Coupling of Fluoroborylene Ligands in Manganese Carbonyl Chemistry to Give A Difluorodiborene Ligand

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Supporting Information

Tables S1-S4: Theoretical harmonic vibrational frequencies (in cm^{-1}) for optimized structures of $Mn_2(BF)_2(CO)_8$, $Mn_2(BF)_2(CO)_7$ and $Mn_2(BF)_2(CO)_6$ using the BP86/TZP method.

Table S5: Theoretical Cartesian coordinates for $Mn_2(BF)_2(CO)_8$ (2 structures), $Mn_2(BF)_2(CO)_7$ (5 structures) and $Mn_2(BF)_2(CO)_6$ (8 structures) at M06-L/TZP level Complete Gaussian 09 reference (Reference 44)

Table S1. Theoretical harmonic vibrational frequencies (in cm^{-1}) for optimized structures of $Mn_2(BF)_2(CO)_8$ using the BP86/TZP method (infrared intensities in parentheses are in km/mol).

8-1S (D_{2h})	8-2S(C_s)
3.3 (a_u,0.0)	17.0 (a'',0.1)
37.2 (b_{1g},0.0)	37.4 (a'',0.1)
38.8 (b_{3g},0.0)	37.7 (a',0.5)
45.3 (b_{1u},0.0)	49.2 (a',0.0)
46.5 (b_{2u},0.0)	51.1 (a'', 0.1)
56.8 (b_{3u},0.4)	60.1 (a',1.2)
81.7 (b_{2g},0.0)	76.2 (a'',0.2)
83.1 (a_g,0.0)	82.1 (a',0.0)
89.5 (b_{1u},0.8)	86.6 (a'',0.2)
93.3 (a_u,0.0)	91.6 (a'',0.3)
93.6 (b_{2u},0.8)	92.7 (a',0.8)
96.3 (b_{3g},0.0)	94.0 (a'',0.0)
104.5 (b_{3u},0.0)	99.4 (a',0.3)
111.0 (a_g,0.0)	102.2 (a',0.0)
112.7 (b_{1g},0.0)	109.4 (a'',0.1)
113.8 (b_{2g},0.0)	113.6 (a'',0.3)
118.0 (b_{1u},0.3)	115.1 (a',1.9)
209.4 (b_{3u},1.0)	196.6 (a',13.9)
212.2 (a_g,0.0)	207.2 (a',12.7)
234.6 (b_{1g},0.0)	228.1 (a',0.5)
359.5 (b_{1g},0.0)	335.1 (a',20.7)
363.8 (a_g,0.0)	360.9 (a',2.0)
371.2 (b_{2u},0.1)	367.3 (a',2.1)
379.4 (b_{3g},0.0)	379.1 (a'',0.6)
400.1 (b_{1u},0.1)	404.2 (a'',0.4)
416.2 (a_u,0.0)	409.3 (a'',0.2)
436.3 (b_{2g},0.0)	419.9 (a',3.3)
439.9 (b_{3u},1.0)	434.2 (a'',0.5)
443.9 (a_g,0.0)	438.8 (a',2.2)
450.2 (b_{2u},1.6)	446.9 (a',1.2)
468.6 (b_{1g},0.0)	468.1 (a',8.4)
469.6 (b_{1u},2.8)	474.1 (a'',3.9)
475.1 (b_{3g},0.0)	478.5 (a',22.3)
491.0 (b_{3u},28.0)	481.6 (a',0.5)
502.7 (b_{1g},0.0)	483.9 (a'',0.3)
503.7 (b_{2u},8.8)	497.0 (a',11.4)
509.8 (a_g,0.0)	502.3 (a',7.9)
520.8 (b_{3u},91.0)	507.2 (a',10.9)
531.3 (b_{2g},0.0)	513.4 (a'',0.1)
540.8 (a_g,0.0)	536.8 (a'',6.2)
555.3 (b_{3u},186.5)	538.1 (a',136.3)
556.7 (b_{1u},25.3)	554.5 (a',135.8)
570.7 (a_u,0.0)	561.1 (a'',12.6)
573.8 (b_{3g},0.0)	572.4 (a'',1.1)
636.6 (b_{2g},0.0)	624.6 (a'',15.9)
655.1 (b_{1u},216.4)	651.2 (a'',190.5)
675.6 (b_{1g},0.0)	667.9 (a',341.6)
681.6 (b_{3u},691.7)	677.4 (a',289.0)
682.0 (b_{2u},161.7)	680.1 (a',113.3)
698.0 (a_g,0.0)	689.8 (a',6.6)
1295.7 (b_{2u},662.0)	1259.9 (a',271.7)
1319.1 (a_g,0.0)	1454.5 (a',738.4)
1975.2 (b_{2g},0.0)	1863.9 (a',300.7)
1995.7 (b_{1g},0.0)	1968.5 (a'',53.7)

1997.5 (b_{3u},736.8)	1994.2 (a',813.5)
2000.6 (b_{2u},1574.9)	1997.8 (a',182.7)
2008.0 (a_g,0.0)	2001.5 (a'',2204.4)
2008.3 (b_{1u},2229.8)	2010.2 (a',441.4)
2048.4 (b_{3u},1070.1)	2036.7 (a',1126.3)
2087.7 (a_g,0.0)	2081.7 (a',145.8)

Table S2. Theoretical harmonic vibrational frequencies (in cm^{-1}) for optimized structures of Mn$_2$(BF)$_2$(CO)$_7$ using the BP86/TZP method (infrared intensities in parentheses are in km/mol).

