Supplementary Material (ESI) for Dalton Transactions

Supplementary File

for

Dimerization of a Fluorocarbyne Complex to a Tetrahedrane Derivative: Fluorocarbyne and Difluoroacetylene Cobalt Carbonyl Complexes

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Tables S1-S19: Theoretical harmonic vibrational frequencies for the structures of $Co_2(CF)_2(CO)_n$ (n = 6, 5, 4, 3, 2) and $Co(CF)(CO)_m$ (m = 3, 2, 1) using the BP86 and B3LYP method.

Tables S20-S60: Theoretical Cartesian coordinates for the structures of $Co_2(CF)_2(CO)_n$ (n = 6, 5, 4, 3, 2) and $Co(CF)(CO)_m$ (m = 3, 2, 1) using the BP86/DZP method.

Table S61-S62: Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), and numbers of imaginary vibrational frequencies (NImag) for more $Co_2(CF)_2(CO)_n$ (n = 6, 4) structures with higher energies.

Figure S1-S2: More optimized structures of $Co_2(CF)_2(CO)_n$ (n = 6, 4) with relative high energies.

Complete Gaussian 03 reference (Reference 44).

Table S1. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Co(CF)(CO)_m$ (m = 3, 2, 1). The corresponging IR intensities (in km/mol) are listed in parentheses for Tables S1-S19.

13S-1(C_{3v})		**12S-1(C_s)**		**11S-1(C_s)**	
B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
45.9(0.0)	44.3(0.1)	57.6(0.1)	58.0(0.0)	78.4(0.8)	80.6(1.0)
45.9(0.0)	44.3(0.1)	61.9(0.6)	66.0(0.7)	266.8(6.9)	266.3(3.8)
76.6(0.0)	74.5(0.0)	72.7(0.2)	75.0(0.3)	294.7(3.9)	293.1(3.6)
76.6(0.0)	74.5(0.0)	266.5(4.7)	268.6(4.0)	387.6(9.3)	390.6(10.0)
87.7(0.0)	84.7(0.0)	284.1(1.4)	273.9(0.6)	524.2(30.7)	539.9(11.4)
288.6(0.6)	283.6(0.1)	313.4(1.0)	316.6(1.8)	545.0(7.7)	551.3(11.6)
288.6(0.6)	283.6(0.1)	443.1(8.0)	469.2(1.0)	696.8(16.2)	682.8(11.2)
331.2(0.0)	331.3(0.0)	483.7(42.8)	505.6(19.2)	1395(693)	1352(606)
404.6(6.8)	421.3(2.2)	488.1(7.5)	511.7(19.8)	2077(847)	1981(648)
465.1(11.1)	481.3(1.7)	510.6(27.5)	517.3(6.7)		
465.1(11.1)	481.3(1.7)	579.9(40.5)	561.6(43.9)		
489.4(57.4)	484.6(49.3)	657(18.2)	643.9(18.1)		
512.2(22.7)	519.2(16.1)	1398(822)	1353(719)		
512.2(22.8)	519.2(16.1)	2068(1313)	1974(1112)		
601.8(62.2)	593.3(76.2)	2124(436)	2028(352)		
601.8(62.2)	593.4(76.2)				
611.9(0.3)	598.2(0.0)				
1452(919)	1418(826)				
2096(971)	2007(868)				
2096(971)	2007(868)				
2149(286)	2061(220)				

Table S2. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the triplet structures of $Co(CF)(CO)_m$ (m = 2, 1).

12T-1(C_s/C_{2v})		**11T-1**(C_s)	
B3LYP	BP86	B3LYP	BP86
34(0.4)	41.2 (0.2)	47.0 (0.5)	55.4 (0.9)
53.8 (1.8)	68.6 (0.0)	188.3(1.8)	196.1(0.0)
70.2 (0.2)	69.3 (0.0)	269.4(6.9)	273.2(5.8)
233.6 (1.8)	251.8(0.5)	317.6(1.5)	322.8(0.2)
268.1 (0.8)	295.0(0.1)	431.7(42.9)	487.3(16.5)
288.9 (0.2)	299.5(0.0)	456.0(10.8)	497.3(8.8)
312.3 (8.5)	416.3(9.5)	507.8(1.2)	566.8(2.1)
372.2(65.4)	471.1(19.2)	1395.1(699.6)	1371.2(628.3)
390.7(13.9)	484.6(22.9)	2086.8(1087.4)	1982.6(793.5)
467.0(7.0)	507.5(12.1)		
498.9(11.3)	529.5(1.5)		
519.7(8.8)	555.9(41.3)		
1413.3(824.9)	1392.4(720.7)		
2075.7(1086.3)	1982.6(1085.8)		
2125.3(660.5)	2031.6(416.1)		

Table S3. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Co_2(CF)_2(CO)_6$.

26S-1(C_{2v})		**26S-2(C_1)**	
B3LYP	BP86	B3LYP	BP86
22.6(0.0)	17.2(0.0)	27.8(0.4)	22.5(0.7)
47.7(0.1)	40.9(0.0)	44.5(0.0)	40.4(0.1)
63.5(0.0)	61.3(0.0)	46.7(0.2)	44.8(0.1)
63.8(0.0)	61.9(0.0)	61.0(0.2)	64.5(0.0)
67.1(0.0)	64.5(0.0)	65.6(0.2)	66.2(0.2)
76.1(0.0)	71.9(0.0)	82.6(0.2)	77.4(0.1)
76.6(0.1)	73.2(0.0)	85.7(0.2)	82.3(0.0)
84.0(0.0)	80.0(0.0)	86.1(0.7)	85.9(0.2)
85.8(0.0)	82.7(0.0)	90.0(0.1)	88.4(0.0)
87.3(0.2)	84.3(0.1)	93.7(0.3)	90.0(0.1)
92.3(0.0)	89.3(0.0)	98.6(0.1)	96.5(0.2)
96.9(0.0)	94.7(0.0)	119.9(0.6)	115.1(0.8)
181.9(4.3)	177.3(0.0)	185.5(0.9)	186.4(0.3)
184.5(0.0)	178.4(2.2)	222.4(7.7)	217.5(1.2)
213.9(0.6)	209.6(0.8)	231.7(1.0)	221.6(2.4)
219.8(3.0)	214.7(1.6)	245.6(4.9)	237.8(2.5)
295.3(5.3)	289.6(2.3)	272.1(2.9)	276.1(0.5)
352.6(0.0)	352.1(0.0)	295.7(5.7)	310.5(0.1)
359.5(0.0)	357.5(0.0)	345.3(33.7)	344.2(21.1)
379.9(6.1)	385.2(3.6)	360.6(1.9)	356.4(14.9)
381.2(15.5)	392.8(3.5)	376.0(16.3)	378.6(1.8)
405.4(0.0)	404.9(0.0)	384.3(6.6)	386.3(2.2)
427.7(1.5)	436.7(0.1)	396.9(25.7)	415.5(5.0)
430.2(2.7)	436.9(0.1)	404.6(4.3)	421.8(8.6)
433.6(11.5)	442.7(1.7)	427.5(24.2)	429.3(4.4)
444.6(4.0)	460.6(6.1)	435.0(4.8)	444.8(9.5)
463.1(3.8)	472.9(0.4)	442.9(4.3)	448.8(3.5)
468.0(0.0)	473.7(0.0)	451.8(15.6)	463.3(5.0)
477.4(3.1)	482.3(4.9)	454.2(4.2)	476.5(13.4)
488.6(9.5)	490.4(3.1)	479.9(9.6)	491.3(5.9)
492.8(0.0)	493.5(0.0)	494.9(32.1)	496.6(24.9)
497.4(33.9)	504.9(75.6)	516.0(20.4)	527.4(14.8)
524.6(153.8)	529.2(71.6)	532.9(4.7)	542.2(15.2)
525.0(63.7)	530.4(76.1)	545.8(14.7)	549.3(34.5)
527.3(73.4)	537.7(62.7)	551.0(93.3)	554.6(106.1)
543.6(6.1)	545.2(5.3)	554.5(44.0)	559.0(44.7)
567.5(0.0)	556.5(0.0)	573.0(37.5)	577.1(5.5)
637.1(308.6)	626.5(271.1)	583.2(53.5)	588.7(90.0)
721.6(1.7)	689.2(1.1)	846.5(73.9)	792.4(65.2)

870.8(203.8)	854.0(188.5)	1048.6(215.7)	973.6(206.6)
1197.0(257.8)	1165.4(274.9)	1129.1(142.2)	1114.5(156.7)
1629.9(163.9)	1597.4(193.1)	1614.6(357.5)	1548.9(388.1)
2092.4(0.0)	2002.5(0.0)	1966.2(515.3)	1888.7(402.3)
2092.9(1.9)	2003.5(35.8)	2095.3(268.0)	2002.2(170.6)
2109.8(1043.1)	2017.9(923.6)	2107.7(909.7)	2017.5(911.8)
2112.7(1493.6)	2022.0(1326.6)	2119.4(768.0)	2021.8(669.8)
2123.9(1921.3)	2041.3(1413.5)	2128.6(1756.8)	2037.0(1410.6)
2167.0(139.3)	2075.6(114.2)	2167.6(241.8)	2073.7(219.6)

Table S4. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Co_2(CF)_2(CO)_6$.

26S-3(C_s)		**26S-4(C_{2v})**	
B3LYP	BP86	B3LYP	BP86
35.4 (0.1)	-37.2 (0.0)	-60.6 (0.0)	-48.3 (0.0)
39.9 (0.1)	36.0 (0.0)	-50.3 (0.0)	-41.9 (0.0)
55.4 (1.3)	58.4 (0.0)	54.4 (0.2)	58.8 (0.2)
60.5 (2.1)	64.4 (0.0)	69.1 (0.0)	68.2 (0.0)
63.0 (0.1)	66.4 (0.1)	73.7 (0.0)	71.9 (0.0)
74.0 (0.1)	73.4 (0.0)	74.5 (0.0)	73.7 (0.0)
82.8 (0.0)	74.0 (0.0)	81.4 (0.1)	78.7 (0.1)
85.2 (0.2)	79.9 (0.0)	81.5 (0.0)	79.3 (0.0)
88.3 (0.2)	80.9 (0.0)	90.8 (0.0)	89.8 (0.0)
94.0 (0.3)	87.9 (0.3)	96.6 (0.1)	94.3 (0.1)
99.6 (0.3)	91.9 (0.1)	99.8 (0.0)	98.0 (0.0)
109.9 (0.1)	93.5 (0.0)	116.8 (0.0)	113.9 (0.0)
150.0 (4.8)	171.9(0.1)	155.7 (0.0)	161.8 (0.0)
166.5 (1.6)	182.0 (2.3)	188.1 (3.2)	184.8 (1.4)
193.6 (3.8)	212.1 (1.2)	204.2 (2.5)	202.2 (2.3)
217.9 (3.9)	218.5 (0.6)	224.9 (0.0)	219.3 (0.1)
269.2 (0.5)	291.6 (1.1)	281.9 (0.0)	288.4 (0.0)
286.0 (11.3)	298.7 (0.9)	284.8 (0.3)	289.5 (0.0)
340.3 (0.3)	348.1 (1.9)	301.9 (4.1)	303.0 (1.5)
359.0 (9.4)	352.8 (0.0)	329.9 (0.0)	340.7 (0.0)
369.2 (44.7)	374.3 (0.6)	339.1 (0.0)	348.7 (0.0)
382.1 (0.3)	385.5 (2.6)	377.4 (3.2)	379.0 (3.7)
398.5 (17.7)	424.5 (1.4)	401.6 (0.7)	401.9 (5.0)
409.7 (6.1)	425.3 (0.5)	408.0 (0.0)	409.9 (1.2)
415.0 (3.0)	448.7 (3.8)	437.1 (34.9)	451.7 (0.0)
427.6 (8.2)	453.1 (1.5)	443.0 (0.0)	458.7 (3.0)
432.6 (6.9)	467.4 (3.9)	462.6 (0.3)	473.2 (0.0)
458.3 (1.5)	471.2 (4.3)	477.4 (4.7)	486.8 (1.6)
460.8 (2.2)	484.5 (1.1)	484.8 (12.1)	487.0 (0.6)
479.6 (23.9)	496.9 (7.4)	491.6 (24.0)	501.1 (146.2)
500.3 (9.2)	507.8 (139.3)	503.5 (73.5)	503.2 (8.8)
515.1 (56.5)	509.1 (16.1)	511.4 (2.2)	518.5 (7.0)
530.6 (91.0)	512.5 (12.5)	515.7 (125.7)	523.1 (0.0)
532.2 (12.0)	535.9 (39.8)	522.1 (76.0)	523.4 (17.1)
535.2 (66.3)	536.0 (59.8)	526.6 (0.0)	533.3 (75.6)
559.9 (56.7)	546.3 (26.9)	536.3 (0.0)	534.0 (46.0)
571.2 (16.8)	547.2 (1.0)	536.7 (43.6)	545.9 (0.0)
601.0 (116.6)	616.3 (257.5)	624.8 (303.3)	617.6 (264.8)
755.3 (4.3)	692.0 (0.6)	718.6 (0.4)	690.1 (0.2)

911.1 (183.0)	863.4 (183.4)	892.5 (187.0)	873.8 (172.3)
1208.0 (238.9)	1167.0 (235.2)	1194.1 (178.9)	1161.4 (189.4)
1702.2 (156.8)	1615.8 (187.9)	1675.4 (149.8)	1623.4 (178.0)
1961.9 (461.4)	1995.5 (242.9)	2075.6 (48.2)	1992.3 (2.5)
2098.2 (25.8)	2006.3 (398.0)	2094.8 (1801.0)	2008.5 (1559.7)
2103.1 (1718.9)	2016.2 (733.1)	2094.9 (0.0)	2008.9 (0.0)
2110.0 (595.4)	2018.5 (1092.6)	2101.2 (1170.9)	2015.3 (997.7)
2125.9 (1847.0)	2036.0 (1434.2)	2112.4 (2119.9)	2033.0 (1605.0)
2163.2 (85.1)	2073.1 (131.0)	2156.5 (88.7)	2067.6 (73.6)

Table S5. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the triplet structures of $Co_2(CF)_2(CO)_6$.

