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$Fe_3(BF)_3(CO)_8$ Structures with Face-Semibridging Fluoroborylene Ligands and a Bicapped Tetrahedral Fe_3B_3 Cluster Isoelectronic with $Os_6(CO)_{18}$

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Supporting Information

Tables S1-S3: Theoretical harmonic vibrational frequencies for $Fe_3(BF)_3(CO)_8$ (15 structures) from B3LYP/DZP.

Tables S4-S18: Theoretical Cartesian coordinates for $Fe_3(BF)_3(CO)_8$ (15 structures), using BP86/DZP method.

Table S19 Wiberg bond indices from NBO analysis for 8-1S, 9-1S and $Fe(BF)(CO)_4$.

Complete Gaussian 03 reference (reference 44**).**

Table S1. Theoretical harmonic vibrational frequencies (in cm^{-1}) for optimized structures of $Fe_3(BF)_3(CO)_8$ using the BP86/DZP method (infrared intensities in parentheses are in km/mol).

8-1S(C_s)	**8-2S(C_{2V})**	**8-3S(C_s)**	**8-4S(C_1)**	**8-5S(C_s)**
11.5(a",0.0)	22.0(b_2,0.0)	16.3(a",0.1)	9.7 (a, 0.1)	24.2*i*(a",0.0)
33.9(a",0.0)	27.0(a_2,0.0)	24.6(a",0.1)	38.7 (a, 0.1)	28.9(a',0.1)
42.6(a",0.0)	45.0(b_2,0.0)	39.9(a",0.1)	53.3 (a, 0.1)	48.0(a",0.0)
50.7(a",0.0)	56.3(b_2,0.1)	48.8(a",0.0)	54.6 (a, 0.0)	49.4(a',0.0)
56.1(a',0.2)	59.1(a_2,0.0)	55.4(a',0.2)	56.1 (a, 0.0)	54.2(a",0.0)
69.8(a",0.0)	70.5(a_1,0.0)	65.8(a',0.5)	74.6 (a, 0.0)	66.7(a",0.0)
72.7(a',0.2)	73.6($b_1$0.0)	68.6(a",0.1)	78.0 (a, 0.0)	71.4(a',0.0)
80.2(a",0.5)	82.9(a_2,0.0)	77.7(a",0.2)	79.2 (a, 0.0)	78.6(a',0.3)
83.9(a',0.1)	83.7(b_2,0.4)	84.8(a',0.0)	86.2 (a, 0.1)	83.8(a',0.1)
84.2(a",0.1)	90.3(a_1,0.0)	84.9(a',0.6)	89.7 (a, 0.1)	87.9(a",0.2)
89.4(a',0.0)	93.0(b_1,0.0)	88.2(a",0.1)	91.6 (a, 0.1)	90.8(a',0.0)
93.9(a",0.0)	93.0(a_1,0.1)	91.3(a",0.1)	92.8 (a, 0.1)	94.4(a',0.0)
95.8(a',0.0)	96.5(b_2,0.3)	92.6(a',0.4)	100.1 (a, 0.0)	95.3(a",0.2)
98.5(a',0.0)	96.5(b_1,0.1)	94.0(a',0.0)	101.2 (a, 0.0)	99.3(a",0.0)
103.9(a',0.0)	108.6(a_1,0.7)	104.2(a',0.0)	104.1 (a, 0.3)	108.9(a',0.1)
112.6(a',0.2)	111.6(b_1,1.0)	108.7(a',0.0)	105.2 (a, 0.0)	111.1(a",0.0)
115.9(a",0.0)	116.9(a_2,0.0)	117.1(a",0.1)	128.7 (a, 0.0)	144.3(a',0.1)
155.7(a',0.1)	153.9(b_2,0.1)	127.1(a',2.8)	134.1 (a, 0.3)	149.4(a",0.1)
163.4(a",0.0)	182.0(a_1,0.1)	140.8(a",0.1)	157.9 (a, 0.8)	163.8(a",0.3)
173.9(a',0.4)	192.3(b_1,0.0)	151.8(a',1.2)	185.6 (a, 0.1)	172.1(a',0.4)
207.6(a',0.2)	200.5(b_1,0.1)	168.4(a',2.1)	193.7 (a, 0.3)	211.8(a',0.2)
210.7(a',1.1)	225.5(b_1,0.1)	209.0(a',0.5)	206.4 (a, 0.2)	224.6(a",0.5)
235.9(a",0.0)	240.9(a_1,1.7)	234.3(a',1.3)	225.3 (a, 0.5)	233.1(a',0.9)
250.2(a',0.1)	247.8(a_2,0.0)	242.8(a',1.3)	235.4 (a, 0.4)	237.6(a",0.0)
262.1(a',0.2)	260.9(a_1,0.2)	245.5(a",0.1)	250.9 (a, 0.9)	262.1(a',0.7)
337.0(a',1.0)	318.5(b_1,2.3)	343.3(a',9.1)	349.8 (a, 0.9)	285.8(a",0.3)
352.2(a",0.2)	355.2(b_1,2.8)	363.0(a",0.5)	367.5 (a, 0.4)	315.9(a",0.0)
357.3(a',3.6)	361.6(b_2,0.0)	368.6(a',0.0)	373.7 (a, 0.3)	351.9(a',1.8)
375.1(a',3.2)	376.8(a_1,5.1)	380.9(a',2.6)	380.6 (a, 0.1)	365.2(a",4.0)
376.0(a",0.0)	379.7(a_2,0.0)	382.8(a",0.4)	392.5 (a, 0.4)	369.4(a',0.8)
380.7(a",0.3)	387.6(a_1,0.0)	393.9(a",1.8)	396.3 (a, 2.0)	380.7(a',0.4)
393.2(a',18.9)	397.5(b_2,0.8)	402.9(a",0.0)	407.6 (a, 4.9)	386.7(a',4.4)
397.5(a",0.1)	406.7(a_1,9.0)	404.1(a',12.2)	417.5 (a, 1.2)	393.3(a",4.2)
414.2(a",0.2)	410.1(b_2,0.5)	409.7(a",0.2)	426.7 (a, 2.2)	393.3(a',8.4)
425.4(a",0.2)	410.9(a_2,0.0)	415.4(a",0.0)	432.4 (a, 2.6)	399.7(a",14.5)
430.9(a',11.4)	417.4(b_1,4.4)	435.0(a",0.6)	433.3 (a, 0.5)	409.3(a",11.3)
444.0(a",0.9)	421.6(b_2,0.7)	442.1(a',4.5)	441.6 (a, 4.5)	421.3(a',2.9)
451.2(a',0.7)	427.3(a_1,6.3)	449.3(a",0.5)	448.6 (a, 2.3)	426.4(a',2.6)
458.5(a",0.0)	436.6(b_1,11.0)	466.4(a",0.2)	468.0 (a, 0.1)	431.9(a',0.2)
466.2(a",0.0)	442.9(b_2,0.8)	473.7(a',0.2)	478.4 (a, 2.6)	451.8(a",0.1)
469.5(a',4.3)	463.5(a_2,0.0)	480.5(a",0.2)	488.3 (a, 4.6)	464.7(a',0.9)
477.1(a",0.1)	476.2(a_2,0.0)	491.8(a',2.5)	493.4 (a, 1.0)	474.0(a",6.0)
492.4(a",1.7)	482.2(b_2,0.0)	502.5(a',8.7)	502.9 (a, 2.6)	479.0(a',6.0)
499.2(a',4.3)	489.8(a_1,102.7)	502.5(a",3.3)	511.6 (a, 2.6)	493.0(a",10.2)
507.6(a',4.2)	502.5(b_2,0.6)	513.5(a',0.1)	514.4 (a, 5.9)	503.0(a',2.9)
526.2(a',4.8)	502.5(a_2,0.0)	517.0(a",0.3)	522.2 (a, 2.2)	514.2(a",4.8)
527.6(a",0.6)	520.3(b_1,24.9)	528.4(a',6.1)	532.7 (a, 0.0)	517.6(a',0.4)
536.2(a',14.4)	525.5(a_1,41.2)	537.0(a',13.3)	544.6 (a, 9.8)	535.8(a',5.5)

