-11)		-64.8	(27-2-8-1)	-129.8			
(27-2-8-3)	-179.8	(27-2-8-4)		132.5	(27-2-8-9)	-145.8			
(27-2-8-10)	-32.5	(27-2-8-11)		67.7	(1-3-4-2)	0.0			
(1-3-4-7)	177.9	(1-3-4-8)		-65.9	(6-3-4-2)	-175.0			
(6-3-4-7)	2.9	(6-3-4-8)		119.1	(8-3-4-2)	65.9			
(8-3-4-7)	-116.2	(1-3-8-2)		51.0	(1-3-8-4)	99.2			

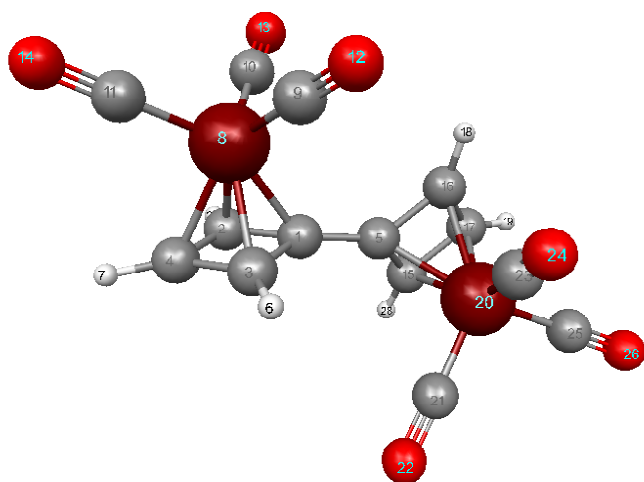
(1-3-8-9)	-111.0	(1-3-8-10)	-5.3	(1-3-8-11)	149.3
(4-3-8-1)	-99.2	(4-3-8-2)	-48.2	(4-3-8-9)	149.8
(4-3-8-10)	-104.6	(4-3-8-11)	50.1	(6-3-8-1)	129.4
(6-3-8-2)	-179.6	(6-3-8-4)	-131.4	(6-3-8-9)	18.4
(6-3-8-10)	124.0	(6-3-8-11)	-81.3	(2-4-8-1)	-50.6
(2-4-8-3)	-100.0	(2-4-8-9)	-138.1	(2-4-8-10)	20.7
(2-4-8-11)	122.1	(3-4-8-1)	49.4	(3-4-8-2)	100.0
(3-4-8-9)	-38.1	(3-4-8-10)	120.6	(3-4-8-11)	-137.9
(7-4-8-1)	179.6	(7-4-8-2)	-129.8	(7-4-8-3)	130.2
(7-4-8-9)	92.1	(7-4-8-10)	-109.1	(7-4-8-11)	-7.7
(1-5-15-17)	159.2	(1-5-15-20)	-131.2	(1-5-15-28)	-10.6
(16-5-15-17)	0.0	(16-5-15-20)	69.7	(16-5-15-28)	-169.8
(20-5-15-17)	-69.7	(20-5-15-28)	120.5	(1-5-16-17)	-158.7
(1-5-16-18)	16.4	(1-5-16-20)	133.0	(15-5-16-17)	0.0
(15-5-16-18)	175.0	(15-5-16-20)	-68.3	(20-5-16-17)	68.3
(20-5-16-18)	-116.7	(1-5-20-15)	130.3	(1-5-20-16)	-133.6
(1-5-20-17)	178.8	(1-5-20-21)	42.9	(1-5-20-23)	-58.7
(1-5-20-25)	164.3	(15-5-20-16)	96.1	(15-5-20-17)	48.5
(15-5-20-21)	-87.4	(15-5-20-23)	171.0	(15-5-20-25)	34.0
(16-5-20-15)	-96.1	(16-5-20-17)	-47.6	(16-5-20-21)	176.5
(16-5-20-23)	74.9	(16-5-20-25)	-62.1	(1-8-9-12)	-8.4
(2-8-9-12)	2.7	(3-8-9-12)	31.7	(4-8-9-12)	55.3
(10-8-9-12)	-109.1	(11-8-9-12)	151.3	(1-8-10-13)	15.7
(2-8-10-13)	-27.0	(3-8-10-13)	19.3	(4-8-10-13)	-40.4
(9-8-10-13)	122.2	(11-8-10-13)	-138.5	(1-8-11-14)	-47.1
(2-8-11-14)	-23.2	(3-8-11-14)	-89.5	(4-8-11-14)	-59.6
(9-8-11-14)	174.7	(10-8-11-14)	74.3	(5-15-17-16)	0.0
(5-15-17-19)	-177.9	(5-15-17-20)	67.1	(20-15-17-16)	-67.1
(20-15-17-19)	115.0	(28-15-17-16)	169.7	(28-15-17-19)	-8.2
(28-15-17-20)	-123.2	(5-15-20-16)	-50.0	(5-15-20-17)	-97.6
(5-15-20-21)	97.3	(5-15-20-23)	-16.0	(5-15-20-25)	-162.5
(17-15-20-5)	97.6	(17-15-20-16)	47.6	(17-15-20-21)	-165.1
(17-15-20-23)	81.7	(17-15-20-25)	-64.8	(28-15-20-5)	-129.8
(28-15-20-16)	-179.8	(28-15-20-17)	132.5	(28-15-20-21)	-32.5
(28-15-20-23)	-145.8	(28-15-20-25)	67.7	(5-16-17-15)	0.0
(5-16-17-19)	177.9	(5-16-17-20)	-65.9	(18-16-17-15)	-175.0
(18-16-17-19)	2.9	(18-16-17-20)	119.1	(20-16-17-15)	65.9
(20-16-17-19)	-116.2	(5-16-20-15)	51.0	(5-16-20-17)	99.2
(5-16-20-21)	-5.3	(5-16-20-23)	-111.0	(5-16-20-25)	149.3
(17-16-20-5)	-99.2	(17-16-20-15)	-48.2	(17-16-20-21)	-104.6
(17-16-20-23)	149.8	(17-16-20-25)	50.1	(18-16-20-5)	129.4
(18-16-20-15)	-179.6	(18-16-20-17)	-131.4	(18-16-20-21)	124.0
(18-16-20-23)	18.4	(18-16-20-25)	-81.3	(15-17-20-5)	-50.6
(15-17-20-16)	-100.0	(15-17-20-21)	20.7	(15-17-20-23)	-138.1
(15-17-20-25)	122.1	(16-17-20-5)	49.4	(16-17-20-15)	100.0
(16-17-20-21)	120.6	(16-17-20-23)	-38.1	(16-17-20-25)	-137.9
(19-17-20-5)	179.6	(19-17-20-15)	-129.8	(19-17-20-16)	130.2
(19-17-20-21)	-109.1	(19-17-20-23)	92.1	(19-17-20-25)	-7.7
(5-20-21-22)	15.7	(15-20-21-22)	-27.0	(16-20-21-22)	19.3
(17-20-21-22)	-40.4	(23-20-21-22)	122.2	(25-20-21-22)	-138.5
(5-20-23-24)	-8.4	(15-20-23-24)	2.7	(16-20-23-24)	31.7
(17-20-23-24)	55.3	(21-20-23-24)	-109.1	(25-20-23-24)	151.3
(5-20-25-26)	-47.1	(15-20-25-26)	-23.2	(16-20-25-26)	-89.5
(17-20-25-26)	-59.6	(21-20-25-26)	74.3	(23-20-25-26)	174.7