26T-1(C_2)		**26T-2(C_s)**		**26T-3(C_{2v})**	
B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
22.6(0.2)	26.2(0.2)	14.9(0.0)	13.8(0.0)	8.1(0.0)	-14.8(0.0)
31.1(0.0)	27.2(0.0)	24.7(0.1)	24.0(0.0)	16.0(0.1)	3.9(0.0)
39.1(0.2)	39.4(0.0)	43.1(0.0)	44.4(0.1)	39.0(0.0)	41.4(0.1)
55.0(1.0)	60.0(1.1)	60.5(0.0)	59.9(0.0)	58.5(0.1)	59.7(0.1)
63.3(0.0)	60.8(0.0)	62.7(0.0)	63.5(0.0)	59.2(0.0)	60.0(0.0)
65.4(0.1)	64.5(0.0)	63.1(0.0)	64.4(0.0)	62.3(0.0)	62.1(0.0)
68.9(0.1)	69.1(0.1)	65.6(0.0)	65.8(0.0)	63.4(0.0)	64.3(0.0)
71.7(0.0)	71.7(0.1)	72.8(0.0)	73.0(0.0)	72.1(0.0)	73.1(0.0)
79.3(0.0)	78.7(0.0)	73.5(0.2)	74.1(0.0)	75.5(0.0)	75.8(0.0)
84.5(0.4)	82.9(0.4)	80.9(0.1)	80.6(0.1)	77.5(0.1)	76.5(0.0)
87.7(0.4)	85.9(0.0)	82.0(0.0)	83.7(0.0)	77.8(0.6)	77.9(0.1)
90.9(0.0)	90.6(0.0)	85.2(0.8)	85.7(0.2)	85.0(0.2)	84.7(0.0)
102.8(0.3)	104.8(0.0)	132.2(1.1)	139.4(0.1)	139.8(2.2)	143.2(0.4)
136.7(2.7)	147.6(0.9)	184.6(0.1)	184.6(1.5)	172.3(0.0)	180.7(0.0)
183.3(0.0)	178.4(0.1)	187.2(2.9)	188.4(0.0)	185.8(2.1)	184.5(1.1)
224.3(6.4)	228.5(2.0)	211.7(11.5)	217.8(3.9)	207.8(15.5)	214.6(6.7)
250.3(0.7)	257.7(0.4)	272.8(8.3)	283.0(4.0)	269.3(5.8)	281.3(2.9)
300.9(1.9)	301.7(3.1)	288.3(0.0)	297.5(0.1)	285.8(0.0)	292.4(0.0)
303.8(8.2)	314.8(0.3)	298.2(0.8)	302.3(0.2)	299.6(1.3)	299.6(0.7)
311.1(5.6)	320.0(5.6)	313.7(2.1)	322.8(2.0)	312.3(1.2)	308.9(1.7)
351.9(9.5)	355.0(3.3)	341.8(10.8)	346.1(1.5)	335.8(29.8)	324.6(0.0)
355.1(70.7)	372.7(10.3)	351.7(22.7)	360.6(0.3)	353.8(11.5)	349.7(3.3)
361.9(0.9)	385.6(5.9)	366.3(7.1)	389.6(2.1)	355.0(13.6)	400.8(0.6)
387.1(21.0)	401.3(27.4)	383.2(1.2)	414.0(8.5)	362.3(0.0)	411.2(10.8)
391.5(5.4)	419.8(0.6)	393.3(1.8)	414.8(0.2)	380.7(5.4)	418.3(0.0)
393.2(1.5)	429.8(18.3)	407.9(7.0)	427.0(0.2)	413.6(22.6)	427.4(6.4)
410.4(0.1)	444.9(2.3)	408.7(15.4)	434.2(15.9)	420.8(4.5)	431.9(0.2)
421.4(5.6)	455.5(0.0)	424.7(0.0)	449.9(12.6)	423.1(0.0)	443.8(37.5)
440.4(51.0)	456.3(0.5)	437.5(13.1)	456.4(0.4)	446.4(9.9)	459.9(0.0)
450.2(0.5)	471.4(0.1)	451.5(3.8)	457.1(11.7)	457.8(0.0)	470.0(0.0)
454.7(17.1)	478.2(13.0)	462.1(9.0)	470.1(0.7)	459.6(0.7)	470.2(0.2)
480.3(66.6)	491.1(0.4)	472.5(142.8)	488.5(58.3)	472(111.5)	488.9(78.4)
481.1(0.9)	495(103.0)	473.7(44.5)	489.5(14.6)	476.2(66.4)	490.5(7.2)
493.9(29.7)	515.9(30.5)	481.5(0.2)	497.2(13.7)	477.3(19.4)	495.5(2.8)
495.4(8.1)	516.8(2.0)	483.6(6.0)	500.0(55.1)	481.6(0.2)	498.2(52.4)
508.3(72.1)	524.0(80.4)	487.1(37.9)	505.2(51.7)	488.3(48.0)	500.3(0.0)
522.1(5.6)	526.4(12.4)	540.7(6.2)	516.9(14.3)	508.3(0.0)	506.2(69.7)
556.6(9.3)	540.8(2.0)	562.9(53.3)	606.0(54.6)	562.8(62.1)	606.7(55.4)
844.7(51.7)	823.8(57.0)	676.3(0.0)	631.3(0.5)	679.6(0.0)	630.4(0.7)

1026(206)	1025(210)	816.7(124.6)	795.1(94.7)	811.9(95.8)	776.7(61.3)
1101(172)	1087(127)	1140(213)	1129(223)	1137(217)	1126(232)
1643(277)	1528(404)	1604(126)	1465(223)	1607(143)	1448(241)
2076(170)	1992(3.8)	2092(286)	1993(227)	2090(0.0)	1999(0.0)
2093(379)	1997(71)	2096(405)	2005(971)	2102(26.0)	2000(284)
2109(1427)	2007(1387)	2104(1354)	2005(201)	2103(1741)	2006(1043)
2111(682.8)	2013(722)	2106(961)	2011(1337)	2109(1287)	2013(1487)
2128(1796)	2028(1748)	2127(1651)	2031(1540)	2130(1521)	2030(1338)
2163(100.2)	2065(168)	2161(68.4)	2063(81.1)	2162(54.9)	2064(138)

Table S6. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Co_2(CF)_2(CO)_5$.

25S-1(C_1)		**25S-2(C_2)**	
B3LYP	BP86	B3LYP	BP86
19.2 (0.2)	20.6 (0.0)	-57.2 (1.3)	-54.4 (1.6)
29.9 (0.2)	36.5 (0.1)	29.0 (0.1)	31.0 (0.0)
56.8 (0.2)	52.9 (0.3)	47.3 (0.1)	46.6 (0.0)
66.4 (0.4)	54.4 (0.1)	72.3 (0.1)	70.3 (0.0)
76.2 (0.2)	74.3 (0.0)	76.6 (1.1)	76.0 (0.5)
80.3 (0.2)	79.3 (0.1)	80.0 (0.2)	76.5 (0.0)
90.2 (0.2)	84.9 (0.0)	89.4 (0.0)	84.8 (0.0)
101.9 (0.0)	91.4 (0.0)	91.2 (0.1)	86.0 (0.0)
106.6 (0.2)	99.2 (0.1)	103.7 (0.1)	102.9 (0.0)
117.2 (1.1)	114.1 (0.2)	128.0 (1.4)	124.3 (0.8)
181.5 (2.7)	176.7 (1.6)	148.8 (1.9)	149.6 (2.0)
206.9 (1.1)	209.5 (1.3)	202.5 (0.7)	207.3 (0.1)
221.5 (3.5)	218.6 (3.4)	223.5 (5.0)	218.2 (2.9)
239.3 (6.6)	234.7 (1.6)	232.6 (2.3)	231.4 (1.7)
292.3 (3.9)	289.9 (2.4)	279.9 (5.9)	274.1 (2.6)
343.6 (16.5)	331.4 (11.3)	328.4 (7.4)	319.8 (3.6)
371.5 (3.7)	363.2 (1.1)	379.1 (2.3)	364.2 (0.3)
392.0 (9.1)	378.7 (2.0)	388.8 (26.8)	387.8 (9.0)
397.8 (3.8)	398.6 (18.0)	400.3 (53.6)	403.3 (0.4)
423.0 (13.8)	415.7 (1.0)	407.6 (0.1)	415.8 (26.6)
436.1 (8.0)	435.7 (8.3)	422.8 (2.6)	420.2 (1.8)
441.3 (9.2)	443.0 (1.1)	425.2 (0.1)	430.8 (0.3)
451.7 (6.2)	452.9 (4.5)	440.9 (6.5)	450.3 (7.0)
467.6 (5.9)	462.9 (2.6)	445.4 (9.5)	458.4 (30.5)
481.0 (4.7)	474.0 (17.1)	462.2 (0.1)	461.9 (0.4)
489.9 (3.8)	486.7 (3.4)	507.9 (0.1)	506.9 (5.3)
504.5 (6.4)	503.1 (3.7)	511.3 (14.1)	507.0 (6.6)
527.4 (70.1)	528.4 (30.0)	523.7 (49.3)	511.5 (8.8)
542.8 (45.4)	545.1 (26.4)	525.6 (2.5)	529.8 (30.7)
567.4 (6.8)	557.0 (29.1)	546.5 (57.4)	548.5 (32.6)
582.4 (66.2)	574.3 (28.2)	574.9 (88.9)	567.5 (90.9)
593.9 (136.9)	576.3 (140.5)	591.2 (25.8)	589.3 (25.9)
607.4 (3.2)	596.3 (3.4)	594.3 (0.4)	593.7 (0.1)
796.5 (26.9)	761.2 (28.0)	815.9 (42.8)	771.3 (48.9)
960.7 (182.4)	920.5 (153.8)	971.5 (158.0)	920.5 (134.2)
1179.5 (205.2)	1157.3 (227.8)	1180.1 (206.9)	1160.6 (234.5)
1618.2 (370.2)	1557.7 (384.7)	1627.0 (333.7)	1575.1 (372.4)
1960.3 (439.8)	1889.9 (392.9)	1959.4 (464.1)	1878.9 (364.8)
2096.3 (666.0)	2003.8 (278.4)	2098.8 (174.6)	2003.7 (123.1)

2107.3 (923.5)	2010.6(1132.9)	2103.6 (1438.3)	2008.6 (1258.3)
2123.1 (2031.4)	2032.6(1671.1)	2120.7 (2021.4)	2031.4 (1714.7)
2155.9 (95.6)	2060.8(74.1)	2154.1 (118.9)	2059.8 (83.0)

Table S7. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Co_2(CF)_2(CO)_5$.