567.1(a',7.8)	549.1(a_1,9.4)	552.8(a',19.4)	559.4 (a, 3.7)	561.1(a',55.4)
568.9(a",48.8)	563.0(b_2,13.7)	573.7(a",26.8)	566.9 (a, 21.0)	570.3(a",3.5)
578.3(a',46.1)	570.4(b_1,50.5)	578.4(a',48.3)	577.6 (a, 11.0)	572.4(a',37.4)
582.2(a",3.7)	575.7(a_2,0.0)	582.7(a",9.6)	587.5 (a, 20.1)	581.5(a',23.8)
599.8(a',76.8)	588.4(b_2,112.9)	596.1(a',98.1)	596.3 (a, 125.6)	591.5(a",20.3)
610.3(a',80.0)	605.5(b_1,15.1)	599.5(a",79.2)	600.5 (a, 125.0)	599.0(a',82.3)
610.9(a",71.1)	610.9(a_1,87.1)	613.1(a',41.3)	617.9 (a, 27.7)	601.4(a",39.6)
626.1(a',55.7)	625.4(a_1,121.8)	631.6(a',277.8)	631.8 (a, 73.0)	626.0(a",159.5)
644.6(a',415.3)	649.2(b_1,321.7)	634.0(a',207.1)	636.3 (a, 138.9)	633.7(a',27.6)
652.3(a',151.9)	670.3(a_1,52.3)	655.5(a',44.4)	653.5 (a, 330.5)	650.5(a',387.4)
1307.8(a",593.9)	1317.6(b_2,594.1)	1307.6(a",583.7)	1190.9 (a, 196.1)	1311.8(a',253.6)
1322.7(a',22.5)	1338.4(a_1,136.0)	1324.9(a',10.3)	1318.2 (a, 381.4)	1346.3(a",727.0)
1355.1(a',432.5)	1349.7(a_1,432.2)	1371.1(a',499.1)	1333.3 (a, 482.8)	1362.7(a',357.9)
1902.3(a',579.9)	1883.8(b_1,806.4)	1938.9(a',279.1)	1847.1 (a, 312.8)	1846.9(a',245.3)
1982.3(a",121.4)	1904.1(a_1,209.1)	1976.7(a",383.3)	1977.4 (a, 19.9)	1906.4(a',607.8)
1986.7(a",783.2)	1992.2(b_2,141.1)	1991.1(a",542.4)	1986.6 (a, 41.3)	1989.8(a",4.0)
2001.5(a',23.2)	1998.3(a_2,0.0)	1997.0(a',50.2)	1992.7 (a, 233.8)	1993.5(a',661.4)
2004.2(a",977.1)	2003.1(b_2,1680.5)	2006.1(a",934.2)	2002.3 (a, 1085.4)	2001.6(a',1061.6)
2011.9(a',1928.3)	2013.5(b_1,1958.1)	2006.8(a',1977.7)	2015.9 (a, 2000.1)	2015.8(a',1757.6)
2019.5(a',1388.6)	2021.7(a_1,1367.0)	2025.1(a',1485.1)	2024.3 (a, 1708.2)	2018.2(a",1471.5)
2057.3(a',164.4)	2054.0(a_1,8.4)	2058.6(a',176.2)	2055.3 (a, 35.0)	2051.1(a',1.8)

Table S2. Theoretical harmonic vibrational frequencies (in cm^{-1}) for optimized structures of $Fe_3(BF)_3(CO)_8$ using the BP86/DZP method (infrared intensities in parentheses are in km/mol).