Frequencies (cm ⁻¹):	18.3	23.9	33.0	45.1	65.3	87.8	88.6	89.4		
	92.9	106.3	107.8	132.9	133.3	139.1	149.5	252.3	258.8	342.4
	358.6	368.0	384.4	410.7	417.4	445.4	452.8	468.2	475.4	475.6
	484.1	496.7	514.5	518.8	519.1	522.2	527.4	534.4	598.3	606.5
	607.1	611.4	619.6	627.9	649.5	659.4	766.3	768.8	827.6	831.4
	840.1	841.9	937.9	941.1	967.1	985.5	986.7	1071.7	1101.6	1132.9

1203.5 1205.3 1275.5 1340.4 1349.0 1367.0 1384.0 1567.2 2080.0 2081.5
 2087.7 2092.2 2122.2 2141.6 3265.6 3265.7 3279.0 3279.3 3290.8 3291.1

(12 TS) B3LYP/6-31G(d)+LANL2DZ C₁ Geometry

Nuclear repulsion energy	2086.30750923	Hartrees
B3LYP/6-31G(d)+LANL2DZ energy	-1235.28009214	Hartrees
Zero-point energy correction	0.162741	Hartrees
Thermal correction to Enthalpy	0.185028	Hartrees
Thermal correction to Gibbs Free Energy	0.109971	Hartrees