25S-3(C_1)		**25S-4(C_1)**	
B3LYP	BP86	B3LYP	BP86
18.3 (0.2)	20.2 (0.0)	20.1 (0.0)	22.1 (0.1)
30.8 (0.1)	34.8 (0.0)	26.1 (0.0)	28.7 (0.0)
42.2 (0.5)	41.7 (0.4)	41.4 (0.1)	42.5 (0.1)
62.1 (0.0)	52.1 (0.8)	49.8 (0.4)	54.6 (0.6)
65.1 (0.0)	63.8 (0.0)	61.4 (0.1)	60.6 (0.1)
69.2 (0.0)	67.2 (0.0)	68.3 (0.0)	69.2 (0.0)
75.3 (0.0)	70.2 (0.1)	73.0 (0.2)	72.4 (0.3)
77.1 (0.2)	74.2 (0.2)	78.4 (0.1)	77.0 (0.4)
85.1 (0.1)	82.7 (0.1)	80.5 (0.9)	81.4 (0.9)
94.4 (0.4)	92.5 (0.2)	83.7 (0.0)	81.5 (0.0)
97.1 (0.3)	104.8 (0.4)	93.7 (0.3)	91.6 (0.3)
102.1 (0.4)	128.5 (3.7)	104.1 (0.4)	103.7 (0.3)
200.5 (0.4)	214.7 (0.4)	177.2 (1.4)	178.4 (0.1)
246.7 (0.0)	242.0 (0.2)	245.7 (0.2)	244.6 (0.2)
300.6 (0.4)	269.2 (0.6)	291.1 (0.6)	290.5 (1.8)
314.3 (0.4)	299.7 (1.3)	315.6 (3.2)	305.9 (2.0)
332.4 (7.1)	328.6 (7.5)	335.7 (2.4)	332.8 (1.4)
347.6 (4.4)	339.4 (0.3)	357.7 (9.6)	352.8 (7.0)
388.0 (2.4)	382.8 (2.1)	382.4 (3.3)	377.0 (1.7)
406.5 (3.5)	420.6 (28.6)	389.7 (17.9)	402.7 (10.9)
412.5 (24.7)	430.5 (2.7)	426.2 (0.9)	432.0 (0.3)
431.9 (6.4)	432.4 (3.1)	444.3 (1.7)	454.3 (11.7)
443.8 (26.4)	439.4 (34.7)	448.9 (14.1)	455.6 (9.1)
457.8 (3.7)	456.5 (5.2)	459.0 (31.5)	466.0 (19.0)
471.2 (16.0)	471.9 (13.2)	462.8 (25.3)	478.9 (4.5)
480.3 (13.7)	480.2 (31.8)	483.1 (1.7)	489.9 (2.0)
497.3 (26.7)	499.8 (26.6)	498.9 (11.8)	503.5 (16.2)
510.0 (67.2)	513.1 (22.5)	513.0 (33.4)	520.8 (46.7)
528.2 (23.9)	524.5 (44.1)	523.3 (29.6)	526.8 (33.9)
542.3 (31.6)	534.1 (11.7)	541.3 (26.0)	538.5 (2.4)
549.4 (2.4)	551.3 (29.7)	557.2 (55.7)	546.1 (22.1)
575.7 (29.3)	559.5 (17.2)	561.3 (57.4)	553.2 (66.2)
588.7 (47.3)	573.5 (80.3)	577.2 (40.1)	569.5 (50.1)
621.1 (45.1)	607.6 (28.8)	645.0 (45.2)	633.7 (55.3)
757.8 (434.8)	698.6 (353.9)	750.7 (398.9)	744.4 (359.3)
1270.2(514.0)	1258.2 (645.9)	1287.5 (469.3)	1256.6(423.7)
1386.8 (458.3)	1317.1 (268.6)	1404.6 (1039.9)	1354.2 (919.2)
2084.1 (806.0)	1997.0 (542.4)	2076.6 (67.2)	1990.9 (19.4)
2090.3 (552.2)	2002.0(1113.5)	2091.1 (657.6)	1999.2 (721.7)

2094.3 (1313.5)	2005.2 (613.3)	2094.5 (1293.4)	2007.6(1060.3)
2114.2 (1615.5)	2024.5(1441.7)	2105.9 (1532.8)	2021.3(1300.2)
2147.3 (40.3)	2056.9 (77.9)	2148.4 (382.1)	2058.6 (285.7)

Table S8. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the triplet structures of $Co_2(CF)_2(CO)_5$ and $Co_2(CF)_2(CO)_4$

25T-1(C_s/C_1)		**24T-1**(C_2/C_1)	
B3LYP	BP86	B3LYP	BP86
19.2 (0.1)	24.8 (0.0)	33.4 (0.0)	30.7 (0.2)
37.7 (0.1)	45.5 (0.0)	36.9 (0.0)	37.5 (0.0)
40.7 (0.0)	45.6 (0.2)	47.2 (1.0)	40.3 (0.0)
58.6 (0.0)	65.4 (0.0)	52.4 (0.0)	63.7 (0.2)
64.7 (0.2)	73.9 (0.0)	67.3 (0.0)	70.4 (0.1)
67.8 (0.1)	74.3 (0.7)	76.5 (0.4)	72.0 (0.0)
70.7 (0.1)	77.6 (0.2)	79.0 (0.0)	76.2 (0.1)
74.0 (0.0)	81.0 (0.1)	80.5 (0.2)	78.9 (0.1)
75.9 (0.1)	85.0 (0.1)	108.2 (1.7)	121.4 (0.9)
84.1 (0.2)	143.8 (0.1)	149.7 (1.0)	177.4 (0.4)
102.5 (0.8)	173.2 (0.5)	200.9 (0.3)	194.1 (0.6)
165.0 (1.1)	188.1 (2.7)	215.5 (5.7)	208.6 (2.6)
178.9 (0.3)	234.0 (1.6)	271.5 (4.2)	275.3 (0.1)
206.3 (6.4)	236.9 (0.1)	350.2 (3.3)	328.4 (9.9)
260.2 (8.5)	262.2 (0.7)	360.1 (4.5)	354.3 (1.5)
290.6 (3.3)	288.3 (1.2)	364.1 (1.8)	367.4 (3.4)
315.7 (2.2)	313.0 (0.6)	380.8 (5.2)	384.1 (2.5)
340.3 (32.1)	364.1 (0.4)	412.5 (21.7)	416.2 (2.6)
360.2 (5.5)	379.3 (0.4)	425.1 (0.6)	426.1 (2.9)
374.9 (17.2)	380.7 (0.5)	443.3 (0.5)	429.3 (4.2)
397.9 (11.3)	386.1 (0.4)	445.2 (59.7)	445.7 (11.3)
405.1 (3.7)	397.6 (0.0)	460.1 (7.8)	469.2 (3.8)
412.7 (15.7)	406.1 (3.1)	464.9 (5.6)	479.2 (1.5)
417.1 (8.9)	425.3 (0.3)	488.0 (76.6)	487.8 (19.1)
438.8 (52.4)	432.6 (2.9)	488.5 (25.6)	508.2 (65.2)
457.7 (9.4)	461.3 (13.9)	512.9 (50.7)	512.0 (36.5)
468.9 (6.8)	475.4 (11.6)	528.3 (10.7)	517.0 (27.2)
472.4 (31.2)	496.2 (8.3)	592.6 (12.2)	542.5 (2.6)
478.2 (4.2)	500.9 (3.8)	818.6 (28.8)	735.5 (4.3)
483.9 (36.2)	503.0 (53.8)	985.2 (192.4)	880.5 (162.7)
502.9 (34.4)	517.7 (18.9)	1137.0 (188.5)	1165.0 (241.8)
512.1 (17.7)	544.6 (74.4)	1621.2 (199.4)	1623.2 (257.6)
529.2 (2.3)	546.3 (14.0)	2075.1 (572.6)	1991.1 (568.7)
776.3 (10.3)	683.8 (0.1)	2095.1(1040.7)	1991.4 (848.1)
914.1 (214.2)	845.0 (176.8)	2124.2(1933.2)	2004.3(2082.5)
1168.2 (225.2)	1173.0 (257.8)	2153.4 (79.3)	2048.8 (207.5)
1710.0 (173.8)	1681.5 (237.2)		
2073.3 (586.9)	1900.0 (360.6)		
2093.2 (49.5)	1999.2 (2.7)		

2102.0 (1518.3)	2002.6(1467.4)
2119.0 (1669.9)	2011.4(2065.7)
2156.7 (223.5)	2051.6(101.4)

Table S9. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Co_2(CF)_2(CO)_4$.

24S-1(C_{2h})		**24S-2(C_1)**	
B3LYP	BP86	B3LYP	BP86
24.0 (0.1)	33.2 (0.2)	29.1 (0.1)	30.1 (0.1)
44.7 (0.0)	41.7 (0.0)	38.9 (0.3)	41.1 (0.1)
66.0 (0.0)	65.8 (0.3)	48.1 (0.8)	52.2 (0.4)
71.7 (0.4)	66.4 (0.0)	57.7 (0.4)	61.7 (0.5)
82.7 (0.0)	78.7 (0.0)	67.6 (0.5)	70.7 (0.3)
90.6 (0.0)	86.1 (0.0)	81.4 (0.1)	72.1 (0.0)
95.3 (1.1)	91.5 (0.7)	85.3 (0.1)	81.6 (0.0)
101.1 (0.0)	95.4 (0.0)	91.1 (0.0)	83.8 (0.1)
113.1 (0.0)	107.2 (0.0)	104.3 (1.4)	152.8 (1.3)
216.7 (0.1)	207.4 (0.1)	173.7 (2.3)	178.9 (3.7)
255.2 (0.0)	252.5 (0.0)	190.9 (0.1)	197.5 (3.0)
276.9 (0.0)	273.7 (0.0)	220.9 (4.5)	214.6 (1.7)
325.5 (0.4)	329.7 (1.9)	260.4 (2.4)	278.6 (3.3)
359.2 (1.6)	350.1 (0.0)	328.2 (11.2)	326.6 (1.0)
365.4 (0.0)	352.6 (0.4)	377.1 (1.1)	368.2 (1.3)
421.8 (0.0)	415.6 (0.0)	399.5 (2.7)	400.7 (5.6)
446.3 (26.9)	438.3 (19.6)	402.1 (15.6)	403.4 (1.3)
461.9 (22.7)	454.9 (0.0)	423.2 (8.3)	429.7 (0.2)
462.7 (0.0)	470.7 (5.5)	434.1 (5.4)	447.4 (0.4)
467.9 (20.3)	480.3 (2.6)	453.4 (2.9)	455.2 (0.8)
485.5 (0.0)	491.0 (0.0)	463.7 (3.2)	463.0 (3.0)
486.5 (0.0)	495.1 (0.0)	478.7 (3.5)	492.1 (16.9)
501.4 (0.0)	508.9 (0.0)	494.7 (7.5)	501.7 (13.2)
553.3 (0.0)	544.5 (0.0)	513.4 (24.0)	533.5 (16.9)
554.7 (38.9)	546.3 (35.4)	548.7 (9.7)	536.8 (8.2)
568.6 (80.2)	554.3 (45.6)	558.6 (79.5)	543.8 (28.8)
574.7 (8.0)	571.8 (42.5)	583.5 (7.9)	551.9 (47.2)
589.7 (0.0)	590.0 (0.0)	611.1 (25.2)	582.9 (44.7)
619.4 (0.0)	605.8 (0.0)	827.2 (29.3)	697.0 (0.8)
673.6 (159.1)	673.1 (142.9)	1033.3 (220.5)	838.3 (173.7)
1258.5 (965.7)	1242.2(939.5)	1159.6 (139.7)	1159.0 (297.2)
1293.5 (0.0)	1272.4 (0.0)	1544.4 (419.7)	1583.5 (273.9)
2088.8 (0.0)	1996.3 (0.0)	2066.1 (575.9)	1986.3 (352.0)
2097.0 (1722.9)	2004.3(1523.0)	2094.3 (1002.2)	1992.6(1024.2)
2111.4 (2347.5)	2023.8(1888.7)	2101.4 (1302.7)	2013.3(1409.4)
2146.2 (0.0)	2052.6 (0.0)	2144.3 (529.9)	2045.7 (317.2)

Table S10. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Co_2(CF)_2(CO)_4$.

24S-3(C_s)		**24S-4(C_s)**	
B3LYP	BP86	B3LYP	BP86
-58.0 (12.7)	-55.5 (11.6)	10.4 (0.0)	18.3 (0.1)
-26.0 (0.0)	-26.7 (0.0)	24.8 (0.0)	27.0 (0.0)
30.0 (0.3)	33.5 (0.2)	46.3 (0.1)	42.2 (0.0)
37.5 (1.4)	34.4 (2.1)	54.9 (0.0)	46.2 (0.1)
46.8 (0.1)	60.9 (0.2)	65.9 (0.0)	65.3 (0.0)
70.1 (1.6)	68.0 (0.8)	72.1 (0.6)	72.3 (0.0)
82.8 (0.0)	77.3 (0.2)	73.1 (0.1)	72.4 (1.1)
88.5 (0.1)	86.6 (0.1)	81.6 (0.9)	79.5 (0.6)
99.5 (0.5)	94.0 (1.5)	87.4 (0.1)	85.5 (0.0)
139.7 (1.4)	161.1 (1.4)	90.8 (0.4)	87.9 (0.4)
197.8 (6.1)	194.8 (0.2)	200.4 (2.0)	203.2 (0.7)
241.4 (5.7)	230.4 (3.1)	250.1 (0.2)	244.8 (0.2)
248.3 (0.0)	250.5 (0.4)	324.1 (0.3)	321.0 (0.7)
280.3 (5.4)	280.6 (3.4)	338.1 (2.0)	334.6 (0.4)
335.6 (32.2)	325.9 (34.5)	343.5 (0.1)	341.0 (0.3)
381.0 (4.3)	373.6 (1.1)	371.3 (26.3)	362.3 (20.9)
393.7 (28.0)	394.7 (4.2)	404.5 (18.2)	407.5 (11.7)
403.0 (0.5)	399.8 (13.0)	434.9 (1.6)	431.3 (0.2)
436.9 (8.6)	433.4 (3.2)	442.4 (1.5)	439.3 (1.8)
443.0 (8.1)	461.5 (2.5)	452.6 (13.4)	465.0 (11.4)
463.7 (2.9)	465.7 (2.4)	474.9 (8.9)	482.2 (10.1)
472.5 (0.5)	477.9 (0.0)	482.4 (1.3)	487.0 (1.8)
475.8 (0.7)	479.1 (1.2)	490.3 (22.8)	494.8 (2.8)
519.0 (4.8)	520.0 (19.8)	506.1 (7.0)	501.2 (1.5)
550.3 (44.4)	551.6 (31.7)	525.9 (24.1)	530.5 (35.6)
587.8 (32.8)	572.8 (1.2)	542.4 (46.1)	539.8 (31.8)
601.6 (36.8)	604.6 (48.8)	569.2 (52.8)	557.1 (55.7)
607.3 (54.9)	605.0 (30.1)	576.1 (99.5)	569.7 (59.3)
853.9 (38.5)	829.0 (36.7)	625.4 (65.8)	606.4 (74.2)
1104.2 (285.7)	1064.3 (304.6)	750.8 (203.0)	735.7 (154.3)
1139.4 (74.6)	1102.6 (97.5)	1300.0 (485.8)	1274.3 (471.3)
1425.7 (534.8)	1368.7 (471.8)	1482.9 (1160.4)	1442.5 (1028.3)
2071.0 (25.6)	1974.6 (7.8)	2079.6 (85.4)	1992.0 (57.8)
2086.6 (1701.4)	1992.5(1412.7)	2086.2 (922.1)	1997.7 (819.8)
2095.2 (1286.1)	2001.7(1129.6)	2099.8 (1626.8)	2011.4 (1413.9)
2139.6 (676.1)	2042.5(515.0)	2144.1 (606.2)	2055.4 (478.8)

Table S11. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Co_2(CF)_2(CO)_4$.