8-6S(C_s)	**8-7S(C_s)**	**8-1T(C_s)**	**8-2T(C_s)**	**8-3T(C_s)**
40.5*i*(a",0.0)	3.9*i*(a",0.0)	9.0(a",0.0)	20.9(a",0.0)	7.3 (a", 0.0)
27.1(a",0.0)	15.8(a",0.0)	35.5(a",0.0)	33.3(a",0.1)	34.6 (a", 0.0)
39.4(a',0.3)	34.2(a',0.1)	43.4(a",0.0)	44.5(a",0.0)	41.8 (a", 0.0)
41.2(a",0.0)	46.1(a",0.1)	56.6(a",0.1)	50.5(a',0.0)	51.4 (a', 0.3)
60.7(a",0.1)	48.0(a",0.4)	59.5(a',0.6)	54.0(a",0.1)	52.2 (a", 0.0)
64.3(a',0.0)	60.4(a',0.0)	61.5(a',0.1)	67.4(a',0.4)	68.7 (a', 0.4)
70.7(a",0.0)	69.9(a',0.3)	69.5(a",0.0)	73.0(a",0.0)	73.5 (a", 0.0)
74.6(a',0.2)	72.4(a",0.0)	79.0(a",0.4)	77.2(a",0.2)	77.5 (a", 0.3)
81.8(a",0.0)	85.0(a',0.4)	81.4(a',0.2)	79.4(a',0.6)	79.0 (a', 0.1)
83.7(a',0.5)	91.1(a",0.1)	83.0(a",0.0)	85.2(a',0.3)	83.4 (a', 0.0)
86.8(a',0.3)	93.5(a',0.1)	83.1(a',0.2)	85.5(a",0.0)	83.4 (a", 0.2)
86.9(a",0.5)	95.1(a',0.0)	85.5(a',0.2)	88.3(a',0.0)	89.7 (a', 0.3)
95.7(a',0.2)	95.5(a",0.0)	98.6(a',0.1)	89.9(a",0.2)	91.9 (a", 0.0)
103.8(a',0.2)	101.3(a",0.1)	100.4(a",0.0)	93.1(a',0.4)	96.6 (a', 0.1)
107.3(a",0.0)	101.4(a',0.1)	101.8(a',0.3)	101.1(a',0.5)	101.5 (a', 0.2)
109.0(a',0.9)	107.5(a',0.1)	107.2(a',0.0)	109.9(a',0.3)	112.9 (a", 0.0)
112.2(a",0.0)	112.9(a",0.1)	113.3(a",0.0)	116.7(a",0.0)	119.5 (a', 0.3)
147.1(a',0.6)	117.5(a',0.0)	131.3(a',0.3)	122.2(a',1.5)	161.4 (a', 0.6)
165.9(a",0.0)	126.4(a',0.1)	161.7(a',0.0)	139.3(a",0.1)	167.8 (a", 0.1)
170.2(a',0.1)	163.3(a",0.7)	174.0(a",0.0)	141.5(a',0.6)	169.1 (a', 0.2)
189.3(a',0.0)	183.7(a',0.4)	186.6(a',0.2)	165.3(a',0.4)	200.0 (a', 4.9)
201.2(a",0.1)	200.9(a",0.5)	210.9(a',0.2)	216.4(a',0.4)	205.0 (a', 0.9)
224.1(a',0.5)	223.9(a',1.2)	222.2(a",0.0)	231.0(a',0.2)	220.9 (a", 0.0)
233.8(a',0.4)	225.7(a",0.0)	231.2(a',0.1)	238.2(a",0.0)	224.8 (a', 0.8)
261.1(a',0.3)	249.3(a',0.9)	239.3(a',0.1)	241.5(a',1.9)	251.1 (a', 0.8)
294.2(a",0.0)	349.3(a",3.1)	316.0(a',7.9)	333.3(a",1.1)	306.6 (a', 1.7)
324.3(a",0.0)	364.3(a',2.4)	325.4(a",1.0)	355.8(a',9.6)	313.2 (a", 0.1)
352.7(a',7.5)	380.9(a",1.1)	357.0(a",0.1)	367.3(a',1.4)	339.4 (a', 1.9)
358.6(a",0.0)	382.8(a',2.6)	358.3(a',3.0)	378.0(a",0.1)	353.5 (a", 0.0)
371.9(a',2.3)	395.8(a",0.1)	372.0(a',3.1)	379.5(a',1.3)	369.2 (a", 1.8)
375.5(a",1.0)	400.6(a',0.7)	377.2(a',0.2)	386.2(a",0.9)	370.9 (a', 1.2)
387.1(a',0.8)	404.7(a",1.5)	379.4(a",0.6)	387.1(a",0.4)	384.1 (a', 10.0)
389.4(a",0.0)	409.4(a',2.7)	388.0(a",0.2)	396.3(a",0.2)	389.8 (a", 0.2)
403.7(a",0.4)	420.3(a',0.5)	395.1(a",1.0)	403.2(a',5.4)	390.7 (a", 0.5)
408.9(a',0.9)	423.1(a",2.5)	411.3(a",0.3)	405.4(a",0.7)	407.2 (a', 16.7)
423.3(a",1.0)	432.8(a",0.0)	416.5(a",0.1)	417.7(a",0.1)	409.5 (a", 0.0)
439.6(a",0.0)	438.4(a',1.3)	424.5(a',0.0)	437.7(a",1.0)	412.5 (a", 0.0)
447.9(a',3.2)	457.4(a",0.3)	437.2(a",0.0)	440.7(a',0.3)	427.6 (a", 0.1)
448.4(a",1.6)	472.5(a',0.2)	442.8(a",1.3)	442.0(a",0.1)	444.1 (a', 6.7)
452.6(a',11.6)	472.7(a",0.4)	445.4(a',1.4)	463.6(a',0.3)	454.1 (a', 2.0)
463.0(a",0.5)	480.0(a",2.1)	469.1(a",0.5)	467.9(a",1.8)	458.2 (a", 0.8)
482.2(a',4.4)	483.6(a',1.0)	477.4(a',16.9)	486.6(a',6.7)	463.4 (a", 0.3)
488.3(a",2.8)	504.2(a",13.5)	480.7(a',0.2)	495.2(a',16.5)	474.7 (a', 46.9)
489.4(a',7.1)	504.2(a',8.9)	486.5(a",0.6)	496.7(a',6.6)	485.5 (a", 0.7)
513.1(a',6.8)	515.4(a',36.9)	502.0(a',33.9)	507.4(a",3.4)	495.6 (a', 5.9)

522.1(a',1.2)	524.7(a",28.0)	508.1(a',1.3)	512.5(a",0.6)	509.9 (a', 0.8)
526.5(a",0.0)	535.0(a',1.4)	519.2(a',7.4)	516.0(a',16.0)	514.8 (a', 2.8)
535.6(a',0.5)	537.0(a",49.0)	526.6(a",0.0)	523.4(a',4.7)	520.6 (a", 5.7)
554.7(a",9.8)	548.8(a',23.1)	527.7(a',4.5)	537.2(a',4.7)	526.3 (a', 18.5)
555.5(a',3.9)	562.8(a",4.7)	540.0(a",15.8)	548.5(a',62.4)	535.5 (a", 17.5)
562.4(a',46.3)	571.9(a',14.9)	555.0(a',24.2)	561.4(a",11.9)	554.8 (a', 102.2)
582.1(a",26.8)	587.7(a",6.5)	563.4(a",40.1)	566.8(a',68.4)	559.8 (a", 29.5)
586.1(a',144.6)	600.2(a',111.1)	572.6(a',121.8)	568.5(a",40.8)	572.6 (a', 66.5)
590.9(a',53.8)	603.4(a",122.4)	591.2(a',55.5)	590.5(a",58.2)	586.1 (a', 18.3)
592.3(a",74.5)	611.3(a',73.4)	599.4(a",63.7)	597.5(a',110.7)	598.9 (a", 66.9)
613.5(a',41.8)	628.9(a',141.7)	606.5(a',53.3)	599.0(a',190.4)	600.3 (a', 132.4)
621.9(a',387.6)	630.3(a',83.1)	612.0(a',96.7)	609.9(a',121.4)	622.5 (a', 59.6)
639.0(a',185.6)	640.5(a",248.8)	632.7(a',427.5)	630.0(a',175.6)	635.8 (a', 490.9)
1262.4(a",465.4)	1296.3(a',222.3)	1293.7(a",539.5)	1296.2(a",500.9)	1295.3 (a", 520.4)
1287.2(a',17.3)	1314.2(a",101.6)	1304.9(a',15.1)	1317.9(a',10.6)	1314.4 (a', 7.5)
1367.4(a',426.0)	1350.4(a',741.3)	1357.0(a',456.8)	1359.0(a',459.1)	1367.7 (a', 479.5)
1957.5(a',232.0)	1950.0(a",0.3)	1949.8(a',335.1)	1968.3(a',72.3)	1891.9 (a', 480.2)
1963.2(a",513.4)	1971.0(a",99.7)	1973.2(a",528.6)	1979.0(a",63.7)	1983.8 (a", 287.2)
1978.8(a',1.4)	1980.0(a',944.8)	1988.0(a',495.8)	1984.2(a",998.5)	1989.8 (a", 578.0)
1991.5(a",296.6)	1981.2(a",416.5)	1992.4(a",220.1)	1988.3(a',74.5)	1990.7 (a', 45.9)
1992.5(a',2023.6)	1987.5(a',17.3)	1998.7(a",1290.4)	1999.6(a',2296.8)	2001.3 (a", 1203.4)
1998.8(a",1299.8)	2009.4(a",1810.4)	2002.3(a',1813.0)	2002.6(a",968.3)	2003.2 (a', 2083.9)
2011.5(a',1415.5)	2009.9(a',2157.8)	2011.9(a',1399.5)	2012.9(a',1533.6)	2013.7 (a', 1498.8)
2049.5(a',201.1)	2047.4(a',88.7)	2053.5(a',213.0)	2054.1(a',174.0)	2052.3 (a', 77.8)

Table S3. Theoretical harmonic vibrational frequencies (in cm^{-1}) for optimized structures of $Fe_3(BF)_3(CO)_8$ using the BP86/DZP method (infrared intensities in parentheses are in km/mol).