	X	Y	Z
C1	0.615936	0.358339	-0.847745
C2	1.674179	0.533933	-1.855460
C3	1.093000	1.586835	-0.192850
C4	2.123217	1.728084	-1.188628
C5	-0.615794	-0.422363	-0.827413
H6	0.721195	2.201773	0.614879
H7	2.897619	2.458137	-1.380290
Fe8	2.429107	0.039893	-0.005062
C9	1.966581	-0.272440	1.685322
C10	2.771453	-1.630907	-0.513179
C11	4.113596	0.554013	0.298210
O12	1.646131	-0.475860	2.773433
O13	2.965785	-2.713644	-0.857122
O14	5.198511	0.892212	0.489911
C15	-1.688331	-0.632607	-1.817232
C16	-1.095227	-1.611940	-0.114273
C17	-2.137214	-1.794219	-1.086782
H18	-0.733232	-2.177751	0.733304
H19	-2.915247	-2.530529	-1.234327
Fe20	-2.427729	-0.041822	-0.000495
C21	-2.582167	1.662646	-0.483611
O22	-2.651492	2.764195	-0.815351
C23	-2.087663	0.191010	1.733404
O24	-1.853315	0.343270	2.851245
C25	-4.168778	-0.414272	0.146367
O26	-5.292873	-0.655443	0.226816
H27	1.926315	0.037160	-2.782446
H28	-1.931198	-0.193143	-2.774885

(1-2)	1.472	(1-3)	1.472	(1-5)	1.458	(1-8)	2.025	(2-4)	1.440
(2-8)	2.059	(2-27)	1.082	(3-4)	1.440	(3-6)	1.081	(3-8)	2.053
(4-7)	1.081	(4-8)	2.084	(5-15)	1.475	(5-16)	1.467	(5-20)	2.028
(8-9)	1.780	(8-10)	1.780	(8-11)	1.787	(9-12)	1.152	(10-13)	1.153
(11-14)	1.152	(15-17)	1.444	(15-20)	2.048	(15-28)	1.081	(16-17)	1.437
(16-18)	1.081	(16-20)	2.062	(17-19)	1.081	(17-20)	2.082	(20-21)	1.778
(20-23)	1.782	(20-25)	1.786	(21-22)	1.153	(23-24)	1.152	(25-26)	1.152
(2-1-3)	88.4	(2-1-5)	132.9	(2-1-8)	70.1	(3-1-5)	135.6		
(3-1-8)	69.9	(5-1-8)	131.8	(1-2-4)	90.3	(1-2-8)	67.6		
(1-2-27)	134.4	(4-2-8)	70.6	(4-2-27)	134.9	(8-2-27)	125.1		
(1-3-4)	90.3	(1-3-6)	134.1	(1-3-8)	67.8	(4-3-6)	135.0		
(4-3-8)	70.8	(6-3-8)	125.7	(2-4-3)	90.9	(2-4-7)	134.5		
(2-4-8)	68.7	(3-4-7)	134.5	(3-4-8)	68.5	(7-4-8)	122.8		
(1-5-15)	132.9	(1-5-16)	135.8	(1-5-20)	131.3	(15-5-16)	88.5		
(15-5-20)	69.5	(16-5-20)	70.2	(1-8-2)	42.2	(1-8-3)	42.3		
(1-8-4)	60.3	(1-8-9)	101.0	(1-8-10)	101.6	(1-8-11)	150.4		
(2-8-3)	59.9	(2-8-4)	40.7	(2-8-9)	143.2	(2-8-10)	92.2		
(2-8-11)	115.4	(3-8-4)	40.7	(3-8-9)	92.9	(3-8-10)	143.8		