24S-5(C_1)		**24S-6(C_{2v})**	
B3LYP	BP86	B3LYP	BP86
16.8 (0.4)	17.3 (0.3)	-89.8 (1.7)	-92.3 (0.5)
30.7 (0.2)	23.9 (0.2)	34.9 (0.0)	36.4 (0.0)
55.8 (0.6)	53.8 (0.6)	40.8 (0.2)	38.3 (0.1)
58.0 (0.6)	56.1 (0.1)	56.9 (0.0)	56.8 (0.0)
65.3 (0.2)	61.2 (0.3)	64.0 (0.0)	58.1 (0.0)
73.4 (0.0)	71.9 (0.1)	66.5 (0.1)	67.0 (0.2)
75.5 (0.1)	74.5 (0.1)	83.7 (0.0)	84.1 (0.0)
82.3 (0.3)	77.0 (0.2)	89.6 (0.8)	86.5 (0.1)
92.1 (0.2)	89.4 (0.2)	90.3 (0.2)	88.2 (0.6)
97.7 (0.2)	92.8 (0.2)	219.3(0.0)	211.9 (4.5)
203.5(0.5)	207.2(0.9)	220.1 (0.0)	217.6 (0.1)
251.4 (0.2)	248.0 (0.1)	227.6 (1.2)	220.7 (0.0)
314.0 (0.2)	301.8 (1.1)	239.5 (13.5)	225.5 (1.0)
330.9 (2.2)	330.7 (2.6)	310.8 (0.0)	309.0 (0.4)
341.9 (3.0)	337.7 (1.6)	314.6 (0.0)	316.6 (0.0)
368.0 (12.4)	376.4 (9.0)	347.1 (4.3)	357.6 (0.2)
402.0 (10.6)	393.7 (6.4)	356.1 (46.5)	373.9 (26.2)
426.5 (5.0)	435.0 (8.7)	365.7 (20.5)	384.0 (20.5)
446.0 (3.1)	455.9 (10.3)	409.9 (0.0)	414.9 (0.0)
467.0 (6.7)	464.9 (3.3)	426.5 (0.0)	423.2 (4.3)
474.6 (5.4)	479.2 (10.1)	427.3 (2.5)	424.9 (0.0)
481.2 (4.2)	487.6 (23.2)	430.9 (6.0)	426.4 (0.0)
494.5 (89.2)	502.6 (8.8)	478.7 (0.0)	495.0 (0.0)
509.3 (19.5)	514.7 (25.1)	498.6 (53.6)	509.4 (52.8)
523.2 (22.7)	521.5 (48.4)	511.3 (9.6)	515.1 (2.4)
536.8 (28.9)	533.2 (19.0)	512.7 (2.7)	518.8 (6.4)
549.7 (64.5)	551.9 (21.5)	513.9 (35.7)	526.9 (1.5)
564.0 (29.7)	562.3 (32.1)	549.1 (39.8)	542.2 (38.0)
652.1 (16.7)	652.9 (38.7)	603.0 (24.6)	593.5 (29.8)
755.3 (275.0)	712.3 (193.6)	687.8 (46.8)	675.7 (39.2)
1279.8 (531.7)	1267.1 (524.5)	1235.3 (510.2)	1205.5(494.1)
1386.0 (529.4)	1336.5 (591.4)	1271.1 (569.2)	1238.6 (503.4)
2091.1 (864.9)	1987.1 (707.9)	2081.0 (69.0)	1989.1 (46.4)
2094.5 (798.5)	1996.7 (795.3)	2090.8 (2672.0)	2000.6 (1252.6)
2096.6 (1853.5)	2013.9(1479.1)	2091.9 (1374.9)	2004.5 (2148.6)
2140.6 (254.6)	2045.1 (184.5)	2142.9 (317.8)	2049.1 (266.6)

Table S12. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Co_2(CF)_2(CO)_4$.

24S-7(C_1)		**24S-8(C_1)**	
B3LYP	BP86	B3LYP	BP86
23.6 (0.1)	20.8 (1.0)	24.0 (0.1)	31.6 (0.3)
26.0 (0.1)	34.3 (0.3)	33.3 (0.3)	34.2 (0.1)
46.1 (0.6)	47.9 (0.6)	41.5 (0.0)	42.9 (0.3)
51.8 (0.1)	56.1 (0.1)	51.2 (0.1)	48.0 (0.7)
57.7 (0.9)	58.6 (0.1)	52.5 (1.2)	54.9 (0.3)
65.2 (0.1)	64.0 (0.2)	75.0 (0.0)	74.1 (0.3)
75.5 (0.2)	78.3 (0.0)	77.4 (0.3)	77.8 (0.1)
90.3 (0.3)	89.6 (0.3)	89.3 (0.3)	89.7 (0.2)
92.4 (0.5)	92.6 (0.1)	95.7 (1.1)	95.1 (0.9)
99.2 (0.4)	160.6 (2.5)	99.5 (0.7)	161.3 (2.3)
192.8 (3.1)	203.4 (0.5)	197.2 (4.9)	213.9 (2.6)
247.8 (0.8)	231.7 (0.5)	247.4 (0.7)	241.0 (0.4)
285.5 (2.8)	260.5 (0.2)	292.5 (2.9)	273.8 (6.4)
308.9 (1.3)	318.4 (3.3)	317.3 (1.1)	302.0 (2.9)
348.9 (9.6)	331.9 (2.4)	329.1 (10.2)	316.7 (10.0)
358.9 (2.3)	371.2 (9.2)	359.5 (2.2)	344.5 (0.3)
413.7 (28.5)	385.4 (0.8)	415.2 (1.5)	401.7 (1.5)
418.7 (3.1)	394.0 (2.4)	417.5 (30.1)	424.8 (6.4)
426.8 (15.6)	438.5 (9.8)	436.2 (8.1)	438.5 (1.5)
447.5 (2.8)	443.5 (4.7)	445.2 (5.4)	453.6 (4.9)
471.8 (10.5)	460.8 (14.0)	474.9 (17.6)	466.5 (11.8)
491.8 (3.9)	482.7 (1.9)	484.4 (11.3)	480.1 (5.1)
497.9 (25.1)	497.7 (6.4)	497.8 (13.5)	488.4 (12.3)
517.3 (2.0)	521.3 (35.4)	516.8 (15.8)	527.9 (1.4)
542.7 (57.9)	526.4 (6.3)	542.7 (33.3)	531.1 (64.1)
565.1 (28.3)	545.8 (13.8)	555.4 (70.5)	546.5 (31.6)
570.7 (15.6)	551.9 (36.0)	585.7 (28.2)	553.1 (21.9)
579.4 (117.0)	561.0 (44.5)	595.6 (66.7)	581.5 (26.3)
637.6 (14.8)	632.6 (35.9)	625.6 (17.3)	607.5 (62.6)
767.9 (312.8)	700.6 (96.1)	762.5 (277.6)	724.7 (153.3)
1297.1 (524.5)	1270.2 (507.7)	1297.4 (491.9)	1276.4 (479.9)
1437.8 (1020.8)	1379.7 (889.3)	1470.7 (1151.6)	1427.3 (1003.3)
2051.1 (451.8)	1913.5 (523.0)	2042.8 (599.3)	1919.9 (523.2)
2076.6 (1116.9)	1988.8 (795.2)	2075.5 (967.1)	1984.1 (627.8)
2104.1 (1886.9)	2012.7(1689.4)	2098.4 (1307.7)	2008.3 (1497.8)
2133.1 (180.8)	2039.1 (201.2)	2133.7 (640.9)	2038.4 (403.5)

Table S13. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Co_2(CF)_2(CO)_3$.

23S-1(C_1/C_s)		**23S-2**(C_s)	
B3LYP	BP86	B3LYP	BP86
8.4 (0.3)	35.3 (0.1)	36.4 (0.6)	36.6 (0.1)
43.7 (0.2)	39.8 (0.1)	38.4 (0.1)	41.1 (0.1)
62.6 (0.1)	63.6 (0.1)	66.8 (0.5)	64.1 (0.1)
74.6 (0.4)	68.0 (0.4)	67.0 (0.1)	68.9 (0.4)
80.1 (0.7)	72.9 (0.5)	75.9 (0.6)	73.1 (0.5)
82.3 (0.2)	77.5 (0.2)	77.2 (0.2)	78.9 (0.2)
92.2 (0.6)	90.7 (0.5)	90.5 (0.4)	91.0 (0.5)
159.7 (0.8)	219.9(2.1)	223.0 (2.6)	220.3 (2.0)
241.1 (0.5)	227.0 (0.2)	226.8 (1.0)	227.7 (0.2)
260.4 (0.3)	228.3 (1.3)	236.6 (0.6)	228.5 (1.3)
277.1 (1.3)	259.2 (2.1)	253.2 (4.3)	259.8 (2.0)
326.5 (2.4)	283.2 (6.6)	314.9 (13.9)	283.5 (6.7)
382.3 (6.8)	371.2 (6.7)	375.2 (6.9)	371.9 (6.8)
420.3 (6.6)	399.5 (18.1)	388.1 (33.5)	399.9 (18.1)
436.1 (15.0)	421.5 (2.0)	426.9 (0.0)	422.0 (1.9)
448.7 (23.9)	442.4 (3.2)	434.2 (0.0)	443.6 (3.4)
462.2 (4.6)	449.9 (1.5)	453.6 (0.4)	450.5 (1.3)
475.1 (11.5)	478.8 (4.2)	466.0 (4.9)	479.2 (4.1)
490.0 (19.2)	490.4 (4.5)	473.8 (17.3)	491.3 (4.6)
524.7 (42.6)	508.7 (27.8)	487.1 (51.9)	509.2 (27.7)
540.7 (28.6)	526.3 (9.6)	508.4 (10.2)	526.7 (9.9)
550.5 (9.4)	527.5 (1.7)	528.6 (1.0)	528.2 (1.6)
591.2 (42.2)	537.8 (33.6)	541.1 (50.5)	538.7 (33.5)
620.5 (24.6)	601.1 (26.5)	605.5 (54.7)	602.1 (26.4)
714.7 (141.9)	624.6 (28.3)	623.3 (17.6)	625.6 (28.3)
1261.9 (933.5)	1219.9 (682.0)	1253.1 (733.8)	1220.4 (680.7)
1301.0 (28.6)	1249.7 (293.2)	1284.6 (321.9)	1250.2 (294.5)
2086.3 (2103.7)	1986.4 (1757.9)	2077.4 (2302.2)	1986.4 (1756.1)
2090.0 (944.7)	1994.1 (947.0)	2086.2 (1061.6)	1994.0 (948.8)
2131.8 (337.6)	2031.2 (312.6)	2124.6 (276.0)	2031.1 (311.4)

Table S14. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(CF)_2(CO)_3$.

23S-3(C_s)		**23S-4(C_1)**	
B3LYP	BP86	B3LYP	BP86
15.9 (0.0)	-9.8 (0.0)	37.1 (0.1)	37.3 (0.0)
35.7 (0.0)	29.4 (0.0)	42.1 (0.2)	42.3 (0.2)
47.1 (0.2)	48.3 (0.1)	52.3 (0.1)	53.3 (0.4)
62.0 (0.0)	60.1 (0.0)	59.4 (0.5)	55.2 (0.4)
66.8 (0.3)	68.0 (0.2)	72.6 (1.3)	72.2 (1.0)
74.6 (0.1)	74.8 (0.2)	78.0 (0.8)	75.6 (1.0)
96.0 (0.6)	96.1 (0.4)	96.2 (0.4)	93.2 (0.4)
105.9 (0.2)	130.4 (0.7)	121.9 (0.7)	129.3(1.0)
224.1 (0.9)	223.2 (1.8)	225.5 (0.5)	226.7 (0.7)
231.9 (3.2)	240.4 (1.7)	240.8 (2.5)	245.6 (1.5)
313.5 (0.0)	316.7 (0.1)	296.6 (2.0)	287.8 (2.9)
330.5 (1.0)	324.7 (0.8)	312.1 (1.9)	302.6 (0.8)
348.2 (18.9)	326.3 (8.7)	355.6 (10.9)	366.0 (23.2)
368.1 (0.7)	355.6 (0.1)	429.0 (2.3)	419.3 (0.5)
406.4 (15.3)	415.1 (11.1)	432.0 (6.1)	425.0 (4.6)
442.0 (4.6)	426.0 (0.1)	440.8 (4.5)	436.7 (3.0)
451.2 (2.2)	431.2 (1.1)	456.1 (15.7)	447.7 (5.7)
453.0 (0.5)	462.3 (1.9)	492.5 (34.9)	499.2 (25.3)
465.9 (12.8)	470.7 (2.0)	511.2 (23.1)	512.5 (3.7)
490.8 (23.9)	482.4 (6.9)	520.3 (12.7)	516.1 (12.3)
493.9 (12.4)	504.8 (29.8)	550.0 (19.4)	540.6 (27.0)
527.2 (34.3)	522.6 (33.4)	576.5 (34.6)	562.7 (22.9)
627.5 (111.7)	604.1 (79.3)	607.1 (111.3)	596.0 (109.2)
629.7 (26.7)	619.1 (12.9)	630.1 (20.7)	611.4 (22.1)
711.9 (101.9)	691.3 (77.8)	767.1 (212.0)	753.1 (181.7)
1319.3(494.4)	1291.5 (464.8)	1318.2 (416.8)	1285.8 (393.5)
1479.8 (1261.2)	1442.2(1105.7)	1456.5 (1097.0)	1416.1 (965.5)
1990.4 (687.4)	1886.8 (571.6)	1969.7 (656.8)	1873.0 (518.6)
2087.5 (1065.3)	1992.1(921.7)	2085.3 (1772.6)	1995.3 (1514.2)
2129.0 (914.7)	2033.5 (745.5)	2116.8 (441.5)	2026.8 (397.4)

Table S15. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Co_2(CF)_2(CO)_3$.