8-4T(C_2)	**8-5T(C_{2V})**	**8-6T(C_s)**	**8-7T(D_{3h})**	**8-8T(C_1)**
103.0*i*(b,7.2)	185.3*i* (a_2, 0.0)	10.4(a",0.1)	30.9(?a,0.0)	22.0(a,0.1)
18.6(b,0.0)	15.5*i* (b_2, 0.0)	29.4(a',0.0)	30.9(?a,0.0)	28.9(a,0.0)
24.1(a,0.4)	36.4 (a_2, 0.0)	43.0(a",0.0)	50.0(?a,0.0)	33.7(a,0.0)
37.3(a,0.1)	46.6 (b_2, 0.0)	48.7(a',0.1)	50.0(?a,0.0)	41.4(a,0.0)
41.0(b,0.1)	55.9 (b_2, 0.0)	55.3(a",0.0)	51.0(?a,0.0)	56.1(a,0.1)
64.2(a,0.3)	58.6 (a_2, 0.0)	61.6(a",0.0)	51.7(?a,0.0)	64.6(a,0.0)
68.9(b,0.0)	63.7 (a_1, 0.0)	61.9(a',0.2)	69.2(e',0.2)	71.3(a,0.1)
71.7(b,0.8)	66.6 (b_1, 0.0)	73.3(a',0.3)	69.2(e',0.2)	78.9(a,0.1)
76.7(a,0.1)	77.2 (b_2, 1.3)	78.0(a',0.2)	72.2(a_2",0.4)	85.2(a,0.1)
78.6(a,0.0)	84.0 (a_1, 0.1)	90.2(a',0.1)	90.9(a_1',0.0)	90.1(a,0.2)
81.4(b,0.2)	85.0 (b_1, 0.3)	90.7(a",0.5)	93.5(?b,0.0)	90.2(a,0.3)
89.9(b,0.0)	90.6 (a_1, 0.0)	91.4(a",0.0)	94.6(?b,0.4)	92.4(a,0.3)
91.2(a,0.2)	93.3 (b_2, 0.0)	95.9(a',0.1)	94.6(?b,0.4)	98.5(a,0.2)
97.6(b,0.2)	94.2 (b_1, 0.1)	104.4(a",0.0)	113.5(e",0.0)	102.3(a,0.1)
106.8(a,0.1)	105.7 (a_2, 0.0)	111.6(a',0.0)	113.5(e",0.0)	112.1(a,0.2)
108.5(a,0.0)	107.6 (a_1, 0.2)	135.4(a",0.3)	131.9(e",0.0)	124.7(a,0.0)
109.0(b,0.3)	149.8 (b_1, 0.4)	137.5(a',0.1)	131.9(e",0.0)	125.2(a,0.3)
129.7(b,0.2)	160.2 (b_2, 0.1)	141.8(a",0.1)	135.2(e',0.1)	133.0(a,0.0)
140.9(a,0.9)	169.9 (a_1, 0.1)	169.1(a",1.4)	135.2(e',0.1)	149.2(a,0.6)
182.1(b,0.1)	179.7 (b_1, 1.4)	171.8(a',1.4)	181.1(e',1.2)	177.7(a,0.5)
195.8(a,0.7)	189.3 (a_2, 0.0)	179.3(a',0.1)	181.1(e',1.2)	186.7(a,0.5)
196.8(b,0.3)	191.6 (b_1, 3.1)	193.1(a",0.1)	221.9(e',5.4)	201.4(a,0.1)
202.4(a,0.0)	214.2 (a_1, 0.0)	226.8(a',2.1)	221.9(e',5.4)	210.9(a,0.1)
225.8(b,0.0)	225.4 (a_2, 0.0)	228.6(a",3.1)	233.3(a_2',0.0)	222.7(a,1.3)
228.2(a,0.9)	246.7 (b_1, 0.0)	258.6(a',1.2)	262.6(a_1',0.0)	225.9(a,0.0)
290.1(b,3.3)	255.6 (a_1, 0.3)	286.1(a',0.3)	297.4(e",0.0)	333.2(a,2.3)
314.1(b,4.1)	301.6 (b_2, 0.3)	300.2(a",0.1)	297.5(e",0.0)	337.4(a,1.8)
315.3(a,1.3)	316.7 (b_1, 0.6)	311.2(a",2.2)	313.7(a_2',0.0)	371.2(a,3.5)
334.1(a,1.0)	318.8 (a_1, 0.4)	345.3(a',1.3)	346.6(e',0.0)	372.9(a,2.7)
366.5(a,0.1)	323.9 (a_2, 0.0)	353.9(a",0.2)	346.6(e',0.0)	382.1(a,0.6)
370.4(b,0.0)	346.6 (b_1, 2.5)	376.4(a',1.1)	369.2(a_1',0.0)	388.4(a,1.1)
386.4(b,0.8)	369.2 (b_2, 0.8)	378.8(a',0.8)	378.4(a_2",0.2)	393.7(a,0.2)
387.2(a,0.1)	372.4 (a_1, 0.9)	381.1(a",0.4)	383.6(a_1',0.0)	397.0(a,1.7)
399.4(b,0.1)	377.9 (a_1, 8.3)	381.7(a',0.9)	392.2(e",0.0)	405.8(a,1.3)
407.5(a,0.4)	384.5 (a_1, 0.1)	392.5(a',2.6)	392.2(e",0.0)	415.7(a,1.4)
408.2(b,1.2)	385.4 (b_2, 0.0)	399.6(a',1.2)	395.3(e',0.3)	418.6(a,0.5)
419.8(a,0.0)	393.8 (b_2, 2.1)	403.6(a",0.2)	395.3(e',0.3)	429.0(a,16.5)
423.0(b,0.4)	408.1 (b_1, 6.7)	423.7(a',0.9)	431.5(?C,7.1)	447.5(a,3.9)
431.9(a,16.2)	417.6 (a_2, 0.0)	425.1(a",11.8)	443.4(?C,0.5)	453.7(a,0.1)
451.6(b,2.0)	422.8 (b_2, 10.0)	436.4(a",14.7)	446.7(?C,0.0)	457.5(a,11.6)
456.8(a,0.8)	433.8 (a_1, 7.2)	439.4(a',2.5)	446.7(?C,0.0)	465.5(a,8.4)
457.8(b,2.2)	438.3 (b_2, 4.6)	447.0(a",0.2)	448.9(?C,0.0)	474.4(a,1.8)
469.8(b,0.2)	443.2 (a_2, 0.0)	449.5(a',1.1)	454.3(?C,0.0)	486.5(a,8.4)
474.8(a,18.2)	451.5 (a_2, 0.0)	455.3(a",8.9)	454.3(?C,0.0)	498.2(a,19.3)
488.3(a,26.8)	476.1 (b_2, 5.0)	467.4(a',0.5)	487.5(e',29.7)	513.9(a,8.6)
491.2(b,59.7)	484.3 (a_1, 37.4)	489.1(a',27.1)	487.5(e',29.7)	515.3(a,0.6)