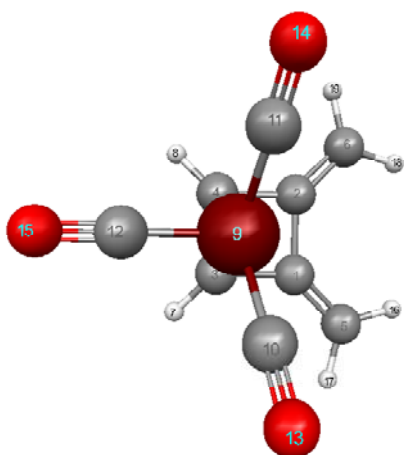
(3-8-11)	114.3	(4-8-9)	130.0	(4-8-10)	128.8	(4-8-11)	90.1
(9-8-10)	99.0	(9-8-11)	97.7	(10-8-11)	97.9	(8-9-12)	178.9
(8-10-13)	178.5	(8-11-14)	179.6	(5-15-17)	90.1	(5-15-20)	68.0
(5-15-28)	134.4	(17-15-20)	70.8	(17-15-28)	134.8	(20-15-28)	126.0
(5-16-17)	90.6	(5-16-18)	134.1	(5-16-20)	67.7	(17-16-18)	135.0
(17-16-20)	70.5	(18-16-20)	124.8	(15-17-16)	90.9	(15-17-19)	134.6
(15-17-20)	68.3	(16-17-19)	134.5	(16-17-20)	69.0	(19-17-20)	122.9
(5-20-15)	42.4	(5-20-16)	42.0	(5-20-17)	60.3	(5-20-21)	98.4
(5-20-23)	104.5	(5-20-25)	149.9	(15-20-16)	59.9	(15-20-17)	40.9
(15-20-21)	93.8	(15-20-23)	146.3	(15-20-25)	111.4	(16-20-17)	40.6
(16-20-21)	140.4	(16-20-23)	91.7	(16-20-25)	118.4	(17-20-21)	132.6
(17-20-23)	126.2	(17-20-25)	90.2	(21-20-23)	99.0	(21-20-25)	97.9
(23-20-25)	97.7	(20-21-22)	178.2	(20-23-24)	179.3	(20-25-26)	179.3
(3-1-2-4)	0.3	(3-1-2-8)	69.1	(3-1-2-27)	-173.0		
(5-1-2-4)	162.0	(5-1-2-8)	-129.1	(5-1-2-27)	-11.3		
(8-1-2-4)	-68.8	(8-1-2-27)	117.8	(2-1-3-4)	-0.3		
(2-1-3-6)	171.7	(2-1-3-8)	-69.4	(5-1-3-4)	-161.1		
(5-1-3-6)	10.9	(5-1-3-8)	129.8	(8-1-3-4)	69.1		
(8-1-3-6)	-118.9	(2-1-5-15)	-44.4	(2-1-5-16)	110.2		
(2-1-5-20)	-144.9	(3-1-5-15)	109.0	(3-1-5-16)	-96.4		
(3-1-5-20)	8.5	(8-1-5-15)	-146.4	(8-1-5-16)	8.2		
(8-1-5-20)	113.2	(2-1-8-3)	95.8	(2-1-8-4)	47.8		
(2-1-8-9)	177.9	(2-1-8-10)	-80.4	(2-1-8-11)	49.8		
(3-1-8-2)	-95.8	(3-1-8-4)	-48.0	(3-1-8-9)	82.1		
(3-1-8-10)	-176.2	(3-1-8-11)	-46.0	(5-1-8-2)	130.3		
(5-1-8-3)	-133.9	(5-1-8-4)	178.2	(5-1-8-9)	-51.7		
(5-1-8-10)	49.9	(5-1-8-11)	-179.9	(1-2-4-3)	-0.3		
(1-2-4-7)	-178.2	(1-2-4-8)	66.1	(8-2-4-3)	-66.4		
(8-2-4-7)	115.7	(27-2-4-3)	173.0	(27-2-4-7)	-5.0		
(27-2-4-8)	-120.6	(1-2-8-3)	-50.7	(1-2-8-4)	-98.7		
(1-2-8-9)	-3.4	(1-2-8-10)	104.8	(1-2-8-11)	-155.3		
(4-2-8-1)	98.7	(4-2-8-3)	48.0	(4-2-8-9)	95.3		
(4-2-8-10)	-156.4	(4-2-8-11)	-56.6	(27-2-8-1)	-129.5		
(27-2-8-3)	179.8	(27-2-8-4)	131.8	(27-2-8-9)	-132.9		
(27-2-8-10)	-24.6	(27-2-8-11)	75.2	(1-3-4-2)	0.3		
(1-3-4-7)	178.2	(1-3-4-8)	-66.3	(6-3-4-2)	-171.6		
(6-3-4-7)	6.3	(6-3-4-8)	121.8	(8-3-4-2)	66.6		
(8-3-4-7)	-115.4	(1-3-8-2)	50.6	(1-3-8-4)	98.6		
(1-3-8-9)	-103.2	(1-3-8-10)	6.3	(1-3-8-11)	157.0		
(4-3-8-1)	-98.6	(4-3-8-2)	-47.9	(4-3-8-9)	158.3		
(4-3-8-10)	-92.3	(4-3-8-11)	58.5	(6-3-8-1)	129.2		
(6-3-8-2)	179.9	(6-3-8-4)	-132.2	(6-3-8-9)	26.1		
(6-3-8-10)	135.5	(6-3-8-11)	-73.7	(2-4-8-1)	-49.9		
(2-4-8-3)	-99.9	(2-4-8-9)	-128.8	(2-4-8-10)	30.8		
(2-4-8-11)	131.0	(3-4-8-1)	50.0	(3-4-8-2)	99.9		
(3-4-8-9)	-28.9	(3-4-8-10)	130.7	(3-4-8-11)	-129.0		
(7-4-8-1)	180.0	(7-4-8-2)	-130.1	(7-4-8-3)	130.0		
(7-4-8-9)	101.1	(7-4-8-10)	-99.3	(7-4-8-11)	0.9		
(1-5-15-17)	162.8	(1-5-15-20)	-128.0	(1-5-15-28)	-8.5		
(16-5-15-17)	0.3	(16-5-15-20)	69.5	(16-5-15-28)	-171.1		
(20-5-15-17)	-69.2	(20-5-15-28)	119.4	(1-5-16-17)	-162.0		
(1-5-16-18)	12.0	(1-5-16-20)	129.5	(15-5-16-17)	-0.3		
(15-5-16-18)	173.7	(15-5-16-20)	-68.8	(20-5-16-17)	68.5		
(20-5-16-18)	-117.6	(1-5-20-15)	129.8	(1-5-20-16)	-134.3		
(1-5-20-17)	178.1	(1-5-20-21)	43.4	(1-5-20-23)	-58.2		
(1-5-20-25)	165.6	(15-5-20-16)	95.9	(15-5-20-17)	48.3		
(15-5-20-21)	-86.4	(15-5-20-23)	172.0	(15-5-20-25)	35.8		
(16-5-20-15)	-95.9	(16-5-20-17)	-47.7	(16-5-20-21)	177.6		
(16-5-20-23)	76.0	(16-5-20-25)	-60.1	(1-8-9-12)	10.7		
(2-8-9-12)	13.1	(3-8-9-12)	52.6	(4-8-9-12)	71.0		
(10-8-9-12)	-93.1	(11-8-9-12)	167.6	(1-8-10-13)	-0.2		
(2-8-10-13)	-41.8	(3-8-10-13)	-4.5	(4-8-10-13)	-61.3		