23S-5(C_s)		**23S-6(D_{3h})**	
B3LYP	BP86	B3LYP	BP86
-43.1 (0.0)	-9.0 (0.6)	40.8 (0.0)	40.1 (0.3)
37.5 (0.3)	45.2 (0.1)	40.8 (0.0)	40.1 (0.3)
46.5 (0.0)	58.5 (0.5)	56.6 (0.0)	59.7 (0.0)
50.5 (0.5)	65.9 (0.7)	56.6 (0.0)	59.7 (0.0)
62.0 (0.3)	66.6 (0.2)	87.4 (0.3)	86.7 (0.3)
75.1 (0.2)	80.1 (0.7)	87.4 (0.3)	86.7 (0.3)
91.8 (0.1)	148.8 (0.4)	130.3 (0.0)	161.0 (0.0)
96.8 (0.3)	167.3 (1.2)	130.3 (0.0)	192.2 (0.0)
179.2 (4.5)	218.9 (1.3)	152.3 (2.3)	192.2 (0.0)
238.2 (1.1)	223.6 (1.4)	244.1 (0.0)	261.8 (0.0)
277.6 (1.2)	236.1 (4.8)	244.1 (0.0)	261.8 (0.0)
330.6 (1.9)	288.1 (0.1)	288.0 (0.0)	293.4 (0.0)
368.8 (7.6)	293.2 (15.2)	307.6 (35.9)	348.4 (0.0)
408.9 (12.7)	377.4 (6.1)	348.5 (0.0)	369.6 (17.0)
419.6 (1.5)	378.7 (3.9)	376.7 (17.5)	394.2 (8.2)
437.6 (0.2)	427.5 (0.9)	376.7 (17.5)	394.2 (8.2)
441.9 (7.6)	458.2 (0.0)	385.2 (0.0)	404.8 (0.0)
484.5 (13.4)	462.3 (4.6)	488.5 (1.8)	492.5 (0.5)
486.9 (19.8)	479.2 (1.1)	488.5 (1.8)	492.5 (0.5)
527.6 (6.9)	506.0 (5.4)	582.1 (18.3)	569.1 (0.0)
552.2 (14.8)	512.9 (2.4)	582.1 (0.0)	569.1 (0.0)
583.8 (114.7)	570.7 (26.4)	582.1 (18.3)	578.0 (18.5)
616.4 (44.5)	596.7 (19.4)	582.1 (0.0)	578.1 (18.5)
625.3 (9.6)	625.2 (5.5)	615.7 (32.5)	594.0 (30.4)
757.2 (141.6)	643.2 (25.2)	653.0 (0.0)	637.4 (0.0)
1328.4(372.5)	1302.0 (561.7)	1478.8(2215.7)	1443.2 (1976.8)
1477.8 (1146.2)	1455.3(1079.8)	1492.3 (0.0)	1455.5 (0.0)
2068.4 (979.0)	1922.0(935.5)	2031.4 (1128.0)	1925.0 (966.9)
2068.8 (1506.6)	1934.1 (674.5)	2031.4 (1128.0)	1925.0 (966.9)
2108.9 (341.5)	2003.3 (853.0)	2065.3 (0.0)	1961.7 (0.0)

Table S16. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the triplet structures of $Co_2(CF)_2(CO)_3$

23T-1(C_1/C_s)		**23T-2**(C_s)	
B3LYP	BP86	B3LYP	BP86
10.4 (0.1)	39.3 (0.4)	4.2 (0.0)	-40.8 (0.0)
34.8 (0.3)	43.6 (0.1)	24.8 (0.1)	36.2 (0.1)
59.7 (0.0)	45.0 (0.0)	39.6 (0.1)	40.7 (0.2)
67.9 (0.1)	71.4 (0.2)	66.0 (0.1)	65.3 (0.2)
70.4 (0.1)	81.6 (0.0)	70.9 (0.1)	69.5 (0.0)
79.3 (0.0)	87.3 (0.2)	78.4 (0.1)	78.0 (0.0)
89.9 (2.4)	98.0 (0.3)	97.3 (1.4)	91.3 (0.9)
166.7 (1.9)	186.7 (0.0)	154.6 (1.6)	174.3 (0.1)
220.2 (0.8)	250.3 (1.3)	230.3 (0.2)	237.8 (0.1)
263.9 (0.5)	257.0 (0.4)	281.4 (1.5)	272.3 (0.5)
291.8 (0.3)	326.1 (4.0)	297.2 (0.2)	280.0 (1.4)
329.7 (0.1)	338.9 (1.2)	316.4 (1.2)	338.2 (1.0)
345.4 (0.1)	358.9 (4.1)	342.7 (2.2)	351.3 (3.5)
382.9 (2.0)	381.0 (8.7)	384.4 (0.3)	396.7 (2.9)
418.7 (23.4)	416.6 (1.5)	392.6 (5.5)	414.1 (0.8)
429.3 (11.5)	436.5 (0.6)	417.8 (1.1)	434.0 (0.5)
454.4 (59.8)	449.5 (0.6)	445.1 (46.2)	459.2 (6.5)
484.5 (1.8)	458.9 (10.4)	475.2 (43.6)	471.5 (15.1)
498.3 (20.3)	481.8 (9.7)	489.0 (1.4)	477.3 (2.1)
519.8 (2.7)	512.6 (8.2)	498.4 (14.0)	484.7 (9.5)
524.2 (3.1)	519.5 (23.7)	502.1 (0.0)	500.8 (11.8)
558.6 (61.7)	533.1 (7.4)	521.7 (0.5)	547.5 (25.0)
558.9 (2.6)	574.3 (10.1)	554.4 (61.0)	557.4 (13.3)
591.8 (33.1)	583.2 (22.4)	570.8 (27.3)	563.7 (23.1)
702.3 (229.9)	665.9 (60.1)	673.8 (193.1)	602.5 (54.4)
1290.5 (991.1)	1260.1 (883.4)	1287.8 (996.5)	1255.5 (983.9)
1338.6 (38.3)	1291.2 (10.9)	1331.2 (18.0)	1294.1 (3.6)
2081.1 (994.1)	1985.4 (1733.7)	2079.8 (859.3)	1980.4 (1720.0)
2090.3 (2265.1)	1990.5 (970.8)	2085.9 (2161.2)	1986.2 (952.5)
2125.8 (150.1)	2033.0 (364.4)	2124.3 (242.8)	2028.5 (331.9)

Table S17. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the triplet structures of $Co_2(CF)_2(CO)_3$

23T-3(C_1)		**23T-4**(C_1)	
B3LYP	BP86	B3LYP	BP86
26.5 (0.1)	16.6 (0.3)	19.4 (0.2)	28.6 (0.1)
42.8 (0.2)	41.5 (0.1)	26.6 (0.0)	40.4 (0.3)
55.3 (0.1)	49.9 (0.1)	39.8 (0.3)	50.4 (0.2)
57.3 (0.3)	55.1 (0.3)	60.5 (0.5)	67.0 (0.3)
59.8 (0.1)	58.2 (0.6)	70.2 (0.3)	77.1 (0.2)
72.6 (1.3)	65.7 (1.4)	74.2 (0.4)	82.9 (0.0)
94.8 (0.9)	91.7 (0.9)	85.0 (0.2)	86.8 (0.2)
151.2 (0.6)	173.6 (0.2)	89.1 (0.4)	182.5(0.1)
201.5 (3.0)	222.2 (0.6)	189.0 (4.9)	224.7 (1.7)
225.3 (0.1)	234.8 (3.7)	233.7 (0.2)	244.9 (0.3)
254.6 (14.2)	264.7 (0.6)	262.3 (4.4)	296.5 (6.4)
283.1 (10.5)	293.0 (3.8)	302.7 (3.2)	314.7 (1.5)
317.5 (2.9)	307.4 (2.4)	331.7 (9.4)	345.8 (1.4)
363.3 (1.4)	357.2 (2.5)	358.8 (5.1)	356.2 (0.0)
401.1 (0.5)	382.2 (0.6)	387.3 (3.5)	391.9 (10.9)
419.3 (14.0)	404.3 (3.0)	410.7 (13.1)	409.0 (4.4)
421.1 (11.7)	423.9 (9.8)	417.2 (24.0)	425.7 (2.9)
449.0 (10.8)	441.7 (5.0)	446.9 (10.0)	448.0 (8.4)
463.1 (27.7)	458.2 (5.8)	450.9 (3.2)	470.5 (8.8)
472.0 (37.0)	490.9 (12.0)	486.0 (3.2)	486.5 (3.3)
491.7 (33.3)	505.4 (36.4)	505.7 (18.3)	504.4 (15.3)
550.7 (19.5)	533.6 (16.1)	530.1 (76.0)	545.8 (32.4)
563.1 (69.9)	554.5 (37.5)	538.3 (13.5)	554.3 (16.5)
622.7 (31.3)	593.0 (54.8)	553.0 (48.1)	596.9 (37.6)
689.3 (100.4)	650.0 (40.1)	683.6 (23.9)	640.3 (18.1)
1283.4 (485.4)	1269.0 (473.3)	1301.3 (394.0)	1272.8 (393.9)
1459.5 (988.9)	1425.4 (931.5)	1445.8 (1101.5)	1396.4 (1054.0)
1974.0 (743.7)	1876.9 (584.9)	2041.8 (814.1)	1872.0 (571.3)
2078.0(2211.1)	1983.4 (1696.7)	2073.4 (1264.6)	1984.8 (838.9)
2110.1 (404.3)	2018.6 (461.4)	2115.6 (1129.9)	2023.2 (933.6)

Table S18. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Co_2(CF)_2(CO)_2$.

22S-1(C_{2v})		**22S-2(C_1)**		**22-3(C_1/C_s)**	
B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
43.7 (0.1)	44.4 (0.2)	32.1 (0.2)	30.1 (0.5)	14.5 (0.1)	21.0 (0.1)
68.7 (0.3)	71.3 (0.3)	47.0 (0.3)	48.9 (0.1)	35.6 (0.2)	26.1 (0.4)
76.3 (0.0)	77.5 (0.0)	66.9 (0.4)	68.4 (0.6)	55.3 (0.1)	44.7 (0.0)
90.5 (1.0)	82.9 (0.8)	72.1 (1.2)	73.2 (1.2)	60.0 (0.9)	54.8 (0.6)
90.5 (0.0)	91.8 (0.0)	91.0 (1.5)	89.8 (1.5)	71.7 (0.2)	78.9 (0.6)
221.8 (13.0)	230.7 (1.1)	122.5 (3.2)	120.6 (3.0)	91.6 (0.1)	174.4 (0.3)
234.0 (0.0)	233.7 (0.0)	228.7 (1.4)	225.4 (1.6)	186.9 (1.7)	177.4 (5.1)
241.1 (1.2)	236.5 (0.0)	253.7 (0.5)	261.1 (0.7)	224.8 (1.3)	225.5 (0.0)
241.6 (0.2)	249.1 (8.5)	314.6 (2.4)	307.9 (1.9)	283.3 (5.5)	252.8 (3.1)
377.9 (1.8)	379.3 (2.6)	365.6 (0.9)	348.9 (1.1)	296.7 (2.7)	300.3 (0.5)
449.2 (0.0)	458.6 (0.0)	394.5 (17.3)	385.9 (26.4)	333.5 (27.8)	302.8 (14.6)
455.3 (8.4)	463.2 (10.7)	422.2 (2.2)	421.2 (2.1)	346.1 (4.2)	404.6 (19.5)
459.8 (12.2)	472.1 (0.0)	446.6 (19.7)	446.5 (10.1)	405.2 (0.5)	415.2 (4.2)
469.6 (0.0)	497.2 (1.3)	462.6 (19.7)	478.3 (2.0)	464.3 (9.3)	423.5 (0.1)
484.0 (50.1)	506.8 (24.5)	482.3 (9.6)	483.3 (11.6)	474.9 (29.2)	467.4 (0.4)
487.5 (1.0)	510.5 (0.0)	505.3 (19.0)	521.8 (13.4)	505.0 (18.4)	470.7 (6.7)
506.9 (6.3)	518.9 (2.8)	549.1 (0.5)	542.1 (0.5)	540.8 (36.9)	489.4 (16.5)
527.2 (10.6)	527.9 (3.6)	626.7 (30.5)	612.2 (17.5)	590.4 (27.5)	577.9 (21.9)
592.0 (59.8)	613.7 (32.5)	660.0 (89.2)	637.4 (80.0)	646.8 (63.5)	608.4 (40.6)
654.8 (2.8)	633.1 (2.2)	736(132)	721(93.1)	663.0 (12.2)	635.0 (12.0)
1216(762.9)	1190(711.3)	1315(426.1)	1278(411.3)	1417(1635)	1374(1601)
1255(152.1)	1225(118.2)	1455(1204)	1420(1052)	1447(396.0)	1409(400.4)
2069(2408)	1977(1904)	1881(501)	1796(423.5)	1977 (699)	1880(1132)
2098(252.3)	2001(230.4)	2098(1342)	2002(1121)	2049(627)	1900(33.2)

Table S19. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(CF)_2(CO)_2$.