7-1S(C_s)	7-2S(C_s)	7-3S(C_s)	7-4S(C_1)	7-1T(C_s)
17.0(a",0.0)	15.7(a",0.0)	13.3(a",0.1)	16.2(a,0.1)	22.7(a",0.0)
36.5(a',0.4)	30.5(a",0.0)	16.7(a',0.1)	27.7(a,0.1)	30.4(a",0.0)
36.5(a",0.0)	49.8(a",0.1)	41.6(a',0.0)	41.2(a,0.4)	35.5(a',1.6)
49.8(a",0.1)	68.2(a',0.5)	76.7(a",0.0)	44.8(a,0.2)	45.7(a",0.1)
58.7(a',0.0)	74.4(a',1.9)	82.7(a',0.2)	66.7(a,0.0)	55.6(a',1.3)
66.4(a",0.1)	75.3(a",0.0)	87.1(a",0.0)	75.4(a,0.1)	70.0(a",0.0)
68.7(a',1.7)	86.4(a',0.1)	89.2(a',0.2)	76.8(a,0.2)	73.9(a',0.1)
79.6(a',0.4)	88.9(a",0.4)	91.3(a',0.2)	81.1(a,0.4)	80.4(a',0.2)
86.4(a',0.0)	93.0(a",0.5)	104.2(a',0.9)	85.1(a,0.9)	81.3(a",0.5)
91.2(a",0.0)	96.0(a',0.0)	108.4(a',0.6)	89.4(a,0.5)	86.4(a',0.1)
93.6(a',0.4)	108.6(a',0.4)	115.6(a",0.0)	94.5(a,0.4)	89.2(a",0.8)
96.1(a",0.9)	114.4(a',0.1)	124.1(a",0.3)	100.1(a,0.5)	94.5(a',0.0)
105.0(a',0.0)	116.6(a",0.1)	135.9(a",0.2)	105.3(a,0.1)	102.6(a",0.0)
112.2(a",0.0)	131.8(a',1.0)	137.8(a',0.2)	113.1(a,0.1)	102.9(a',0.8)
112.4(a',0.1)	164.1(a',3.9)	209.5(a",0.0)	123.6(a,1.1)	113.0(a',3.6)
202.2(a',0.3)	199.3(a",0.3)	233.3(a",0.3)	178.1(a,13.3)	189.0(a',0.1)
213.8(a',1.2)	220.1(a',0.6)	235.9(a',3.7)	207.5(a,0.8)	212.6(a",0.0)
238.2(a",0.0)	229.7(a',1.5)	243.3(a",0.2)	228.4(a,0.0)	236.9(a',0.9)
365.1(a",0.0)	346.5(a",2.5)	364.7(a',2.5)	359.4(a,16.9)	286.5(a',1.3)
378.5(a',1.4)	363.3(a',0.4)	371.1(a",8.0)	371.0(a,3.5)	317.5(a",0.1)
383.4(a",0.0)	369.1(a",0.5)	388.1(a",0.1)	383.5(a,1.1)	373.0(a",0.0)
394.0(a",0.0)	397.4(a",0.0)	389.7(a',0.0)	393.4(a,0.8)	382.3(a",0.4)
395.0(a',0.2)	397.9(a',4.1)	393.0(a',0.0)	409.5(a,1.3)	384.6(a',2.9)
411.4(a",0.1)	403.7(a",0.2)	403.7(a',3.0)	416.4(a,7.0)	392.6(a',0.4)
441.3(a',4.1)	426.5(a',10.8)	407.0(a",0.5)	433.6(a,0.3)	415.1(a",0.1)
443.0(a",0.8)	431.7(a",0.8)	412.1(a',0.2)	441.9(a,5.4)	420.7(a",0.0)
452.1(a',3.4)	440.8(a",0.0)	444.2(a',1.9)	447.4(a,8.4)	430.2(a',3.4)
459.0(a",0.1)	444.0(a',5.5)	446.5(a",0.0)	452.8(a,0.3)	435.1(a",0.0)
472.8(a',10.1)	465.2(a",0.7)	451.2(a',0.4)	468.4(a,0.7)	441.2(a",0.3)
485.5(a',3.0)	468.4(a',12.7)	461.6(a",0.0)	474.5(a,3.3)	442.7(a',1.6)
488.1(a",0.7)	475.3(a',8.9)	488.1(a',1.9)	481.6(a,0.4)	460.3(a',16.5)
499.8(a",2.3)	498.6(a",4.8)	493.6(a",35.2)	486.9(a,4.8)	461.4(a',2.1)
512.7(a',6.2)	501.9(a',1.4)	509.3(a',6.7)	488.3(a,7.7)	474.4(a",8.7)
514.1(a',13.5)	513.9(a",4.3)	516.3(a",6.3)	500.0(a,2.7)	483.9(a',0.8)
519.6(a",13.9)	515.1(a',5.3)	521.4(a',0.4)	520.0(a,10.0)	497.2(a",1.2)
533.8(a',36.2)	531.0(a',25.8)	539.8(a',1.9)	525.9(a,16.0)	507.2(a',84.1)
550.7(a',53.4)	552.9(a",2.2)	545.5(a",0.0)	545.1(a,8.1)	523.5(a',56.8)
558.6(a",0.1)	558.8(a',8.3)	558.4(a',5.0)	551.3(a,55.7)	539.8(a',9.4)
566.9(a',14.6)	576.1(a',2.7)	569.5(a",3.7)	568.0(a,0.2)	539.8(a",2.8)
609.6(a',85.1)	605.1(a",27.7)	603.7(a",44.4)	611.4(a,41.6)	599.1(a',31.5)
637.5(a",18.4)	613.6(a',3.1)	617.2(a",0.3)	636.5(a,79.9)	600.3(a",5.5)
647.7(a',123.5)	638.6(a",79.6)	617.3(a',96.7)	640.6(a,103.2)	615.3(a',80.7)
659.3(a",83.2)	640.7(a',169.5)	643.9(a',25.8)	645.8(a,72.9)	626.4(a',455.6)
675.2(a',486.6)	670.6(a',406.5)	664.3(a",378.7)	672.7(a,366.0)	626.8(a",111.9)
685.7(a',25.1)	685.2(a',7.1)	675.7(a',86.0)	689.6(a,23.0)	657.4(a',67.6)
1312.6(a",633.2)	1304.7(a",266.3)	1285.0(a',229.7)	1279.8(a,281.2)	1362.9(a",624.4)
1330.8(a',37.5)	1327.8(a',459.9)	1327.0(a',412.5)	1450.7(a,736.0)	1371.5(a',264.1)
1957.4(a',389.1)	1900.5(a',352.3)	1829.9(a',318.3)	1882.8(a,384.7)	1906.2(a',447.9)
1974.0(a",594.1)	1984.3(a",487.0)	1982.8(a",1.1)	1965.5(a,184.1)	1973.0(a',446.8)
1990.5(a',1113.3)	1995.9(a',359.6)	1989.5(a',1502.1)	1978.7(a,1058.6)	1985.5(a',1010.1)
2000.8(a",946.0)	1997.7(a",1041.4)	2000.1(a",260.8)	1983.7(a,1123.0)	1990.7(a",178.3)
2007.8(a',1427.9)	1999.3(a',1004.4)	2008.5(a',1121.1)	1998.6(a,536.1)	1996.7(a",1304.0)
2015.2(a',743.1)	2024.7(a',2049.5)	2025.9(a",2108.7)	2018.6(a,1637.9)	2011.4(a',2073.2)
2070.7(a',178.5)	2064.6(a',72.5)	2063.8(a',86.2)	2058.2(a,138.9)	2053.6(a',31.8)