(9-8-10-13)	103.0	(11-8-10-13)	-157.8	(1-8-11-14)	3.4
(2-8-11-14)	38.0	(3-8-11-14)	-28.7	(4-8-11-14)	5.1
(9-8-11-14)	-125.4	(10-8-11-14)	134.3	(5-15-17-16)	-0.3
(5-15-17-19)	-177.9	(5-15-17-20)	66.6	(20-15-17-16)	-66.9
(20-15-17-19)	115.4	(28-15-17-16)	171.0	(28-15-17-19)	-6.6
(28-15-17-20)	-122.0	(5-15-20-16)	-50.4	(5-15-20-17)	-98.2
(5-15-20-21)	98.3	(5-15-20-23)	-14.1	(5-15-20-25)	-161.6
(17-15-20-5)	98.2	(17-15-20-16)	47.8	(17-15-20-21)	-163.5
(17-15-20-23)	84.1	(17-15-20-25)	-63.5	(28-15-20-5)	-129.8
(28-15-20-16)	179.9	(28-15-20-17)	132.1	(28-15-20-21)	-31.5
(28-15-20-23)	-143.9	(28-15-20-25)	68.6	(5-16-17-15)	0.3
(5-16-17-19)	177.9	(5-16-17-20)	-66.0	(18-16-17-15)	-173.6
(18-16-17-19)	4.1	(18-16-17-20)	120.1	(20-16-17-15)	66.3
(20-16-17-19)	-116.1	(5-16-20-15)	50.8	(5-16-20-17)	99.1
(5-16-20-21)	-3.7	(5-16-20-23)	-110.0	(5-16-20-25)	150.4
(17-16-20-5)	-99.1	(17-16-20-15)	-48.2	(17-16-20-21)	-102.8
(17-16-20-23)	150.9	(17-16-20-25)	51.3	(18-16-20-5)	129.1
(18-16-20-15)	179.9	(18-16-20-17)	-131.8	(18-16-20-21)	125.4
(18-16-20-23)	19.1	(18-16-20-25)	-80.5	(15-17-20-5)	-50.2
(15-17-20-16)	-99.8	(15-17-20-21)	22.6	(15-17-20-23)	-136.8
(15-17-20-25)	123.6	(16-17-20-5)	49.6	(16-17-20-15)	99.8
(16-17-20-21)	122.4	(16-17-20-23)	-37.0	(16-17-20-25)	-136.6
(19-17-20-5)	179.8	(19-17-20-15)	-130.0	(19-17-20-16)	130.2
(19-17-20-21)	-107.4	(19-17-20-23)	93.2	(19-17-20-25)	-6.5
(5-20-21-22)	4.7	(15-20-21-22)	-37.7	(16-20-21-22)	7.2
(17-20-21-22)	-52.3	(23-20-21-22)	111.0	(25-20-21-22)	-149.9
(5-20-23-24)	16.0	(15-20-23-24)	25.8	(16-20-23-24)	56.6
(17-20-23-24)	79.6	(21-20-23-24)	-85.2	(25-20-23-24)	175.5
(5-20-25-26)	-44.9	(15-20-25-26)	-19.8	(16-20-25-26)	-86.2
(17-20-25-26)	-55.7	(21-20-25-26)	77.4	(23-20-25-26)	177.7