510.3(b,1.8)	508.9 (b_1, 1.4)	512.6(a",63.7)	528.3(e',117.1)	518.4(a,3.6)
511.8(a,0.1)	509.1 (b_2, 19.9)	522.7(a',43.1)	528.4(e',117.1)	526.5(a,3.3)
519.0(b,6.6)	528.1 (a_1, 1.0)	534.3(a',73.7)	532.0(a_1',0.0)	532.1(a,6.2)
525.7(a,6.2)	534.6 (b_1, 0.4)	543.1(a",1.2)	557.9(?D,0.0)	539.1(a,17.5)
546.6(b,51.5)	554.3 (a_2, 0.0)	552.7(a',38.4)	557.9(?D,0.0)	564.4(a,95.1)
560.4(a,33.4)	559.4 (b_1, 145.5)	564.0(a',59.9)	559.9(?D,118.8)	572.2(a,25.3)
579.9(a,0.7)	571.2 (a_1, 138.8)	568.5(a",49.3)	569.2(?b,76.2)	581.6(a,44.4)
589.4(b,49.1)	578.8 (b_2, 82.6)	570.3(a',57.5)	569.2(?b,76.2)	589.6(a,40.1)
594.1(b,110.1)	588.4 (a_1, 0.8)	581.8(a",13.4)	576.1(?b,0.0)	591.5(a,75.0)
599.8(a,150.3)	591.0 (b_1, 18.9)	606.3(a",175.1)	613.4(e',194.7)	601.0(a,50.1)
627.1(a,60.2)	623.7 (a_1, 90.0)	611.6(a',89.1)	613.4(e',194.6)	620.2(a,124.6)
633.2(b,482.9)	631.1 (b_1, 396.7)	625.3(a',125.3)	621.8(a_1',0.0)	635.5(a,187.9)
1302.6(b,629.1)	1325.2 (b_2, 598.0)	1331.4(a',250.7)	1362.1(e',830.1)	1157.4(a,219.1)
1311.8(a,7.1)	1333.9 (a_1, 48.5)	1354.6(a",789.7)	1362.1(e',830.1)	1321.0(a,293.9)
1362.5(a,486.5)	1354.2 (a_1, 508.8)	1374.2(a',366.5)	1393.2(a_1',0.0)	1342.3(a,601.9)
1951.7(a,6.4)	1892.2 (b_1, 812.2)	1803.3(a',245.4)	1776.4(a_2",473.3)	1969.2(a,112.1)
1957.5(b,447.1)	1907.0 (a_1, 218.9)	1906.6(a',498.7)	1796.9(a_1',0.0)	1972.3(a,22.5)
1975.9(b,501.6)	1980.6 (b_2, 717.8)	1986.9(a",40.7)	1988.8(e",0.0)	1982.8(a,309.2)
1994.2(a,246.9)	1992.9 (a_2, 0.0)	1989.1(a',47.8)	1988.8(e",0.0)	1985.4(a,550.7)
1999.6(a,2051.7)	1997.7 (b_2, 1301.0)	1994.6(a',1796.8)	1994.5(a_2",1796.2)	1996.4(a,722.0)
2000.3(b,1477.2)	2010.3 (a_1, 1880.5)	2004.7(a",1794.1)	2008.4(e',1593.6)	2008.0(a,2026.5)
2014.9(b,1518.2)	2012.0 (b_1, 1625.3)	2008.1(a',1661.9)	2008.4(e',1593.4)	2014.3(a,1796.3)
2050.7(a,20.9)	2048.0 (a_1, 1.7)	2043.5(a',6.8)	2040.2(a_1',0.0)	2056.3(a,302.0)

Table S4. Theoretical Cartesian coordinates (in Å) for the structure **8-1S** (C_s) using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.635587	-0.163713	1.272294
2	8	0	3.427778	-0.268163	2.106846
3	26	0	1.407626	0.031779	0.000000
4	5	0	-0.413049	0.090969	1.466737
5	9	0	-0.435759	0.099247	2.777282
6	5	0	-0.413049	0.090969	-1.466737
7	26	0	-0.378519	1.449128	0.000000
8	6	0	-1.214508	2.458344	-1.235908
9	8	0	-1.735931	3.137874	-2.012077
10	9	0	-0.435759	0.099247	-2.777282
11	26	0	-0.940359	-1.196044	0.000000
12	6	0	-2.656393	-0.635543	0.000000
13	8	0	-3.765787	-0.318317	0.000000
14	6	0	2.635587	-0.163713	-1.272294
15	8	0	3.427778	-0.268163	-2.106846
16	5	0	1.061078	-1.820251	0.000000
17	9	0	1.622268	-2.995010	0.000000
18	6	0	-1.113860	-2.346650	1.371575
19	8	0	-1.248857	-3.107945	2.229489
20	6	0	-1.113860	-2.346650	-1.371575
21	8	0	-1.248857	-3.107945	-2.229489
22	6	0	1.357810	2.113517	0.000000
23	8	0	2.113026	3.008550	0.000000
24	6	0	-1.214508	2.458344	1.235908
25	8	0	-1.735931	3.137874	2.012077

Table S5. Theoretical Cartesian coordinates (in Å) for the structure **8-2S** (C_{2v}) using the B3LYP/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	1.266694	0.000000	-0.644499
2	26	0	-1.266694	0.000000	-0.644499
3	26	0	0.000000	0.000000	1.473085
4	6	0	-2.354830	1.293281	-1.244051
5	6	0	0.000000	1.253145	2.744619
6	6	0	2.354830	1.293281	-1.244051
7	6	0	-2.354830	-1.293281	-1.244051
8	6	0	2.354830	-1.293281	-1.244051
9	6	0	0.000000	-1.253145	2.744619
10	8	0	-3.085066	2.087563	-1.657522
11	8	0	0.000000	2.081163	3.546824
12	8	0	3.085066	2.087563	-1.657522
13	9	0	0.000000	0.000000	-3.459266
14	8	0	-3.085066	-2.087563	-1.657522
15	8	0	3.085066	-2.087563	-1.657522
16	8	0	0.000000	-2.081163	3.546824
17	5	0	0.000000	-1.519296	-0.456340
18	5	0	0.000000	1.519296	-0.456340
19	9	0	0.000000	2.829609	-0.501897
20	9	0	0.000000	-2.829609	-0.501897
21	6	0	-1.955508	0.000000	1.223795
22	6	0	1.955508	0.000000	1.223795
23	8	0	-2.958312	0.000000	1.828332
24	8	0	2.958312	0.000000	1.828332
25	5	0	0.000000	0.000000	-2.156168