Table S3. Theoretical harmonic vibrational frequencies (in cm^{-1}) for optimized structures of Mn$_2$(BF)$_2$(CO)$_6$ using the BP86/TZP method (infrared intensities in parentheses are in km/mol).

6-1S(C_s)	6-2S(C_{2v})	6-3S(C_1)	6-4S(C_s)	6-5S(C_s)
20.0(a",0.0)	27.9(a$_2$,0.0)	26.9(a,0.1)	17.6(a",0.2)	49.2i(a",0.0)
46.2(a",0.3)	56.8(a$_1$,0.3)	48.0(a,0.3)	22.0(a",0.0)	22.7(a",0.0)
63.7(a",0.0)	59.1(b$_1$,0.0)	49.9(a,0.1)	32.9(a",0.5)	45.8(a",0.0)
72.5(a',0.2)	59.5(b$_2$,1.2)	58.6(a,0.5)	67.3(a',0.1)	57.5(a',0.7)
78.6(a',0.7)	70.6(a$_2$,0.0)	70.9(a,0.0)	73.2(a",0.2)	73.9(a",0.3)
85.8(a",0.1)	81.3(b$_1$,1.0)	79.9(a,0.6)	75.0(a',0.0)	88.1(a',0.1)
92.2(a',0.0)	81.4(a$_1$,0.0)	83.6(a,0.5)	88.2(a",0.4)	88.6(a",0.2)
94.2(a',0.0)	85.1(b$_1$,0.6)	86.8(a,0.4)	88.6(a',0.5)	94.0(a',1.2)
95.6(a",0.2)	96.4(a$_1$,1.0)	97.4(a,1.0)	98.2(a",0.1)	102.4(a",0.4)
103.1(a",0.1)	101.5(a$_1$,0.0)	99.0(a,0.4)	103.7(a',0.1)	102.7(a',0.0)
106.3(a',0.0)	106.2(b$_2$,0.5)	106.2(a,0.2)	113.2(a",0.1)	110.0(a',0.2)
128.3(a',0.5)	125.7(b$_2$,0.5)	117.9(a,0.5)	113.2(a',0.1)	117.8(a",0.1)
151.7(a',0.3)	127.7(a$_2$,0.0)	141.8(a,0.1)	143.5(a',0.1)	137.2(a',0.8)
171.4(a",0.5)	206.3(b$_2$,0.1)	212.0(a,0.1)	167.5(a',0.4)	146.9(a',0.4)
222.6(a',0.2)	241.2(a$_2$,0.0)	242.3(a,0.1)	227.2(a',1.1)	201.6(a',0.4)
264.5(a',3.1)	252.2(a$_1$,0.1)	248.4(a,0.0)	254.9(a',0.1)	241.6(a',0.3)
320.4(a",5.1)	355.8(b$_2$,0.3)	305.0(a,1.3)	383.2(a",0.0)	361.4(a",0.2)
358.6(a',10.9)	365.8(b$_1$,0.0)	381.2(a,0.9)	388.1(a',1.5)	376.2(a",1.1)
385.5(a",0.1)	375.9(a$_2$,0.0)	395.3(a,1.2)	392.5(a",0.3)	386.9(a",0.2)
408.1(a",1.7)	398.2(a$_1$,0.5)	401.0(a,0.5)	411.9(a',5.8)	397.3(a',11.3)
426.5(a",0.7)	404.3(a$_2$,0.0)	409.7(a,1.0)	412.0(a",0.1)	408.2(a',4.2)
433.6(a",0.2)	410.3(b$_1$,0.9)	413.1(a,1.7)	426.1(a",4.5)	411.6(a",0.1)
437.3(a',2.3)	424.8(a$_1$,0.0)	424.3(a,1.7)	450.4(a',3.0)	437.1(a',13.4)
451.3(a',1.9)	428.7(b$_1$,0.4)	430.3(a,2.6)	459.5(a",0.9)	452.5(a',13.2)
455.2(a",0.5)	458.0(b$_2$,17.3)	457.3(a,1.7)	462.4(a',0.4)	456.9(a',2.3)