Frequencies (cm ⁻¹):	-21.4	13.6	23.6	50.6	58.3	84.8	87.7	90.1		
	90.6	106.0	107.7	130.0	132.8	137.0	155.6	210.1	311.7	346.6
	358.3	368.1	378.6	411.9	415.7	421.8	457.2	472.0	472.1	479.4
	479.8	494.1	516.0	517.4	519.6	524.3	531.0	535.6	602.8	606.6
	608.5	608.9	622.2	626.2	646.1	676.3	762.8	765.8	822.2	828.7
	839.0	841.2	939.4	941.3	969.3	984.9	985.4	1082.7	1100.9	1119.6
	1202.4	1202.5	1275.4	1341.0	1350.4	1363.1	1382.9	1558.6	2080.1	2087.0
	2087.9	2095.3	2127.5	2140.8	3265.4	3265.6	3277.7	3278.3	3291.0	3291.4

3,4-dimethylenecyclobutene-Fe(CO)₃ B3LYP/6-31G(d)+LANL2DZ C_s Geometry

Nuclear repulsion energy	854.42276248	Hartrees
B3LYP/6-31G(d)+LANL2DZ energy	-695.59869412	Hartrees
Zero-point energy correction	0.122502	Hartrees
Thermal correction to Enthalpy	0.136408	Hartrees
Thermal correction to Gibbs Free Energy	0.082160	Hartrees



	X	Y	Z
C1	0.318965	1.932544	0.755138
C2	0.318965	1.932544	-0.755138
C3	1.313336	0.820771	0.729036
C4	1.313336	0.820771	-0.729036
C5	-0.319141	2.650874	1.693640
C6	-0.319141	2.650874	-1.693640
H7	2.069408	0.558433	1.459606
H8	2.069408	0.558433	-1.459606
Fe9	-0.055530	-0.460239	0.000000
C10	-0.974913	-0.986352	1.478684
C11	-0.974913	-0.986352	-1.478684
C12	1.011377	-1.839915	0.000000
O13	-1.528961	-1.320844	2.430184
O14	-1.528961	-1.320844	-2.430184
O15	1.745858	-2.729271	0.000000
H16	-1.032172	3.425187	1.424957
H17	-0.130700	2.496050	2.752200
H18	-1.032172	3.425187	-1.424957
H19	-0.130700	2.496050	-2.752200