Table S6. Theoretical Cartesian coordinates (in Å) for the structure **8-3S** (C_s) using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.505262	0.300665	1.484652
2	9	0	0.512280	0.295951	2.798583
3	26	0	1.148023	-0.837324	0.000000
4	6	0	2.323215	-1.332261	-1.250488
5	8	0	3.088278	-1.706757	-2.034981
6	26	0	0.149823	1.574156	0.000000
7	6	0	-0.479173	2.586244	-1.363193
8	8	0	-0.855230	3.272702	-2.211178
9	26	0	-1.237868	-0.761078	0.000000
10	6	0	-2.143267	-1.605011	-1.283549
11	8	0	-2.691025	-2.161543	-2.132708
12	5	0	0.083186	-2.346208	0.000000
13	9	0	-0.022372	-3.646805	0.000000
14	6	0	2.323215	-1.332261	1.250488
15	8	0	3.088278	-1.706757	2.034981
16	5	0	0.505262	0.300665	-1.484652
17	9	0	0.512280	0.295951	-2.798583
18	6	0	1.804422	2.211488	0.000000
19	8	0	2.879681	2.634555	0.000000
20	6	0	-0.479173	2.586244	1.363193
21	8	0	-0.855230	3.272702	2.211178
22	6	0	-2.263376	0.750368	0.000000
23	8	0	-3.176632	1.467907	0.000000
24	6	0	-2.143267	-1.605011	1.283549
25	8	0	-2.691025	-2.161543	2.132708

Table S7. Theoretical Cartesian coordinates (in Å) for the structure **8-4S** (C_1) using the B3LYP/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.216755	-2.686242	0.595883
2	8	0	1.328308	-3.679268	1.175148
3	26	0	1.036538	-1.146267	-0.282131
4	6	0	0.030583	-1.386058	-1.760310
5	8	0	-0.798744	-1.450989	-2.590531
6	26	0	0.308497	1.441053	0.033335
7	6	0	-0.786901	2.142980	-1.220243
8	8	0	-1.449431	2.655125	-2.019156
9	26	0	-1.397517	-0.650087	-0.318064
10	6	0	-3.040658	-0.038980	-0.749125
11	8	0	-4.100914	0.329212	-1.012250
12	5	0	1.752178	0.277437	0.832645
13	9	0	2.821578	0.518370	1.557305
14	5	0	0.003399	-0.329197	1.215368
15	9	0	-0.117058	-0.551745	2.543705
16	6	0	2.720535	-1.188879	-0.916723
17	8	0	3.804145	-1.228647	-1.313716
18	5	0	-1.450450	0.855379	0.849269
19	9	0	-2.331399	1.404372	1.654730
20	6	0	1.764543	1.921541	-0.916720
21	8	0	2.685017	2.279925	-1.516635
22	6	0	0.388029	2.725530	1.263087
23	8	0	0.443218	3.553972	2.065236
24	6	0	-2.079693	-2.049034	0.536182
25	8	0	-2.511394	-2.929881	1.144166

Table S8. Theoretical Cartesian coordinates (in Å) for the structure **8-5S** (C_s) using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.240815	-1.548894	2.150622
2	8	0	2.075897	-2.040298	2.780116
3	26	0	-0.050287	-0.815208	1.173524
4	6	0	-0.332628	-2.386218	0.000000
5	8	0	-0.516742	-3.540774	0.000000
6	26	0	-0.094661	1.462037	0.000000
7	6	0	-1.634923	0.424334	0.000000
8	8	0	-2.794922	0.225727	0.000000
9	5	0	0.161676	0.997873	1.936397
10	9	0	0.416579	1.568471	3.075002
11	6	0	-1.268046	-1.174742	2.451448
12	8	0	-2.026640	-1.428645	3.282422
13	5	0	1.416873	0.182376	0.000000
14	9	0	2.729953	0.182429	0.000000
15	26	0	-0.050287	-0.815208	-1.173524
16	6	0	1.240815	-1.548894	-2.150622
17	8	0	2.075897	-2.040298	-2.780116
18	6	0	-1.268046	-1.174742	-2.451448
19	8	0	-2.026640	-1.428645	-3.282422
20	5	0	0.161676	0.997873	-1.936397
21	9	0	0.416579	1.568471	-3.075002
22	6	0	1.288266	2.591374	0.000000
23	8	0	2.132107	3.383217	0.000000
24	6	0	-1.221096	2.863498	0.000000
25	8	0	-1.914453	3.787043	0.000000

Table S9. Theoretical Cartesian coordinates (in Å) for the structure **8-6S** (C_s) using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.752487	-1.880530	1.461234
2	8	0	2.099748	-2.514854	2.363968
3	26	0	1.227418	-0.958307	0.000000
4	5	0	0.201239	0.145119	1.469853
5	9	0	0.187384	0.126255	2.793129
6	5	0	0.201239	0.145119	-1.469853
7	26	0	0.463338	1.505352	0.000000
8	6	0	0.144659	2.620919	-1.388383
9	8	0	-0.045085	3.369147	-2.246716
10	9	0	0.187384	0.126255	-2.793129
11	26	0	-1.251321	-0.402978	0.000000
12	6	0	-2.179845	1.143457	0.000000
13	8	0	-2.932566	2.024804	0.000000
14	6	0	1.752487	-1.880530	-1.461234
15	8	0	2.099748	-2.514854	-2.363968
16	5	0	-0.336473	-2.140278	0.000000
17	9	0	-0.575601	-3.416253	0.000000
18	6	0	-2.128017	-1.043238	1.425753
19	8	0	-2.740797	-1.470475	2.309435
20	6	0	-2.128017	-1.043238	-1.425753
21	8	0	-2.740797	-1.470475	-2.309435
22	6	0	2.220109	1.710744	0.000000
23	8	0	3.377464	1.768452	0.000000
24	6	0	0.144659	2.620919	1.388383
25	8	0	-0.045085	3.369147	2.246716