469.5(a',8.7)	461.1(a$_2$,0.0)	461.3(a,4.0)	465.6(a",0.2)	460.3(a",0.4)
472.8(a",1.0)	462.4(b$_1$,0.9)	466.7(a,2.0)	482.3(a',3.0)	471.7(a",0.6)
483.4(a',1.4)	476.1(b$_2$,2.9)	483.8(a,12.1)	487.3(a',1.2)	475.5(a',1.4)
495.7(a",2.7)	476.8(a$_1$,0.1)	489.2(a,1.5)	499.1(a",3.6)	487.4(a',10.9)
519.6(a',3.8)	519.4(a$_2$,0.0)	496.6(a,5.5)	508.4(a',12.4)	509.5(a',2.2)
523.7(a',5.3)	520.4(b$_1$,0.0)	507.1(a,10.9)	526.3(a',0.6)	516.3(a',0.1)
538.7(a',1.2)	523.9(a$_1$,5.8)	523.7(a,9.1)	552.5(a',4.5)	525.2(a",6.1)
556.8(a",1.3)	532.0(b$_2$,26.8)	529.2(a,1.4)	563.3(a",0.1)	548.7(a",0.6)
564.7(a',7.8)	544.9(a$_1$,4.4)	544.1(a,14.0)	571.3(a',2.1)	559.7(a',5.7)
582.2(a",29.0)	612.1(a$_2$,0.0)	600.4(a,61.9)	585.8(a',19.4)	623.2(a',142.2)
600.2(a',10.3)	617.4(b$_1$,69.2)	613.5(a,27.5)	604.4(a",34.0)	628.6(a',29.9)
643.5(a',136.8)	632.0(b$_2$,166.4)	622.9(a,82.9)	645.8(a",72.5)	632.3(a",34.0)
646.1(a",66.2)	639.8(a$_1$,49.9)	634.6(a,28.5)	646.8(a',82.6)	641.1(a',47.0)
669.4(a',26.7)	652.4(b$_2$,71.7)	643.6(a,86.4)	668.2(a',67.2)	656.0(a",84.8)
691.3(a',339.4)	658.5(a$_1$,49.4)	663.7(a,60.6)	711.9(a',217.4)	683.9(a',20.7)
1339.1(a",330.9)	1367.9(b$_1$,649.2)	1323.0(a,294.1)	1224.0(a',237.7)	1360.5(a',271.3)
1364.6(a',383.1)	1369.0(a$_1$,196.2)	1461.8(a,744.3)	1483.1(a',583.3)	1445.2(a',820.9)
1828.4(a',464.9)	1973.4(a$_2$,0.0)	1889.3(a,393.4)	1814.3(a',331.4)	1939.5(a",368.4)
1976.0(a",485.4)	1974.3(b2,126.4)	1967.6(a,416.9)	1960.6(a",665.2)	1953.5(a',32.4)
1991.6(a',681.2)	1976.6(b1,1225.6)	1975.6(a,529.6)	1983.1(a",1245.8)	1972.8(a',526.0)
1993.1(a",1054.9)	1991.3(a1,1334.4)	1984.0(a,1176.9)	1988.2(a',656.4)	1982.8(a',1686.6)
2005.0(a',1741.2)	2009.0(b2,2027.7)	2003.0(a,1661.2)	1999.9(a',1371.5)	1986.4(a",1273.5)
2052.2(a',273.1)	2050.1(a1,126.6)	2046.1(a,374.6)	2046.9(a',388.7)	2046.6(a',462.7)

Table S4. Theoretical harmonic vibrational frequencies (in cm^{-1}) for optimized structures of Mn$_2$(BF)$_2$(CO)$_6$ using the BP86/TZP method (infrared intensities in parentheses are in km/mol).