22T-1(C_1/C_2)		**22T-2**(C_s)	
B3LYP	BP86	B3LYP	BP86
30.9 (0.3)	20.6 (0.1)	28.2 (0.0)	-22.8 (0.2)
41.2 (0.4)	40.2 (0.1)	41.2 (0.7)	41.0 (0.4)
61.9 (0.6)	63.0 (1.3)	60.4 (1.4)	65.9 (0.8)
66.8 (0.0)	73.5 (0.2)	66.5 (0.0)	72.5 (0.2)
84.5 (1.3)	76.7 (3.4)	88.3 (1.3)	93.8 (1.7)
112.6 (0.9)	166.3 (10.2)	89.5 (2.1)	103.3 (1.9)
216.8 (0.2)	220.9 (0.2)	219.4 (0.8)	220.6 (0.3)
245.8 (0.7)	238.4 (0.0)	230.5 (7.5)	245.3 (5.0)
263.9 (1.5)	285.0 (2.5)	302.3 (0.4)	306.3 (0.0)
312.4 (3.0)	328.5 (0.2)	333.6 (0.3)	336.0 (1.0)
347.1 (2.7)	382.1 (0.1)	366.7 (7.4)	378.1 (10.4)
387.6 (0.6)	393.5 (56.9)	397.5 (0.5)	398.6 (0.9)
426.4 (6.7)	403.5 (3.6)	422.4 (13.3)	436.2 (6.3)
447.3 (63.2)	432.5 (15.2)	456.4 (0.2)	444.1 (1.2)
460.2 (23.9)	465.1 (2.9)	470.9 (0.8)	450.0 (0.7)
501.5 (12.8)	470.3 (38.4)	471.4 (41.6)	489.4 (21.3)
507.8 (8.4)	501.6 (0.0)	488.4 (3.6)	498.9 (5.5)
545.8 (12.4)	507.9 (2.1)	561.5 (48.8)	574.9 (20.0)
581.8 (8.3)	565.2 (2.3)	622.9 (89.6)	608.5 (8.9)
594.7 (31.6)	574.9 (5.5)	671.4 (64.7)	640.1 (26.1)
1270.0 (896.9)	1223.1 (864.2)	1318.8 (421.9)	1296.4 (404.1)
1291.4 (2.8)	1252.3 (14.2)	1450.8 (1032.8)	1439.9 (1156.8)
2084.7 (2244.5)	1975.4 (2083.1)	1927.1 (710.5)	1842.1 (583.7)
2115.5 (400.8)	2002.2 (264.2)	2109.2 (1308.6)	2006.8 (1200.7)

Table S20. Theoretical Cartesian coordinates (in Å) for the structure **13S-1** using the BP86/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.642572	-0.685361
2	6	0	-1.422509	-0.821286	-0.685361
3	6	0	1.422509	-0.821286	-0.685361
4	27	0	0.000000	0.000000	0.062358
5	8	0	0.000000	2.730812	-1.108774
6	8	0	2.364953	-1.365406	-1.108774
7	8	0	-2.364953	-1.365406	-1.108774
8	6	0	0.000000	0.000000	1.710042
9	9	0	0.000000	0.000000	3.000351

Table S21. Theoretical Cartesian coordinates (in Å) for the structure **12S-1** using the BP86/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.650401	0.577473	1.466626
2	27	0	-0.372245	-0.404248	0.000000
3	8	0	-0.650401	1.289642	-2.397138
4	8	0	-0.650401	1.289642	2.397138
5	6	0	-0.650401	0.577473	-1.466626
6	6	0	1.104297	-1.121356	0.000000
7	9	0	2.404007	-1.102346	0.000000

Table S22. Theoretical Cartesian coordinates (in Å) for the structure **12T-1** using the BP86/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.498200	-1.004868
2	27	0	0.000000	0.000000	0.029653
3	8	0	0.000000	-2.474851	-1.649316
4	8	0	0.000000	2.474851	-1.649316
5	6	0	0.000000	-1.498200	-1.004868
6	6	0	0.000000	0.000000	1.731415
7	9	0	0.000000	0.000000	3.028707

Table S23. Theoretical Cartesian coordinates (in Å) for the structure **11S-1** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.000000	0.777174	0.000000
2	8	0	2.240897	-1.064851	0.000000
3	6	0	1.432368	-0.206901	0.000000
4	6	0	-1.383059	-0.066148	0.000000
5	9	0	-2.024781	-1.202954	0.000000

Table S24. Theoretical Cartesian coordinates (in Å) for the structure **11T-1** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.000000	0.588875	0.000000
2	8	0	2.685565	-0.648733	0.000000
3	6	0	1.644805	-0.100196	0.000000
4	6	0	-1.528404	-0.128950	-0.000000
5	9	0	-2.464769	-1.037208	-0.000000

Table S25. Theoretical Cartesian coordinates (in Å) for the structure **26S-1** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.000000	1.255914	-0.078926
2	27	0	0.000000	-1.255914	-0.078926
3	6	0	-1.432707	1.608459	-1.147527
4	6	0	1.432707	-1.608459	-1.147527
5	6	0	-0.690054	0.000000	1.239216
6	6	0	0.690054	0.000000	1.239216
7	6	0	0.000000	2.737286	0.913446
8	6	0	1.432707	1.608459	-1.147527
9	6	0	0.000000	-2.737286	0.913446
10	8	0	-2.374009	1.828428	-1.798899
11	8	0	2.374009	-1.828428	-1.798899
12	8	0	0.000000	3.713475	1.552301
13	8	0	2.374009	1.828428	-1.798899
14	8	0	0.000000	-3.713475	1.552301
15	9	0	1.678558	0.000000	2.149925
16	9	0	-1.678558	0.000000	2.149925
17	6	0	-1.432707	-1.608459	-1.147527
18	8	0	-2.374009	-1.828428	-1.798899

Table S26. Theoretical Cartesian coordinates (in Å) for the structure **26S-2** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-1.190547	-0.006881	-0.100610
2	27	0	1.323509	-0.213953	0.146528
3	6	0	-2.054556	-1.455335	-0.716813
4	6	0	0.265821	-0.455993	-1.392582
5	6	0	3.008954	-0.310002	-0.329023
6	6	0	1.206426	1.609353	0.125785
7	6	0	-0.046937	1.430230	0.645901
8	6	0	-2.046309	1.259115	-1.055344
9	6	0	-1.841534	-0.287938	1.575622
10	6	0	1.225747	-1.863198	0.885495
11	8	0	-2.649812	-2.374964	-1.113817
12	8	0	0.380251	-0.733258	-2.539490
13	8	0	4.126538	-0.353024	-0.665937
14	8	0	-2.628722	2.078816	-1.644326
15	8	0	-2.279043	-0.461932	2.640941
16	8	0	1.181860	-2.904553	1.411220
17	9	0	-0.575301	2.268429	1.591043
18	9	0	2.025944	2.664512	0.144206

Table S27. Theoretical Cartesian coordinates (in Å) for the structure **26S-3** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.823049	-1.195293	0.000000
2	6	0	-1.268163	0.013618	0.686394
3	27	0	0.032186	-1.283771	0.000000
4	27	0	0.099310	1.234369	0.000000
5	6	0	-1.268163	0.013618	-0.686394
6	6	0	1.161040	1.567280	-1.448789
7	6	0	1.161040	1.567280	1.448789
8	6	0	-0.866708	2.731788	0.000000
9	6	0	-0.224938	-2.326294	-1.433039
10	6	0	-0.224938	-2.326294	1.433039
11	8	0	-1.473804	3.727728	0.000000
12	8	0	1.795346	1.772528	2.403858
13	8	0	-0.421119	-3.025197	-2.347802
14	8	0	-0.421119	-3.025197	2.347802
15	8	0	2.992435	-1.188279	0.000000
16	9	0	-2.191132	0.043709	-1.660087
17	8	0	1.795346	1.772528	-2.403858
18	9	0	-2.191132	0.043709	1.660087

Table S28. Theoretical Cartesian coordinates (in Å) for the structure **26S-4** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.000000	1.295200	0.071382
2	27	0	0.000000	-1.295200	0.071382
3	6	0	0.000000	1.415988	1.871768
4	6	0	1.436910	-2.315037	-0.234614
5	6	0	-0.683587	0.000000	-1.246272
6	6	0	0.683587	0.000000	-1.246272
7	6	0	-1.436910	2.315037	-0.234614
8	6	0	1.436910	2.315037	-0.234614
9	6	0	-1.436910	-2.315037	-0.234614
10	8	0	0.000000	1.621037	3.021463
11	8	0	2.348129	-3.010131	-0.457312
12	8	0	-2.348129	3.010131	-0.457312
13	8	0	2.348129	3.010131	-0.457312
14	8	0	-2.348129	-3.010131	-0.457312
15	9	0	1.635496	0.000000	-2.191070
16	9	0	-1.635496	0.000000	-2.191070
17	6	0	0.000000	-1.415988	1.871768
18	8	0	0.000000	-1.621037	3.021463

Table S29. Theoretical Cartesian coordinates (in Å) for the structure **26T-1** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.747037	1.269998	-1.759478
2	6	0	-0.243072	0.636707	1.660573
3	27	0	0.000430	1.286030	-0.106613
4	27	0	-0.000430	-1.286030	-0.106613
5	6	0	0.243072	-0.636707	1.660573
6	6	0	1.737822	-1.621963	-0.501806
7	6	0	-0.747037	-1.269998	-1.759478
8	6	0	-0.624366	-2.872668	0.468079
9	6	0	0.624366	2.872668	0.468079
10	6	0	-1.737822	1.621963	-0.501806
11	8	0	-1.003921	-3.905096	0.854842
12	8	0	-1.243667	-1.298436	-2.815808
13	8	0	1.003921	3.905096	0.854842
14	8	0	-2.871724	1.830601	-0.681158
15	8	0	1.243667	1.298436	-2.815808
16	9	0	0.624366	-1.334628	2.756815
17	8	0	2.871724	-1.830601	-0.681158
18	9	0	-0.624366	1.334628	2.756815

Table S30. Theoretical Cartesian coordinates (in Å) for the structure **26T-2** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.040726	1.516047	-0.000000
2	27	0	-0.093925	-1.447730	0.000000
3	6	0	-1.788329	1.369240	-0.000000
4	6	0	-1.112547	-1.836446	1.457257
5	6	0	1.025917	-0.012459	-0.702494
6	6	0	1.025917	-0.012459	0.702494
7	6	0	0.244461	2.612767	-1.432287
8	6	0	0.244461	2.612767	1.432287
9	6	0	0.973354	-2.936014	0.000000
10	8	0	-2.954526	1.321404	-0.000000
11	8	0	-1.730974	-2.064790	2.419528
12	8	0	0.422397	3.296583	-2.359905
13	8	0	0.422397	3.296583	2.359905
14	8	0	1.676737	-3.865981	0.000000
15	9	0	1.977322	-0.053464	1.659964
16	9	0	1.977322	-0.053464	-1.659964
17	6	0	-1.112547	-1.836446	-1.457257
18	8	0	-1.730974	-2.064790	-2.419528

Table S31. Theoretical Cartesian coordinates (in Å) for the structure **26T-3** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.000000	1.497628	-0.075652
2	27	0	-0.000000	-1.497628	-0.075652
3	6	0	-1.444904	1.905090	-1.095855
4	6	0	-1.444904	-1.905090	-1.095855
5	6	0	0.705570	-0.000000	0.951903
6	6	0	-0.705570	0.000000	0.951903
7	6	0	1.444904	1.905090	-1.095855
8	6	0	0.000000	2.966976	1.020822
9	6	0	-0.000000	-2.966976	1.020822
10	8	0	-2.397876	2.137477	-1.727406
11	8	0	-2.397876	-2.137477	-1.727406
12	8	0	2.397876	2.137477	-1.727406
13	8	0	0.000000	3.881564	1.744056
14	8	0	-0.000000	-3.881564	1.744056
15	9	0	-1.672186	0.000000	1.893619
16	9	0	1.672186	-0.000000	1.893619
17	6	0	1.444904	-1.905090	-1.095855
18	8	0	2.397876	-2.137477	-1.727406