Table S10. Theoretical Cartesian coordinates (in Å) for the structure **8-7S** (C_s) using the B3LYP/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.510769	-0.459156	3.018218
2	8	0	-0.415930	-0.834383	4.109095
3	26	0	-0.688234	0.116185	1.348039
4	6	0	-0.197526	1.856486	1.489570
5	8	0	0.148799	2.956504	1.604047
6	26	0	-0.688234	0.116185	-1.348039
7	6	0	-0.197526	1.856486	-1.489570
8	8	0	0.148799	2.956504	-1.604047
9	26	0	1.478104	0.308613	0.000000
10	6	0	2.750286	0.273234	-1.257329
11	8	0	3.579712	0.210232	-2.059225
12	5	0	-1.240152	-1.236108	0.000000
13	9	0	-1.910324	-2.367865	0.000000
14	5	0	0.781901	-1.150747	1.126107
15	9	0	1.262891	-2.278950	1.586298
16	6	0	-2.466039	0.266251	1.570420
17	8	0	-3.607040	0.337182	1.738496
18	5	0	0.781901	-1.150747	-1.126107
19	9	0	1.262891	-2.278950	-1.586298
20	6	0	-2.466039	0.266251	-1.570420
21	8	0	-3.607040	0.337182	-1.738496
22	6	0	-0.510769	-0.459156	-3.018218
23	8	0	-0.415930	-0.834383	-4.109095
24	6	0	2.750286	0.273234	1.257329
25	8	0	3.579712	0.210232	2.059225

Table S11. Theoretical Cartesian coordinates (in Å) for the structure **8-1T** (C_s) using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.004148	-1.716642	1.419806
2	8	0	2.501256	-2.278660	2.296959
3	26	0	1.236090	-0.836175	0.000000
4	5	0	-0.075068	0.270512	1.465575
5	9	0	-0.062561	0.207541	2.779799
6	5	0	-0.075068	0.270512	-1.465575
7	26	0	0.473874	1.491473	0.000000
8	6	0	0.137294	2.701264	-1.305779
9	8	0	-0.045676	3.504579	-2.115950
10	9	0	-0.062561	0.207541	-2.779799
11	26	0	-1.344973	-0.458429	0.000000
12	6	0	-2.446664	0.966864	0.000000
13	8	0	-3.203815	1.838856	0.000000
14	6	0	2.004148	-1.716642	-1.419806
15	8	0	2.501256	-2.278660	-2.296959
16	5	0	-0.142440	-2.166237	0.000000
17	9	0	-0.372729	-3.443509	0.000000
18	6	0	-2.151559	-1.248467	1.398918
19	8	0	-2.701337	-1.765126	2.274205
20	6	0	-2.151559	-1.248467	-1.398918
21	8	0	-2.701337	-1.765126	-2.274205
22	6	0	2.253785	1.484054	0.000000
23	8	0	3.411888	1.580050	0.000000
24	6	0	0.137294	2.701264	1.305779
25	8	0	-0.045676	3.504579	2.115950

Table S12. Theoretical Cartesian coordinates (in Å) for the structure **8-2T** (C_s) using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.583088	0.317716	1.503485
2	9	0	0.514813	0.279780	2.815517
3	26	0	1.224234	-0.863982	0.000000
4	6	0	2.006394	-1.705439	-1.397174
5	8	0	2.502131	-2.276016	-2.272144
6	26	0	0.396326	1.566765	0.000000
7	6	0	-0.270210	2.568518	-1.342910
8	8	0	-0.686428	3.248535	-2.178855
9	26	0	-1.279266	-0.582259	0.000000
10	6	0	-2.120716	-1.377741	-1.411037
11	8	0	-2.663164	-1.896999	-2.288630
12	5	0	-0.134290	-2.245261	0.000000
13	9	0	-0.273592	-3.536671	0.000000
14	6	0	2.006394	-1.705439	1.397174
15	8	0	2.502131	-2.276016	2.272144
16	5	0	0.583088	0.317716	-1.503485
17	9	0	0.514813	0.279780	-2.815517
18	6	0	2.051788	2.207433	0.000000
19	8	0	3.132945	2.617962	0.000000
20	6	0	-0.270210	2.568518	1.342910
21	8	0	-0.686428	3.248535	2.178855
22	6	0	-2.391021	0.854502	0.000000
23	8	0	-3.211468	1.670230	0.000000
24	6	0	-2.120716	-1.377741	1.411037
25	8	0	-2.663164	-1.896999	2.288630

Table S13. Theoretical Cartesian coordinates (in Å) for the structure **8-3T** (C_s) using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.764289	-1.323187	0.000000
2	26	0	1.327524	0.281334	0.000000
3	26	0	-0.817730	1.311429	0.000000
4	6	0	2.500339	0.186528	1.366420
5	6	0	-1.408700	2.382836	1.373281
6	6	0	-0.749122	-2.477266	1.376195
7	6	0	2.500339	0.186528	-1.366420
8	6	0	-0.749122	-2.477266	-1.376195
9	6	0	-1.408700	2.382836	-1.373281
10	8	0	3.283930	0.136132	2.214917
11	8	0	-1.754716	3.080948	2.225018
12	8	0	-0.761272	-3.253996	2.231650
13	9	0	2.035752	-2.700708	0.000000
14	8	0	3.283930	0.136132	-2.214917
15	8	0	-0.761272	-3.253996	-2.231650
16	8	0	-1.754716	3.080948	-2.225018
17	5	0	-0.401229	0.011806	-1.493750
18	5	0	-0.401229	0.011806	1.493750
19	9	0	-0.358207	-0.009685	2.805864
20	9	0	-0.358207	-0.009685	-2.805864
21	6	0	1.233169	2.171826	0.000000
22	6	0	-2.547188	-1.065410	0.000000
23	8	0	1.662854	3.252475	0.000000
24	8	0	-3.697771	-0.961705	0.000000
25	5	0	1.304259	-1.625107	0.000000

Table S14. Theoretical Cartesian coordinates (in Å) for the structure **8-4T** (C_2) using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.295134	-0.046072	-0.598877
2	26	0	1.295134	0.046072	-0.598877
3	26	0	0.000000	0.000000	1.682430
4	6	0	2.066851	-1.356950	-1.413556
5	6	0	0.498671	-1.448213	2.758071
6	6	0	-1.998209	-1.444485	-1.462895
7	6	0	1.998209	1.444485	-1.462895
8	6	0	-2.066851	1.356950	-1.413556
9	6	0	-0.498671	1.448213	2.758071
10	8	0	2.606178	-2.224134	-1.956432
11	8	0	0.801615	-2.335370	3.427128
12	8	0	-2.486953	-2.325321	-2.031835
13	9	0	0.000000	0.000000	-3.406796
14	8	0	2.486953	2.325321	-2.031835
15	8	0	-2.606178	2.224134	-1.956432
16	8	0	-0.801615	2.335370	3.427128
17	5	0	0.000000	1.450744	0.189718
18	5	0	0.000000	-1.450744	0.189718
19	9	0	0.045610	-2.772148	0.195767
20	9	0	-0.045610	2.772148	0.195767
21	6	0	2.483473	0.078862	0.753393
22	6	0	-2.483473	-0.078862	0.753393
23	8	0	3.340728	0.111808	1.533479
24	8	0	-3.340728	-0.111808	1.533479
25	5	0	0.000000	0.000000	-2.107800