6-1T(C_s）	6-2T(C_s)	6-3T(C_s)
17.3(a'',0.0)	-12.2(a'',0.0)	24.9(a'',0.0)
26.5(a',1.0)	39.1(a'',0.0)	40.9(a',0.3)
38.5(a'',0.1)	47.9(a',0.3)	46.2(a'',0.0)
60.4(a'',0.7)	68.4(a'',0.3)	54.1(a'',0.0)
68.3(a',1.2)	71.2(a',0.2)	64.8(a',2.6)
72.8(a'',0.0)	81.3(a'',1.6)	75.8(a',0.1)
78.2(a',0.1)	84.8(a',1.0)	84.4(a'',0.3)
81.7(a'',1.6)	86.1(a'',0.0)	88.2(a'',0.9)
83.4(a',0.1)	88.5(a',0.2)	88.5(a',0.1)
85.9(a',0.1)	92.6(a',0.2)	96.1(a',0.0)
98.0(a',0.7)	113.5(a',0.4)	111.9(a',0.1)
105.5(a'',0.0)	121.3(a',0.6)	117.5(a'',0.4)
111.0(a',0.1)	128.4(a'',0.0)	152.5(a',0.1)
191.5(a',0.0)	213.1(a',0.0)	221.4(a'',0.0)
236.2(a',0.3)	227.7(a',0.0)	223.8(a',0.4)
240.7(a'',0.0)	248.9(a'',0.2)	235.2(a',0.5)
327.3(a'',1.0)	339.4(a'',1.1)	328.2(a',1.8)
369.7(a'',0.1)	375.3(a',0.2)	346.3(a'',0.7)
372.4(a',2.9)	382.4(a'',0.3)	360.7(a'',0.0)
390.4(a',2.0)	389.1(a',1.4)	380.4(a'',0.5)
398.4(a'',1.0)	396.5(a'',0.0)	405.9(a'',0.1)
410.6(a',1.3)	405.7(a'',1.4)	406.1(a',1.9)
410.8(a'',0.0)	414.6(a'',0.4)	412.1(a',8.8)
420.4(a'',0.5)	421.2(a',1.4)	426.3(a'',0.0)
432.4(a',3.5)	429.4(a'',0.7)	439.2(a'',0.0)
434.5(a'',1.1)	442.3(a',3.1)	440.0(a',3.1)
443.0(a'',0.3)	448.1(a',13.6)	442.4(a'',0.3)
456.2(a',24.7)	455.2(a'',0.2)	461.2(a',1.4)
476.3(a',26.4)	464.9(a',3.9)	466.2(a',3.5)
486.5(a'',1.3)	483.5(a'',0.2)	484.9(a'',4.7)
491.9(a',11.6)	496.2(a',1.1)	486.5(a',1.4)
503.3(a'',9.2)	528.3(a',8.1)	505.3(a',2.1)
534.3(a',2.4)	529.1(a'',0.4)	522.7(a',21.9)
547.3(a',3.3)	554.1(a',4.3)	540.3(a'',0.3)
588.3(a',63.5)	588.2(a'',19.1)	540.4(a',26.3)
589.6(a'',24.0)	589.9(a',35.4)	562.3(a'',7.5)
613.0(a',5.3)	599.2(a',133.0)	598.0(a',108.7)
617.7(a',146.8)	610.6(a'',46.8)	641.8(a',103.8)
618.4(a'',37.3)	630.2(a',69.4)	647.2(a'',71.8)
653.9(a',65.3)	654.9(a',79.2)	664.8(a',329.5)
1351.4(a'',740.8)	1330.3(a'',625.8)	1331.3(a'',489.4)
1361.2(a',107.7)	1334.7(a',123.7)	1342.8(a',196.2)
1960.6(a',232.4)	1961.1(a',1.1)	1901.9(a',686.8)
1971.9(a'',495.0)	1967.9(a'',460.3)	1950.3(a'',670.8)
1975.0(a',1192.4)	1980.3(a'',992.9)	1975.7(a',1889.9)
1982.3(a'',966.5)	1980.4(a',1312.3)	1998.3(a'',859.4)
1988.8(a',2700.2)	1996.2(a',2292.6)	1999.9(a',573.4)
2040.5(a',59.3)	2039.8(a',90.9)	2051.7(a',422.0)

Table S5. Theoretical Cartesian coordinates (in Å) for the structures at M06-L/TZP level.