Table S32. Theoretical Cartesian coordinates (in Å) for the structure **25S-1** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	1.224574	0.154980	-0.004211
2	27	0	-1.182101	-0.027228	-0.033447
3	6	0	-0.495146	-1.161392	1.230160
4	6	0	2.084668	1.636125	0.471648
5	6	0	-2.340618	0.922059	0.914904
6	6	0	-0.119044	1.299927	-0.879919
7	6	0	0.266990	-1.483930	0.129948
8	6	0	-2.263410	-0.380561	-1.401815
9	6	0	2.701454	-0.702800	-0.421313
10	8	0	3.674637	-1.237881	-0.783129
11	8	0	2.675066	2.559741	0.875450
12	8	0	-3.102218	1.508199	1.577427
13	8	0	-2.979033	-0.686715	-2.272246
14	8	0	-0.129238	2.249645	-1.589688
15	9	0	0.489111	-2.704110	-0.417211
16	9	0	-0.630203	-1.670309	2.449718

Table S33. Theoretical Cartesian coordinates (in Å) for the structure **25S-2** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.530672	-1.090384	0.031753
2	27	0	0.530672	1.090384	0.031753
3	6	0	-0.391880	0.561241	-1.483839
4	6	0	-2.081695	-1.457928	0.829087
5	6	0	-0.000000	2.769611	-0.028754
6	6	0	0.000000	0.000000	1.513191
7	6	0	0.391880	-0.561241	-1.483839
8	6	0	2.081695	1.457928	0.829087
9	6	0	-0.000000	-2.769611	-0.028754
10	8	0	0.386234	-3.871841	-0.036961
11	8	0	-3.140845	-1.711862	1.250123
12	8	0	-0.386234	3.871841	-0.036961
13	8	0	3.140845	1.711862	1.250123
14	8	0	0.000000	0.000000	2.701268
15	9	0	1.165306	-1.129437	-2.422914
16	9	0	-1.165306	1.129437	-2.422914

Table S34. Theoretical Cartesian coordinates (in Å) for the structure **25S-3** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.130323	-1.442834	-0.482058
2	6	0	1.757953	1.314946	-1.056674
3	6	0	-2.333811	-1.284473	1.026141
4	8	0	2.266234	2.112498	-1.741094
5	8	0	2.820481	-2.331044	-0.797182
6	27	0	-1.370330	-0.011989	0.139633
7	27	0	1.135084	-0.044662	-0.015942
8	6	0	1.902690	0.088246	1.622935
9	6	0	-0.278706	-0.800550	-1.010760
10	6	0	-0.429849	1.169309	0.932812
11	6	0	-2.570883	0.842145	-0.830584
12	8	0	-3.383615	1.404839	-1.457818
13	9	0	-0.118356	2.356638	1.382671
14	8	0	-3.001776	-2.053979	1.595973
15	9	0	-0.271932	-1.481538	-2.134781
16	8	0	2.398418	0.159302	2.677429

Table S35. Theoretical Cartesian coordinates (in Å) for the structure **25S-4** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.176611	1.325498	2.446502
2	8	0	-1.771936	1.698717	-2.407851
3	8	0	-3.434160	-2.047767	-0.399774
4	8	0	2.891212	-0.689437	2.306742
5	8	0	0.829358	2.946466	0.353389
6	27	0	1.315842	0.035142	-0.068255
7	27	0	-1.295321	-0.069078	-0.043844
8	6	0	0.943687	1.794036	0.199563
9	6	0	2.235328	-0.401979	1.382700
10	6	0	-1.594537	1.044167	-1.457367
11	6	0	-1.820396	0.829986	1.450978
12	6	0	-2.582005	-1.258997	-0.263739
13	6	0	-0.036583	-1.268713	0.095544
14	6	0	2.325485	-0.264255	-1.352882
15	9	0	0.096233	-2.575136	0.203189
16	9	0	3.450117	-0.513423	-1.946987

Table S36. Theoretical Cartesian coordinates (in Å) for the structure **25T-1** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.005624	0.021407	1.197787
2	27	0	0.005624	0.021407	-1.197787
3	6	0	0.242456	1.607116	0.000000
4	6	0	1.451930	-0.117385	2.257149
5	6	0	1.451930	-0.117385	-2.257149
6	6	0	0.357939	-1.478841	0.000000
7	6	0	-1.050559	1.210552	0.000000
8	6	0	-1.199829	-0.637057	-2.362500
9	6	0	-1.199829	-0.637057	2.362500
10	8	0	-1.979628	-1.040825	3.131384
11	8	0	2.373850	-0.169972	2.971637
12	8	0	2.373850	-0.169972	-2.971637
13	8	0	-1.979628	-1.040825	-3.131384
14	8	0	0.619958	-2.633045	0.000000
15	9	0	-2.279994	1.740922	0.000000
16	9	0	0.958314	2.737021	0.000000

Table S37. Theoretical Cartesian coordinates (in Å) for the structure **24S-1** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.000000	-0.000000	1.182925
2	27	0	-0.000000	-0.000000	-1.182925
3	6	0	-0.000000	1.329676	-2.359449
4	6	0	-1.118235	0.814390	-0.000000
5	6	0	1.118235	-0.814390	-0.000000
6	6	0	0.000000	-1.329676	-2.359449
7	9	0	-1.928967	1.853527	-0.000000
8	8	0	-0.089512	-2.193633	-3.141827
9	6	0	-0.000000	1.329676	2.359449
10	6	0	0.000000	-1.329676	2.359449
11	8	0	0.089512	2.193633	3.141827
12	8	0	-0.089512	-2.193633	3.141827
13	8	0	0.089512	2.193633	-3.141827
14	9	0	1.928967	-1.853527	-0.000000

Table S38. Theoretical Cartesian coordinates (in Å) for the structure **24S-2** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.412093	-1.507895	0.086436
2	6	0	-2.690382	0.200015	-0.425890
3	6	0	-0.787181	2.064325	-0.543816
4	6	0	-0.343727	-0.730037	1.223182
5	6	0	2.139655	0.896633	0.951577
6	6	0	2.113849	-0.672120	-1.348701
7	8	0	2.665442	1.823314	1.433483
8	8	0	-0.669518	3.225492	-0.589333
9	8	0	-3.859319	0.134205	-0.435744
10	8	0	2.598475	-0.762258	-2.408620
11	9	0	-0.830135	-2.752265	-0.227957
12	9	0	-0.758011	-0.772677	2.497796
13	27	0	-0.941759	0.274938	-0.363712
14	27	0	1.248868	-0.465571	0.212469

Table S39. Theoretical Cartesian coordinates (in Å) for the structure **24S-3** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.638751	-0.478135	0.700963
2	6	0	0.115096	1.223076	2.086917
3	6	0	-1.849970	-0.458708	1.622085
4	6	0	1.638751	-0.478135	-0.700963
5	6	0	0.115096	1.223076	-2.086917
6	6	0	-1.849970	-0.458708	-1.622085
7	8	0	0.269229	2.294165	-2.538011
8	8	0	-2.998654	-0.554600	1.819536
9	8	0	0.269229	2.294165	2.538011
10	8	0	-2.998654	-0.554600	-1.819536
11	9	0	2.755057	-0.815189	1.393442
12	9	0	2.755057	-0.815189	-1.393442
13	27	0	-0.088273	-0.307304	1.327466
14	27	0	-0.088273	-0.307304	-1.327466

Table S40. Theoretical Cartesian coordinates (in Å) for the structure **24S-4** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	1.299112	0.469371	0.000000
2	27	0	-1.062047	-0.239685	0.000000
3	8	0	-1.021506	-2.064707	2.345730
4	6	0	-1.021506	-1.374940	-1.402437
5	6	0	-0.296085	1.356445	0.000000
6	6	0	-1.021506	-1.374940	1.402437
7	6	0	-2.725286	0.387619	0.000000
8	6	0	1.820763	-1.269957	0.000000
9	6	0	2.556151	1.497007	0.000000
10	9	0	3.601271	2.250949	0.000000
11	8	0	2.229014	-2.364134	0.000000
12	8	0	-1.021506	-2.064707	-2.345730
13	9	0	-0.628144	2.632068	0.000000
14	8	0	-3.815260	0.809039	0.000000

Table S41. Theoretical Cartesian coordinates (in Å) for the structure **24S-5** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-1.273828	0.000616	0.321310
2	27	0	1.134634	-0.030226	0.047872
3	8	0	0.924570	1.432702	2.633712
4	6	0	1.822664	1.178108	-1.098390
5	6	0	-0.121774	-1.097005	-0.575019
6	6	0	1.009548	0.865215	1.613240
7	6	0	2.451682	-1.214615	0.178887
8	6	0	-1.770607	1.537439	-0.083461
9	6	0	-2.749858	-0.977880	0.246675
10	8	0	2.270016	1.919001	-1.884077
11	9	0	-0.287046	-2.210668	-1.260614
12	8	0	3.313706	-2.001163	0.254122
13	9	0	-2.183205	2.314415	-1.035497
14	8	0	-3.740722	-1.585770	0.121930

Table S42. Theoretical Cartesian coordinates (in Å) for the structure **24S-6** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.063591	0.000000	-0.726799
2	6	0	0.000000	1.755169	1.896140
3	6	0	0.000000	2.686568	-0.864745
4	6	0	0.000000	-2.686568	-0.864745
5	6	0	0.000000	-1.755169	1.896140
6	6	0	1.063591	0.000000	-0.726799
7	8	0	0.000000	-2.078603	3.015385
8	8	0	0.000000	2.078603	3.015385
9	9	0	-1.777602	0.000000	-1.835664
10	8	0	0.000000	-3.641026	-1.543583
11	8	0	0.000000	3.641026	-1.543583
12	9	0	1.777602	0.000000	-1.835664
13	27	0	0.000000	1.210238	0.108110
14	27	0	0.000000	-1.210238	0.108110

Table S43. Theoretical Cartesian coordinates (in Å) for the structure **24S-7** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.037948	1.035219	-0.773827
2	6	0	2.343704	1.061781	0.706454
3	6	0	2.153017	-1.266595	-0.665590
4	6	0	-2.518113	1.204363	0.032760
5	6	0	-0.058419	-0.788770	1.355082
6	6	0	-2.198031	-1.490904	-0.297515
7	8	0	-0.177279	-1.423859	2.343025
8	8	0	3.138457	1.821440	1.102690
9	8	0	-2.834912	-2.407659	-0.644633
10	9	0	0.102549	2.189779	-1.402218
11	9	0	3.063475	-1.720194	-1.463229
12	8	0	-3.377181	1.993961	0.128745
13	27	0	1.186694	-0.105090	0.034881
14	27	0	-1.225491	0.007761	-0.027244

Table S44. Theoretical Cartesian coordinates (in Å) for the structure **24S-8** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.771087	1.309519	-1.041757
2	6	0	-2.540800	-0.899231	0.496634
3	6	0	-0.262524	0.916841	1.302604
4	6	0	2.565196	-1.229534	0.147922
5	6	0	2.125443	1.471254	-0.173637
6	6	0	0.075613	-1.097870	-0.693993
7	8	0	2.717325	2.379122	-0.613216
8	8	0	-2.197953	2.122807	-1.763259
9	9	0	0.082517	-2.206427	-1.401250
10	8	0	3.451799	-1.993430	0.181044
11	9	0	-3.686782	-1.431295	0.754379
12	8	0	-0.087089	1.565139	2.274136
13	27	0	-1.227144	-0.022679	0.035276
14	27	0	1.235095	-0.076413	0.148634

Table S45. Theoretical Cartesian coordinates (in Å) for the structure **24T-1** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.111889	1.272191	-0.705371
2	6	0	-2.681546	0.107557	-0.584862
3	6	0	-1.505731	-0.951173	1.755341
4	6	0	0.578442	1.377578	0.465582
5	6	0	2.791263	-0.306291	0.343042
6	6	0	0.928529	-1.612880	-1.361344
7	8	0	3.931068	-0.220721	0.584983
8	8	0	-1.703548	-1.734265	2.600616
9	8	0	-3.620952	0.025473	-1.273746
10	8	0	0.856768	-2.308677	-2.296588
11	9	0	-0.248325	2.020634	-1.813034
12	9	0	1.162612	2.370667	1.157787
13	27	0	-1.187571	0.198514	0.398333
14	27	0	1.042027	-0.381406	-0.046453

Table S46. Theoretical Cartesian coordinates (in Å) for the structure **23S-1** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	1.234357	0.630705	-0.000053
2	27	0	-1.041661	0.065834	-0.000059
3	8	0	4.060067	-0.143279	0.000031
4	6	0	-1.965946	1.668302	-0.000148
5	6	0	-2.201213	-1.279616	0.000057
6	6	0	0.258101	-0.285681	-1.201712
7	6	0	0.258011	-0.285371	1.201778
8	6	0	2.951789	0.245450	0.000020
9	8	0	-2.518320	2.695484	-0.000135
10	8	0	-2.931950	-2.195240	0.000140
11	9	0	0.561837	-1.224230	2.073665
12	9	0	0.561983	-1.224745	-2.073356