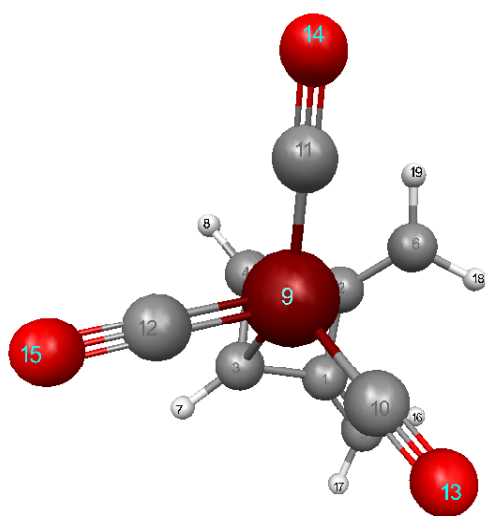
(1-2)	1.510	(1-3)	1.492	(1-5)	1.343	(1-9)	2.537	(2-4)	1.492
(2-6)	1.343	(2-9)	2.537	(3-4)	1.458	(3-7)	1.084	(3-9)	2.012
(4-8)	1.084	(4-9)	2.012	(5-16)	1.086	(5-17)	1.086	(6-18)	1.086
(6-19)	1.086	(10-13)	1.151	(11-14)	1.151	(12-15)	1.153		
(2-1-3)	89.0	(2-1-5)	134.3	(2-1-9)	72.7	(3-1-5)	136.7		
(3-1-9)	52.4	(5-1-9)	130.0	(1-2-4)	89.0	(1-2-6)	134.3		
(1-2-9)	72.7	(4-2-6)	136.7	(4-2-9)	52.4	(6-2-9)	130.0		
(1-3-4)	91.0	(1-3-7)	129.3	(1-3-9)	91.6	(4-3-7)	132.4		
(4-3-9)	68.8	(7-3-9)	124.4	(2-4-3)	91.0	(2-4-8)	129.3		
(2-4-9)	91.6	(3-4-8)	132.4	(3-4-9)	68.8	(8-4-9)	124.4		
(1-5-16)	121.3	(1-5-17)	121.5	(16-5-17)	117.2	(2-6-18)	121.3		
(2-6-19)	121.5	(18-6-19)	117.2	(1-9-2)	34.6	(1-9-3)	36.0		
(1-9-4)	53.6	(2-9-3)	53.6	(2-9-4)	36.0	(3-9-4)	42.5		
(3-1-2-4)	0.0	(3-1-2-6)	-179.8	(3-1-2-9)	50.7				
(5-1-2-4)	179.8	(5-1-2-6)	0.0	(5-1-2-9)	-129.5				
(9-1-2-4)	-50.7	(9-1-2-6)	129.5	(2-1-3-4)	0.0				
(2-1-3-7)	152.4	(2-1-3-9)	-68.8	(5-1-3-4)	-179.8				
(5-1-3-7)	-27.4	(5-1-3-9)	111.4	(9-1-3-4)	68.8				
(9-1-3-7)	-138.9	(2-1-5-16)	1.2	(2-1-5-17)	-177.6				
(3-1-5-16)	-179.1	(3-1-5-17)	2.1	(9-1-5-16)	-104.8				
(9-1-5-17)	76.4	(2-1-9-3)	102.5	(2-1-9-4)	45.5				
(3-1-9-2)	-102.5	(3-1-9-4)	-57.1	(5-1-9-2)	133.9				
(5-1-9-3)	-123.6	(5-1-9-4)	179.4	(1-2-4-3)	0.0				
(1-2-4-8)	-152.4	(1-2-4-9)	68.8	(6-2-4-3)	179.8				
(6-2-4-8)	27.4	(6-2-4-9)	-111.4	(9-2-4-3)	-68.8				
(9-2-4-8)	138.9	(1-2-6-18)	-1.2	(1-2-6-19)	177.6				
(4-2-6-18)	179.1	(4-2-6-19)	-2.1	(9-2-6-18)	104.8				
(9-2-6-19)	-76.4	(1-2-9-3)	-45.5	(1-2-9-4)	-102.5				
(4-2-9-1)	102.5	(4-2-9-3)	57.1	(6-2-9-1)	-133.9				
(6-2-9-3)	-179.4	(6-2-9-4)	123.6	(1-3-4-2)	0.0				
(1-3-4-8)	150.9	(1-3-4-9)	-91.3	(7-3-4-2)	-150.9				
(7-3-4-8)	0.0	(7-3-4-9)	117.8	(9-3-4-2)	91.3				
(9-3-4-8)	-117.8	(1-3-9-2)	43.6	(1-3-9-4)	90.5				
(4-3-9-1)	-90.5	(4-3-9-2)	-46.9	(7-3-9-1)	141.9				
(7-3-9-2)	-174.5	(7-3-9-4)	-127.6	(2-4-9-1)	-43.6				
(2-4-9-3)	-90.5	(3-4-9-1)	46.9	(3-4-9-2)	90.5				
(8-4-9-1)	174.5	(8-4-9-2)	-141.9	(8-4-9-3)	127.6				

Frequencies (cm⁻¹): -35.8 58.4 67.9 73.3 79.7 100.5 107.1 141.4
 251.9 332.6 363.4 389.7 409.2 416.3 454.1 460.1 464.4 467.7

512.5	557.8	581.7	610.7	685.8	688.5	716.5	754.9	778.2	834.9
849.7	880.6	883.3	923.4	950.6	1019.5	1165.3	1206.3	1255.5	1325.0
1452.7	1476.0	1682.8	1715.7	2082.4	2088.5	2135.8	3169.1	3169.5	3231.1
3246.7	3251.4	3252.3							

3,4-dimethylenecyclobutene-Fe(CO)₃ B3LYP/6-31G(d)+LANL2DZ C₁ Geometry

Nuclear repulsion energy	872.87482554 Hartrees
B3LYP/6-31G(d)+LANL2DZ energy	-695.60392954 Hartrees
Zero-point energy correction	0.123687 Hartrees
Thermal correction to Enthalpy	0.137929 Hartrees
Thermal correction to Gibbs Free Energy	0.083339 Hartrees



	X	Y	Z
C1	2.209707	-0.117149	-0.431242
C2	1.360672	1.122987	-0.506232
C3	1.155586	-0.743532	-1.265331
C4	0.560035	0.532421	-1.615948
C5	3.396377	-0.421281	0.099927
C6	0.993684	2.014464	0.457236
H7	1.112499	-1.715573	-1.744562
H8	0.134765	0.947021	-2.520003
Fe9	-0.411899	0.001592	0.012210
C10	-0.135242	-0.772984	1.626057
C11	-1.786459	1.154047	0.133264
C12	-1.448835	-1.276332	-0.623334
O13	0.038372	-1.246862	2.660764
O14	-2.690863	1.866348	0.209719
O15	-2.095607	-2.119491	-1.070523
H16	3.967284	0.314716	0.657708
H17	3.831598	-1.409281	-0.013153
H18	1.548725	2.069353	1.389698
H19	0.266143	2.796570	0.266781