Structures	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
8-1S(D_{2h})	25	-1.363099000	0.000000000	0.000000000
	25	1.363099000	0.000000000	0.000000000
	6	-1.436924000	0.000000000	1.838654000
	6	-2.493478000	1.417274000	0.000000000
	6	-1.436924000	0.000000000	-1.838654000
	6	1.436924000	0.000000000	1.838654000
	6	2.493478000	-1.417274000	0.000000000
	5	0.000000000	1.524072000	0.000000000
	6	1.436924000	0.000000000	-1.838654000
	6	2.493478000	1.417274000	0.000000000
	8	1.548301000	0.000000000	2.976410000
	8	3.192711000	-2.325748000	0.000000000
	8	-1.548301000	0.000000000	2.976410000
	8	-1.548301000	0.000000000	-2.976410000
	8	-3.192711000	2.325748000	0.000000000
	8	1.548301000	0.000000000	-2.976410000
	9	0.000000000	2.819944000	0.000000000
	8	3.192711000	2.325748000	0.000000000
	6	-2.493478000	-1.417274000	0.000000000
	8	-3.192711000	-2.325748000	0.000000000
	5	0.000000000	-1.524072000	0.000000000
	9	0.000000000	-2.819944000	0.000000000
8-2S(C_s)	25	0.412458000	1.265414000	0.000000000
	25	-0.251144000	-1.366687000	0.000000000
	6	0.419130000	1.460963000	1.826803000
	6	1.918828000	2.292116000	0.000000000
	6	0.419130000	1.460963000	-1.826803000
	6	-0.281373000	-1.384395000	1.843397000
	6	-1.899465000	-2.087239000	0.000000000
	6	1.599623000	-0.428856000	0.000000000
	6	-0.281373000	-1.384395000	-1.843397000
	6	0.699244000	-2.928012000	0.000000000
	8	-0.328852000	-1.430259000	2.984726000
	8	-2.958016000	-2.529913000	0.000000000
	8	0.419130000	1.690247000	2.949123000
	8	0.419130000	1.690247000	-2.949123000
	8	2.833265000	2.980256000	0.000000000
	8	-0.328852000	-1.430259000	-2.984726000
	8	2.730021000	-0.701935000	0.000000000
	8	1.283154000	-3.911301000	0.000000000
	5	-0.896567000	2.499842000	0.000000000
	9	-1.827729000	3.367037000	0.000000000
	5	-1.398804000	0.350730000	0.000000000
	9	-2.691193000	0.568013000	0.000000000

7-1S(C_s)	25	0.124289000	-1.246695000	0.000000000
	25	0.202242000	1.281008000	0.000000000
	5	-0.182719000	0.056980000	1.533129000
	6	1.877695000	-0.723921000	0.000000000
	5	-0.182719000	0.056980000	-1.533129000
	6	0.578774000	2.353502000	1.415541000
	6	0.578774000	2.353502000	-1.415541000
	6	-1.481841000	1.780677000	0.000000000
	6	0.348578000	-2.357745000	1.427882000
	6	-1.700876000	-1.509894000	0.000000000
	6	0.348578000	-2.357745000	-1.427882000
	8	2.955402000	-0.326890000	0.000000000
	9	-0.524007000	0.036186000	-2.782364000
	9	-0.524007000	0.036186000	2.782364000
	8	-2.599512000	2.055945000	0.000000000
	8	0.753646000	3.035227000	-2.323658000
	8	0.474346000	-3.043271000	-2.337365000
	8	-2.837133000	-1.626618000	0.000000000
	8	0.753646000	3.035227000	2.323658000
	8	0.474346000	-3.043271000	2.337365000
7-2S(C_s)	25	0.129129000	1.259184000	0.000000000
	25	0.172838000	-1.236871000	0.000000000
	6	1.836348000	-0.368075000	0.000000000
	5	-1.097894000	0.085117000	0.953897000
	5	-1.097894000	0.085117000	-0.953897000
	6	0.757971000	-2.276182000	1.383336000
	6	-1.407391000	-2.131266000	0.000000000
	6	0.757971000	-2.276182000	-1.383336000
	6	1.755272000	2.167496000	0.000000000
	6	-0.586420000	2.317138000	-1.255927000
	6	-0.586420000	2.317138000	1.255927000
	9	-2.142227000	0.032616000	1.727223000
	9	-2.142227000	0.032616000	-1.727223000
	8	2.991623000	-0.288689000	0.000000000
	8	1.105654000	-2.905044000	-2.272830000
	8	-2.393118000	-2.718249000	0.000000000
	8	-1.071962000	2.963461000	2.070483000
	8	-1.071962000	2.963461000	-2.070483000
	8	1.105654000	-2.905044000	2.272830000
	8	2.687346000	2.828043000	0.000000000

7-3S(C_s)	25	0.134082000	-0.083528000	1.240525000
	25	0.134082000	-0.083528000	-1.240525000
	6	1.728269000	-0.072481000	0.000000000
	5	-1.222873000	-0.864781000	0.000000000
	5	-1.034921000	0.973484000	0.000000000
	6	1.520700000	-0.549259000	-2.364517000
	6	-1.036022000	-0.988391000	-2.265833000
	6	-0.100459000	1.468733000	-2.119276000
	6	1.520700000	-0.549259000	2.364517000
	6	-0.100459000	1.468733000	2.119276000
	6	-1.036022000	-0.988391000	2.265833000
	9	-2.372866000	-1.494753000	0.000000000
	9	-1.890834000	1.950453000	0.000000000
	8	2.897523000	-0.052502000	0.000000000
	8	-0.283254000	2.473695000	-2.641645000
	8	-1.766865000	-1.585311000	-2.917573000
	8	-1.766865000	-1.585311000	2.917573000
	8	-0.283254000	2.473695000	2.641645000
	8	2.349977000	-0.812540000	-3.103122000
	8	2.349977000	-0.812540000	3.103122000
7-4S(C_1)	25	-1.256577000	-0.051855000	-0.075803000
	25	1.208787000	-0.163354000	0.007207000
	6	0.623048000	-0.163619000	1.737097000
	6	1.892295000	-1.860380000	0.296712000
	6	2.569864000	0.045886000	-1.169790000
	6	-0.522435000	-1.635445000	-0.764084000
	6	-2.351135000	0.018664000	-1.482748000
	6	-1.915220000	1.551437000	0.441133000
	8	2.400568000	-2.864370000	0.505012000
	8	3.480974000	0.203715000	-1.853233000
	8	0.423047000	-0.141441000	2.871786000
	8	-2.385608000	2.560948000	0.727642000
	8	-0.440116000	-2.660781000	-1.287282000
	8	-3.022043000	0.078215000	-2.411237000
	6	-2.408478000	-1.017616000	0.965410000
	8	-3.130634000	-1.599098000	1.636305000
	5	0.124620000	1.406083000	-0.499955000
	5	2.005510000	1.337401000	0.554158000
	9	0.133038000	2.640413000	-0.937209000
	9	2.601068000	2.405333000	0.913828000