Table S47. Theoretical Cartesian coordinates (in Å) for the structure **23S-2** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.883579	-0.673107	0.000000
2	6	0	-0.157317	-0.351947	1.201159
3	6	0	-0.157317	-0.351947	-1.201159
4	6	0	2.488877	-0.540352	0.000000
5	6	0	1.354124	2.192919	0.000000
6	8	0	-3.818419	-1.384067	0.000000
7	8	0	3.465860	-1.186769	0.000000
8	8	0	1.559416	3.341004	0.000000
9	9	0	-0.157317	-1.340428	-2.071139
10	9	0	-0.157317	-1.340428	2.071139
11	27	0	-1.367622	0.221225	0.000000
12	27	0	0.971626	0.382959	0.000000

Table S48. Theoretical Cartesian coordinates (in Å) for the structure **23S-3** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.394059	1.321890	0.000000
2	27	0	0.562515	-0.856133	0.000000
3	6	0	0.719003	-1.915798	1.440528
4	6	0	0.719003	-1.915798	-1.440528
5	6	0	-1.126062	-0.296154	0.000000
6	6	0	1.419548	1.044143	0.000000
7	6	0	-1.315706	2.663758	0.000000
8	8	0	0.719003	-2.621636	-2.371829
9	8	0	2.599140	0.923766	0.000000
10	9	0	-2.257895	-0.958886	0.000000
11	8	0	0.719003	-2.621636	2.371829
12	9	0	-2.113240	3.681076	0.000000

Table S49. Theoretical Cartesian coordinates (in Å) for the structure **23S-4** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	1.393733	0.354843	-0.111041
2	27	0	-1.031597	0.078226	-0.064360
3	6	0	-2.145882	-0.421760	-1.171368
4	6	0	-1.797956	0.077865	1.550114
5	6	0	0.457170	-1.040798	0.123234
6	6	0	-0.164102	1.670609	-0.232133
7	6	0	3.042811	-0.239678	-0.048324
8	8	0	-2.357795	0.047904	2.575298
9	8	0	0.278158	2.762034	-0.405348
10	9	0	-3.157229	-0.874295	-1.833349
11	8	0	4.120944	-0.700566	0.001454
12	9	0	0.661630	-2.330734	0.281735

Table S50. Theoretical Cartesian coordinates (in Å) for the structure **23S-5** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.683828	0.479784	0.000000
2	6	0	0.221550	-0.902599	1.404768
3	6	0	0.221550	-0.902599	-1.404768
4	6	0	-0.311757	1.302360	0.000000
5	6	0	-2.865021	-0.229273	0.000000
6	8	0	0.221550	-1.472979	-2.436234
7	8	0	0.221550	-1.472979	2.436234
8	8	0	-4.035886	-0.141873	0.000000
9	9	0	3.906256	0.884650	0.000000
10	9	0	-0.641609	2.567075	0.000000
11	27	0	1.092621	0.092092	0.000000
12	27	0	-1.105230	-0.271682	0.000000

Table S51. Theoretical Cartesian coordinates (in Å) for the structure **23S-6** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.000000	0.000000	1.090498
2	27	0	0.000000	0.000000	-1.090498
3	8	0	0.000000	2.806091	0.000000
4	8	0	2.430146	-1.403045	0.000000
5	8	0	-2.430146	-1.403045	0.000000
6	6	0	0.000000	1.626563	0.000000
7	6	0	-1.408645	-0.813281	0.000000
8	6	0	1.408645	-0.813281	0.000000
9	6	0	0.000000	0.000000	2.720277
10	6	0	0.000000	0.000000	-2.720277
11	9	0	0.000000	0.000000	-4.009141
12	9	0	0.000000	0.000000	4.009141

Table S52. Theoretical Cartesian coordinates (in Å) for the structure **23T-1** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	1.374137	-0.278930	-0.446039
2	27	0	-0.928712	0.062141	-0.030525
3	8	0	4.019767	0.126861	0.802413
4	6	0	-2.346908	-0.897618	-0.495202
5	6	0	-1.812511	1.299844	0.877143
6	6	0	0.157153	-1.324434	0.404010
7	6	0	0.343504	1.171759	-0.732118
8	6	0	3.006827	-0.078548	0.249366
9	8	0	-3.288697	-1.493757	-0.853013
10	8	0	-2.383966	2.077808	1.539060
11	9	0	0.508539	2.460179	-0.955373
12	9	0	0.059049	-2.555736	0.859853

Table S53. Theoretical Cartesian coordinates (in Å) for the structure **23T-2** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.250669	-1.936827	0.000000
2	6	0	-0.287474	0.054474	1.404840
3	6	0	-0.287474	0.054474	-1.404840
4	6	0	2.312551	-0.220395	-0.000000
5	6	0	1.310389	2.232887	-0.000000
6	8	0	-2.674345	-3.030334	0.000000
7	8	0	3.358063	-0.748650	-0.000000
8	8	0	1.688812	3.340754	-0.000000
9	9	0	-0.287474	-0.160942	-2.702820
10	9	0	-0.287474	-0.160942	2.702820
11	27	0	-1.415097	-0.357987	0.000000
12	27	0	0.726592	0.554103	-0.000000

Table S54. Theoretical Cartesian coordinates (in Å) for the structure **23T-3** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	1.411361	0.149307	-0.201652
2	27	0	-0.988623	0.013623	-0.019531
3	6	0	-2.270840	-0.397658	-0.979546
4	6	0	-1.616446	0.433391	1.598537
5	6	0	0.304762	-1.250610	0.140403
6	6	0	0.028185	1.575553	-0.493637
7	6	0	3.178568	-0.064344	-0.009716
8	8	0	-2.081658	0.641138	2.651546
9	8	0	-0.037094	2.709630	-0.837767
10	9	0	-3.320212	-0.862391	-1.571255
11	8	0	4.320516	-0.278945	0.153578
12	9	0	0.345387	-2.554463	0.315346

Table S55. Theoretical Cartesian coordinates (in Å) for the structure **23T-4** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-1.328430	-0.445732	-0.448650
2	27	0	0.956207	0.054235	-0.028674
3	6	0	2.414828	-0.806293	-0.596614
4	6	0	1.783051	1.320405	0.884532
5	6	0	-0.398043	1.055385	-0.714213
6	6	0	0.006915	-1.440476	0.620246
7	6	0	-2.894701	-0.244312	0.064137
8	8	0	2.323601	2.144571	1.516776
9	8	0	0.012580	-2.435504	1.268731
10	9	0	-0.673020	2.326604	-0.927326
11	8	0	3.375924	-1.300499	-1.046050
12	9	0	-3.895771	0.339355	0.641052

Table S56. Theoretical Cartesian coordinates (in Å) for the structure **22S-1** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.000000	1.178800	-0.652043
2	27	0	0.000000	-1.178800	-0.652043
3	8	0	0.000000	3.561825	1.060352
4	8	0	0.000000	-3.561825	1.060352
5	6	0	0.000000	2.665136	0.301620
6	6	0	1.235588	0.000000	-0.116421
7	6	0	-1.235588	0.000000	-0.116421
8	6	0	0.000000	-2.665136	0.301620
9	9	0	2.096966	0.000000	0.890129
10	9	0	-2.096966	0.000000	0.890129

Table S57. Theoretical Cartesian coordinates (in Å) for the structure **22S-2** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-1.110233	0.337308	0.103596
2	27	0	1.190419	0.147854	-0.472087
3	6	0	-2.756053	-0.294730	0.165601
4	6	0	0.347787	1.703840	-0.123960
5	6	0	-0.145947	-1.062486	-0.181341
6	6	0	2.667059	-0.324907	0.044852
7	9	0	3.665607	-0.669185	0.790108
8	8	0	-0.359589	2.575568	0.310276
9	8	0	-3.807642	-0.813474	0.159949
10	9	0	-0.277193	-2.367086	-0.039383

Table S58. Theoretical Cartesian coordinates (in Å) for the structure **22S-3** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.972518	0.000007	0.572336
2	27	0	1.089420	-0.000008	-0.367837
3	6	0	-2.586765	0.000010	0.339351
4	6	0	-0.018101	1.509168	-0.245786
5	6	0	-0.018128	-1.509166	-0.245793
6	6	0	2.689267	-0.000015	-0.034521
7	9	0	3.844042	-0.000009	0.551715
8	9	0	-3.705221	0.000006	-0.317159
9	8	0	-0.300186	2.650469	-0.407003
10	8	0	-0.300238	-2.650463	-0.406994

Table S59. Theoretical Cartesian coordinates (in Å) for the structure **22T-1** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-1.178898	-0.036904	-0.513753
2	27	0	1.178898	0.036904	-0.513753
3	8	0	-3.574683	-0.335104	1.169738
4	8	0	3.574683	0.335104	1.169738
5	6	0	-2.668930	-0.212908	0.433088
6	6	0	0.001660	1.354181	-0.258774
7	6	0	-0.001660	-1.354181	-0.258774
8	6	0	2.668930	0.212908	0.433088
9	9	0	-0.001660	2.506453	0.385283
10	9	0	0.001660	-2.506453	0.385283

Table S60. Theoretical Cartesian coordinates (in Å) for the structure **22T-2** using the BP86/DZP method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-1.205936	-0.197649	0.000000
2	27	0	1.151656	-0.236612	0.000000
3	6	0	-2.819258	0.564076	0.000000
4	6	0	0.193171	-1.758549	0.000000
5	6	0	0.000000	1.123192	0.000000
6	6	0	2.777138	0.038361	0.000000
7	9	0	4.042012	0.297850	0.000000
8	8	0	-0.510661	-2.724638	0.000000
9	8	0	-3.838646	1.140224	0.000000
10	9	0	-0.113822	2.435246	0.000000

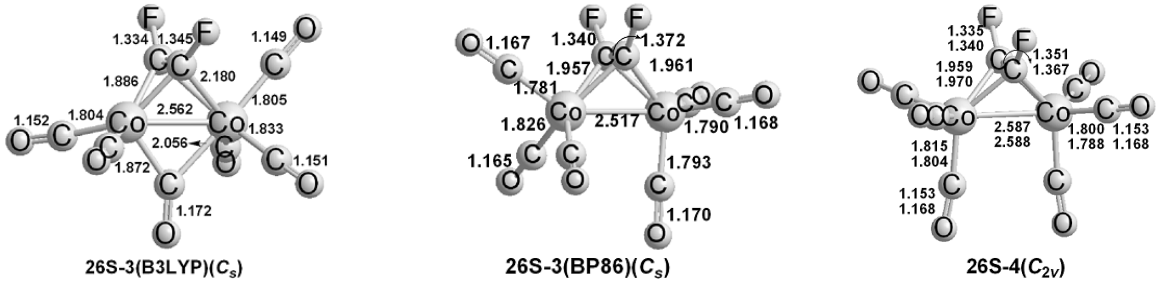

Figure S1. More optimized structures of $Co_2(CF)_2(CO)_6$ with higher energies.

Table S61 Total energies (*E*, in hartree), relative energies (Δ*E*, in kcal/mol), and numbers of imaginary vibrational frequencies (NImag) for the high-lyiing $Co_2(CF)_2(CO)_6$ structures.

Species	B3LYP			BP86		
	$-E_{total}$	ΔE	NImag	$-E_{total}$	ΔE	NImag
26S-3(C_s)	3721.70912	11.1	none	3722.25410	4.4	1 (37*i*)
26S-4(C_{2v})	3721.69911	17.4	2 (60*i*,50*i*)	3722.24158	12.3	2 (48*i*,42*i*)

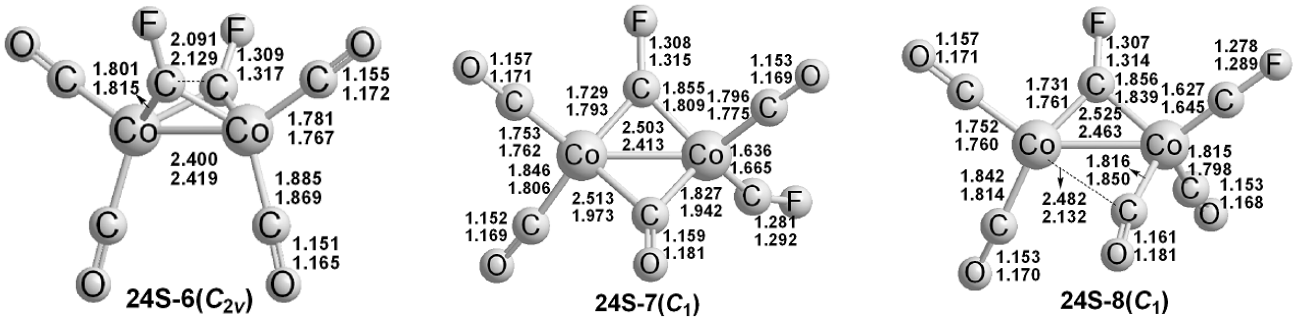

Figure S2. More optimized structures of $Co_2(CF)_2(CO)_4$ with higher energies.

Table S62 Total energies (*E*, in hartree), relative energies (Δ*E*, in kcal/mol), and numbers of imaginary vibrational frequencies (NImag) for the high-lying $Co_2(CF)_2(CO)_4$ structures.

Species	B3LYP			BP86		
	$-E_{total}$	ΔE	Nimag	$-E_{total}$	ΔE	Nimag
24S-6(C_{2v})	3494.94174	32.4	1 (87*i*)	3495.47403	–0.3	1 (90*i*)
24S-7(C_1)	3494.94140	32.6	none	3495.47008	2.2	none
24S-8(C_1)	3494.94074	33.0	none	3495.46940	2.6	none

Complete Gaussian 03 reference (Reference 44)

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