(1-2)	1.505	(1-3)	1.483	(1-5)	1.335	(2-4)	1.490	(2-6)	1.363
(2-9)	2.161	(3-4)	1.451	(3-7)	1.085	(3-9)	2.155	(4-8)	1.082
(4-9)	1.969	(5-16)	1.086	(5-17)	1.086	(6-9)	2.495	(6-18)	1.087
(6-19)	1.085	(10-13)	1.151	(11-14)	1.154	(12-15)	1.153		
(2-1-3)	85.4	(2-1-5)	135.2	(3-1-5)	139.4	(1-2-4)		90.8	
(1-2-6)	131.0	(1-2-9)	91.3	(4-2-6)	129.9	(4-2-9)		62.1	
(6-2-9)	87.1	(1-3-4)	93.2	(1-3-7)	130.9	(1-3-9)		92.2	
(4-3-7)	131.7	(4-3-9)	62.7	(7-3-9)	122.9	(2-4-3)		87.0	
(2-4-8)	133.0	(2-4-9)	75.9	(3-4-8)	134.5	(3-4-9)		76.5	
(8-4-9)	126.9	(1-5-16)	121.2	(1-5-17)	121.5	(16-5-17)		117.4	
(2-6-9)	59.9	(2-6-18)	120.1	(2-6-19)	121.9	(9-6-18)		118.8	
(9-6-19)	99.9	(18-6-19)	117.2	(2-9-3)	56.0	(2-9-4)		42.0	
(2-9-6)	33.1	(3-9-4)	40.9	(3-9-6)	88.6	(4-9-6)		69.6	
(3-1-2-4)	-14.0	(3-1-2-6)	135.4	(3-1-2-9)		48.1			
(5-1-2-4)	162.8	(5-1-2-6)	-47.8	(5-1-2-9)		-135.1			
(2-1-3-4)	14.4	(2-1-3-7)	173.0	(2-1-3-9)		-48.3			
(5-1-3-4)	-162.1	(5-1-3-7)	-3.6	(5-1-3-9)		135.1			
(2-1-5-16)	2.1	(2-1-5-17)	-177.5	(3-1-5-16)		177.2			
(3-1-5-17)	-2.4	(1-2-4-3)	14.3	(1-2-4-8)		-141.2			
(1-2-4-9)	91.1	(6-2-4-3)	-135.6	(6-2-4-8)		68.9			
(6-2-4-9)	-58.9	(9-2-4-3)	-76.8	(9-2-4-8)		127.7			
(1-2-6-9)	-89.2	(1-2-6-18)	18.7	(1-2-6-19)		-172.0			
(4-2-6-9)	49.3	(4-2-6-18)	157.1	(4-2-6-19)		-33.5			
(9-2-6-18)	107.9	(9-2-6-19)	-82.8	(1-2-9-3)		-38.0			
(1-2-9-4)	-90.2	(1-2-9-6)	131.0	(4-2-9-3)		52.2			
(4-2-9-6)	-138.9	(6-2-9-3)	-169.0	(6-2-9-4)		138.9			
(1-3-4-2)	-14.6	(1-3-4-8)	140.3	(1-3-4-9)		-90.8			

(7-3-4-2)	-172.8	(7-3-4-8)	-18.0	(7-3-4-9)	111.0
(9-3-4-2)	76.2	(9-3-4-8)	-129.0	(1-3-9-2)	38.7
(1-3-9-4)	92.5	(1-3-9-6)	32.7	(4-3-9-2)	-53.8
(4-3-9-6)	-59.8	(7-3-9-2)	-177.7	(7-3-9-4)	-123.9
(7-3-9-6)	176.3	(2-4-9-3)	-90.3	(2-4-9-6)	22.5
(3-4-9-2)	90.3	(3-4-9-6)	112.8	(8-4-9-2)	-133.6
(8-4-9-3)	136.0	(8-4-9-6)	-111.1	(2-6-9-3)	9.1
(2-6-9-4)	-28.0	(18-6-9-2)	-110.1	(18-6-9-3)	-101.0
(18-6-9-4)	-138.1	(19-6-9-2)	121.2	(19-6-9-3)	130.3
(19-6-9-4)	93.2				

Frequencies (cm ⁻¹):	57.0	70.3	79.5	96.9	102.6	113.2	159.0	175.3		
	241.7	317.5	375.2	411.2	434.6	447.2	459.1	474.9	480.8	493.2
	530.9	562.3	596.4	632.2	697.8	719.2	753.8	767.7	779.5	805.4
	839.1	856.7	925.4	949.3	958.1	1037.3	1156.4	1190.8	1256.2	1326.6
	1447.4	1474.6	1632.6	1751.0	2076.1	2086.4	2129.4	3173.7	3176.9	3229.7
	3254.3	3263.8	3266.0							