7-1T(*C*ₛ)	25	0.198315000	-1.204247000	0.000000000
	25	0.144835000	1.231189000	0.000000000
	5	-0.887355000	0.064901000	1.210107000
	6	1.849746000	-0.265448000	0.000000000
	5	-0.887355000	0.064901000	-1.210107000
	6	0.831940000	2.253454000	1.406477000
	6	0.831940000	2.253454000	-1.406477000
	6	-1.454173000	2.046707000	0.000000000
	6	0.761856000	-2.237116000	1.412113000
	6	-1.419243000	-2.031861000	0.000000000
	6	0.761856000	-2.237116000	-1.412113000
	8	2.977237000	-0.022183000	0.000000000
	9	-1.845325000	-0.000758000	-2.070291000
	9	-1.845325000	-0.000758000	2.070291000
	8	-2.494147000	2.542422000	0.000000000
	8	1.181301000	2.894325000	-2.286310000
	8	1.081169000	-2.878372000	-2.304580000
	8	-2.442143000	-2.552314000	0.000000000
	8	1.181301000	2.894325000	2.286310000
	8	1.081169000	-2.878372000	2.304580000
6-1S(*C*ₛ)	25	-0.230131000	-1.136836000	0.000000000
	25	-0.435456000	1.263939000	0.000000000
	5	0.909530000	0.415542000	0.972858000
	5	0.909530000	0.415542000	-0.972858000
	9	1.950624000	0.439255000	1.745152000
	9	1.950624000	0.439255000	-1.745152000
	6	1.462737000	-1.801493000	0.000000000
	6	-0.667312000	-2.249325000	1.372232000
	6	-1.802587000	-0.173499000	0.000000000
	6	-0.667312000	-2.249325000	-1.372232000
	6	-0.177820000	2.545299000	-1.250241000
	6	-0.177820000	2.545299000	1.250241000
	8	0.064533000	3.316750000	2.065107000
	8	0.064533000	3.316750000	-2.065107000
	8	-0.935217000	-2.922092000	2.258264000
	8	-0.935217000	-2.922092000	-2.258264000
	8	2.523915000	-2.238329000	0.000000000
	8	-2.705817000	0.581346000	0.000000000
6-2S(*C*₂ᵥ)	25	0.000000000	1.136984000	0.050072000
	25	0.000000000	-1.136984000	0.050072000
	6	1.231092000	-2.339836000	-0.510742000
	6	-1.231092000	-2.339836000	-0.510742000
	6	-1.231092000	2.339836000	-0.510742000
	6	1.231092000	2.339836000	-0.510742000
	5	1.455449000	0.000000000	-0.690069000
	6	0.000000000	-1.604859000	1.815401000
	5	-1.455449000	0.000000000	-0.690069000
	6	0.000000000	1.604859000	1.815401000
	9	-2.583702000	0.000000000	-1.309784000
	8	2.008552000	3.094587000	-0.890336000
	8	-2.008552000	3.094587000	-0.890336000
	8	0.000000000	1.848667000	2.933558000
	8	0.000000000	-1.848667000	2.933558000
	8	2.008552000	-3.094587000	-0.890336000
	9	2.583702000	0.000000000	-1.309784000
	8	-2.008552000	-3.094587000	-0.890336000