Table S15. Theoretical Cartesian coordinates (in Å) for the structure **8-5T** (C_{2v}) using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	1.285318	0.000000	-0.646432
2	26	0	-1.285318	0.000000	-0.646432
3	26	0	0.000000	0.000000	1.456533
4	6	0	-2.294565	1.307693	-1.346191
5	6	0	0.000000	1.312375	2.817559
6	6	0	2.294565	1.307693	-1.346191
7	6	0	-2.294565	-1.307693	-1.346191
8	6	0	2.294565	-1.307693	-1.346191
9	6	0	0.000000	-1.312375	2.817559
10	8	0	-2.975167	2.116539	-1.812790
11	8	0	0.000000	2.041736	3.707886
12	8	0	2.975167	2.116539	-1.812790
13	9	0	0.000000	0.000000	-3.459719
14	8	0	-2.975167	-2.116539	-1.812790
15	8	0	2.975167	-2.116539	-1.812790
16	8	0	0.000000	-2.041736	3.707886
17	5	0	0.000000	-1.507403	-0.245746
18	5	0	0.000000	1.507403	-0.245746
19	9	0	0.000000	2.816023	-0.228497
20	9	0	0.000000	-2.816023	-0.228497
21	6	0	-2.086825	0.000000	1.092419
22	6	0	2.086825	0.000000	1.092419
23	8	0	-3.040168	0.000000	1.769852
24	8	0	3.040168	0.000000	1.769852
25	5	0	0.000000	0.000000	-2.158628

Table S16 Theoretical Cartesian coordinates (in Å) for the structure **8-6T** (C_s) using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.497937	1.326701	2.132497
2	8	0	1.977955	2.184587	2.743667
3	26	0	0.766146	-0.052250	1.257428
4	6	0	2.297617	-0.476426	0.000000
5	8	0	3.433502	-0.747307	0.000000
6	26	0	-1.420901	-0.136703	0.000000
7	6	0	-0.531690	-1.745727	0.000000
8	8	0	-0.246058	-2.874187	0.000000
9	5	0	-1.021594	0.103705	1.991790
10	9	0	-1.701187	0.299728	3.081932
11	6	0	1.265591	-1.244134	2.550140
12	8	0	1.578673	-1.931733	3.422509
13	5	0	0.164650	1.417404	0.000000
14	9	0	0.034042	2.720859	0.000000
15	26	0	0.766146	-0.052250	-1.257428
16	6	0	1.497937	1.326701	-2.132497
17	8	0	1.977955	2.184587	-2.743667
18	6	0	1.265591	-1.244134	-2.550140
19	8	0	1.578673	-1.931733	-3.422509
20	5	0	-1.021594	0.103705	-1.991790
21	9	0	-1.701187	0.299728	-3.081932
22	6	0	-2.471657	1.331897	0.000000
23	8	0	-3.209481	2.219994	0.000000
24	6	0	-2.927614	-1.096467	0.000000
25	8	0	-3.910062	-1.704972	0.000000

Table S17. Theoretical Cartesian coordinates (in Å) for the structure **8-7T** (D_{3h}) using the B3LYP/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.699081	1.275756
2	8	0	0.000000	3.547043	2.060383
3	26	0	0.000000	1.433135	0.000000
4	26	0	-1.241131	-0.716567	0.000000
5	6	0	0.000000	0.000000	-1.503092
6	8	0	0.000000	0.000000	-2.683622
7	5	0	-1.992037	1.150103	0.000000
8	9	0	-3.113237	1.797428	0.000000
9	6	0	0.000000	2.699081	-1.275756
10	8	0	0.000000	3.547043	-2.060383
11	26	0	1.241131	-0.716567	0.000000
12	6	0	2.337473	-1.349541	1.275756
13	8	0	3.071829	-1.773521	2.060383
14	6	0	2.337473	-1.349541	-1.275756
15	8	0	3.071829	-1.773521	-2.060383
16	5	0	0.000000	-2.300206	0.000000
17	9	0	0.000000	-3.594857	0.000000
18	6	0	-2.337473	-1.349541	1.275756
19	8	0	-3.071829	-1.773521	2.060383
20	6	0	-2.337473	-1.349541	-1.275756
21	8	0	-3.071829	-1.773521	-2.060383
22	6	0	0.000000	0.000000	1.503092
23	8	0	0.000000	0.000000	2.683622
24	5	0	1.992037	1.150103	0.000000
25	9	0	3.113237	1.797428	0.000000

Table S18. Theoretical Cartesian coordinates (in Å) for the structure **8-8T** (C_1) using the B3LYP/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.970707	-1.030409	0.080334
2	8	0	4.114022	-1.183841	-0.015229
3	26	0	1.216890	-0.846171	0.250146
4	6	0	1.328294	-0.472221	2.028696
5	8	0	1.497250	-0.206111	3.140772
6	26	0	-1.430773	-0.485026	0.014957
7	6	0	-1.440578	-0.829429	1.810706
8	8	0	-1.573552	-1.047034	2.937534
9	26	0	0.228469	1.551771	-0.086788
10	6	0	-0.950179	2.566180	0.891537
11	8	0	-1.697910	3.217169	1.483308
12	5	0	0.051483	-0.386208	-1.390259
13	9	0	0.063925	-0.698339	-2.710791
14	5	0	1.695674	0.466095	-1.071654
15	9	0	2.615778	0.801742	-1.950197
16	6	0	0.991888	-2.635252	0.105733
17	8	0	0.880214	-3.777000	-0.021058
18	5	0	-1.360251	0.924430	-1.244447
19	9	0	-1.967945	1.604584	-2.181508
20	6	0	-1.875150	-2.049351	-0.731346
21	8	0	-2.189290	-3.034003	-1.244871
22	6	0	-3.120366	0.090814	0.054393
23	8	0	-4.221883	0.442321	0.059606
24	6	0	1.606507	2.756861	-0.061217
25	8	0	2.467858	3.524555	-0.039427

Table 19 Wiberg bond indices from NBO analysis for 8-1S, 9-1S and $Fe(BF)(CO)_4$.

		(Fe-CO)$_t$	*(Fe1-CO)$_{\mu 2}$*	*(Fe2-CO)$_{\mu 2}$*	*(Fe2-BF)$_{\mu 2}$*	*(Fe3-BF)$_{\mu 2}$*	*(Fe1-BF)$_{\mu 3}$*
8-1S	B3LYP	1.15±0.05	0.94	0.58	0.69	0.50	0.52
	BP86	1.22±0.05	0.91	0.63	0.67	0.50	0.51
9-1S	B3LYP	1.13±0.05			0.58	0.58	0.66,0.32
	BP86	1.20±0.3			0.57	0.57	0.61,0.37
$Fe(BF)(CO)_4$	B3LYP	1.24±0.05			1.13		
	BP86	1.27±0.05			1.10		
conti		*(Fe2-BF)$_{\mu 3}$*	*(Fe3-BF)$_{\mu 3}$*	(Fe1-Fe2)	(Fe1-Fe3)	(Fe2-Fe3)	
8-1S	B3LYP	0.26	0.55	0.69	0.27	0.26	
	BP86	0.26	0.54	0.67	0.27	0.27	
9-1S	B3LYP	0.51,0.39	0.51,0.39	0.34	0.34	0.30	
	BP86	0.40,0.48	0.40,0.48	0.33	0.33	0.30	

Complete Gaussian 03 reference (reference 44)

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