6-3S(C_1)	25	-1.110659000	-0.193727000	0.082532000
	25	1.161790000	-0.062966000	-0.043320000
	5	-0.296156000	1.425861000	-0.457993000
	6	2.129994000	1.372323000	-0.486653000
	6	-1.156615000	-0.236674000	1.903654000
	6	-2.649376000	-1.055020000	-0.294020000
	6	-0.150819000	-1.522154000	-0.880294000
	6	1.916652000	-0.198086000	1.586316000
	6	2.465260000	-1.030264000	-0.854631000
	5	-2.338842000	1.038851000	-0.369598000
	8	3.277411000	-1.627905000	-1.397361000
	8	-3.643934000	-1.577447000	-0.554341000
	8	-1.188895000	-0.208410000	3.048782000
	9	-3.251276000	1.857771000	-0.718725000
	8	2.358585000	-0.258881000	2.642369000
	9	-0.262358000	2.668337000	-0.839211000
	8	-0.030056000	-2.453315000	-1.556556000
	8	2.750494000	2.298215000	-0.766287000
6-4S(C_s)	25	0.111587000	-1.317880000	0.000000000
	25	0.384155000	1.161918000	0.000000000
	6	0.682068000	2.237478000	1.408078000
	5	-1.099698000	2.136750000	0.000000000
	6	0.682068000	2.237478000	-1.408078000
	6	0.546856000	-2.384060000	-1.393850000
	6	0.546856000	-2.384060000	1.393850000
	6	-1.533277000	-2.070895000	0.000000000
	5	-1.293116000	0.121425000	0.000000000
	6	1.668529000	-0.418080000	0.000000000
	8	-2.555005000	-2.595214000	0.000000000
	9	-2.063089000	2.965066000	0.000000000
	8	0.815707000	2.921421000	2.322459000
	8	0.815707000	2.921421000	-2.322459000
	8	0.815707000	-3.025351000	2.304882000
	8	0.815707000	-3.025351000	-2.304882000
	9	-2.616243000	0.246221000	0.000000000
	8	2.557917000	0.353001000	0.000000000
6-5S(C_s)	25	-1.133432000	-0.223068000	0.000038000
	25	1.140288000	-0.042110000	-0.000023000
	5	-0.463936000	1.512617000	-0.000187000
	6	2.048972000	1.488117000	-0.000116000
	6	-0.513809000	-0.945606000	1.566516000
	6	-2.758338000	-1.008556000	-0.000022000
	6	-0.513592000	-0.946136000	-1.566133000
	6	2.246570000	-0.671602000	1.266394000
	6	2.246684000	-0.671740000	-1.266273000
	5	-2.442347000	1.010969000	-0.000126000
	8	2.923593000	-1.063299000	-2.103556000
	8	-3.811506000	-1.482436000	-0.000066000
	8	-0.321521000	-1.389595000	2.612928000
	9	-3.414908000	1.840906000	-0.000249000
	8	2.923400000	-1.063071000	2.103784000
	9	-0.403228000	2.806108000	-0.000337000
	8	-0.321298000	-1.390512000	-2.612383000
	8	2.630373000	2.479106000	-0.000172000

6-1T(C_s)	25	0.116376000	1.260807000	0.000000000
	25	-0.021412000	-1.050411000	0.000000000
	5	0.610554000	0.053075000	1.547435000
	5	0.610554000	0.053075000	-1.547435000
	6	-0.793374000	-2.021618000	-1.342956000
	6	1.475017000	-2.016080000	0.000000000
	6	-0.793374000	-2.021618000	1.342956000
	6	0.206519000	2.461544000	-1.393417000
	6	-1.663877000	0.924379000	0.000000000
	6	0.206519000	2.461544000	1.393417000
	9	1.018884000	0.027391000	2.767283000
	9	1.018884000	0.027391000	-2.767283000
	8	-1.262505000	-2.630450000	-2.193467000
	8	0.267071000	3.188413000	-2.278369000
	8	-1.262505000	-2.630450000	2.193467000
	8	2.473867000	-2.584297000	0.000000000
	8	-2.813517000	0.841795000	0.000000000
	8	0.267071000	3.188413000	2.278369000
6-2T(C_s)	25	0.096030000	-1.298999000	0.000000000
	25	-0.001736000	1.058168000	0.000000000
	5	0.639419000	-0.129170000	-1.509399000
	5	0.639419000	-0.129170000	1.509399000
	6	-1.566604000	1.988479000	0.000000000
	6	0.688109000	2.108324000	1.282379000
	6	0.688109000	2.108324000	-1.282379000
	6	0.202630000	-2.472754000	1.421957000
	6	-1.682566000	-0.941652000	0.000000000
	6	0.202630000	-2.472754000	-1.421957000
	9	1.124784000	-0.125925000	-2.709884000
	9	1.124784000	-0.125925000	2.709884000
	8	-2.567901000	2.543153000	0.000000000
	8	0.283994000	-3.175526000	2.323001000
	8	1.152723000	2.807850000	-2.068701000
	8	1.152723000	2.807850000	2.068701000
	8	-2.829470000	-0.848884000	0.000000000
	8	0.283994000	-3.175526000	-2.323001000
6-3T(C_s)	25	-0.214055000	-1.121693000	0.000000000
	25	-0.611211000	1.352516000	0.000000000
	5	0.700494000	0.373637000	1.062059000
	5	0.700494000	0.373637000	-1.062059000
	9	1.721804000	0.447670000	1.865902000
	9	1.721804000	0.447670000	-1.865902000
	6	1.504972000	-1.744341000	0.000000000
	6	-0.550931000	-2.125695000	1.498294000
	6	-1.859339000	-0.343260000	0.000000000
	6	-0.550931000	-2.125695000	-1.498294000
	6	-0.060146000	2.414263000	-1.385436000
	6	-0.060146000	2.414263000	1.385436000
	8	0.349583000	3.094922000	2.217950000
	8	0.349583000	3.094922000	-2.217950000
	8	-0.728744000	-2.732539000	2.453126000
	8	-0.728744000	-2.732539000	-2.453126000
	8	2.585914000	-2.120978000	0.000000000
	8	-2.815917000	0.333434000	0.000000000

Complete Gaussian 09 reference (Reference 45)

Gaussian 09, Revision B.01,

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and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

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