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Mononuclear and Binuclear Cobalt Carbonyl Nitrosyls: Comparison with Isoelectronic Nickel Carbonyls

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Supporting Information

Tables S1-S17: The theoretical harmonic vibrational frequencies for the 32 structures of $Co_2(NO)_2(CO)_n$ (n = 5, 4, 3, 2) and $Co(NO)(CO)_m$ (m = 4, 3, 2, 1) using the BP86 and B3LYP method.

Tables S18-S49: Theoretical Cartesian coordinates for the 32 structures of $Co_2(NO)_2(CO)_n$ (n = 5, 4, 3, 2) and $Co(NO)(CO)_m$ (m = 4, 3, 2, 1) using the BP86/DZP method.

Table S1. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co(NO)(CO)_4$ by BP86/DZP method (infrared intensities in parentheses are in km/mol).

14S-1(C_s)		**14T-1(C_S)**	
BP86	B3LYP	BP86	B3LYP
50.5(a",0.0)	55.9 (a", 0.0)	47.6(a',0.1)	8.7 (a", 0.0)
56.3(a',0.1)	57.1 (a', 0.1)	52.4(a",0.1)	22.5 (a", 0.0)
78.0(a',0.1)	82.5 (a', 0.1)	64.7(a",0.0)	30.7 (a", 0.1)
79.7(a",0.0)	82.8 (a", 0.1)	76.7(a',0.0)	36.4 (a", 0.1)
87.6(a',0.0)	90.2 (a", 0.0)	81.2(a",0.0)	58.5 (a", 0.0)
90.3(a",0.0)	92.9 (a', 0.1)	87.4(a',0.1)	60.7 (a", 0.0)
103.2(a',0.0)	109.1 (a', 0.2)	91.2(a',0.1)	75.5 (a", 0.2)
152.9(a",0.2)	160.7 (a", 1.2)	96.2(a",0.7)	78.1 (a", 0.2)
222.5(a',31.4)	242.2 (a', 27.9)	171.7(a',11.3)	83.6 (a", 0.4)
314.8(a",0.1)	320.2 (a", 0.3)	281.0(a',1.9)	110.7 (a", 0.4)
334.9(a',8.4)	337.4 (a', 17.1)	306.9(a",0.3)	287.2 (a", 0.2)
345.9(a",0.0)	361.2 (a", 0.5)	333.0(a",1.1)	311.9 (a", 0.0)
380.6(a',5.6)	367.6 (a', 6.2)	338.4(a',1.7)	343.8 (a", 4.5)
415.9(a',8.5)	390.2 (a', 11.1)	389.8(a',0.7)	368.1 (a', 0.1)
441.3(a',20.9)	420.3 (a', 22.4)	434.4(a',4.2)	410.8 (a", 18.4)
458.2(a",4.9)	463.5 (a", 12.7)	439.7(a",12.0)	413.9 (a", 2.9)
473.0(a',2.7)	467.4 (a", 35.0)	448.2(a',9.0)	423.5 (a", 0.1)
489.1(a",5.5)	481.7 (a', 3.5)	453.3(a',4.6)	449.0 (a", 17.2)
498.9(a',10.9)	504.6 (a', 21.3)	458.1(a",6.7)	472.8 (a", 65.7)
507.6(a",60.3)	511.8 (a", 29.7)	500.8(a",39.8)	474.3 (a", 25.7)
526.6(a',82.3)	527.8 (a', 78.0)	513.1(a',55.7)	486.7 (a", 56.9)
562.8(a',38.5)	580.5 (a', 29.7)	516.4(a',65.8)	862.1 (a", 216.7)
1693.1(a',734.2)	1714.8 (a', 882.3)	1630.1(a',565.7)	1969.2 (a', 67.1)
1995.9(a",993.4)	2085.4(a",1142.4)	2005.2(a",1017.2)	2074.9(a',1247.3)
2001.7(a',982.4)	2093.0(a',1009.5)	2009.4(a',534.6)	2087.7 (a', 777.8)
2005.3(a',499.2)	2102.0 (a', 597.1)	2011.9(a',831.3)	2155.0 (a', 13.3)
2063.9(a',93.0)	2159.0 (a', 139.6)	2069.8(a',77.8)	2907.4 (a", 269.2)

Table S2. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co(NO)(CO)_3$.

13S-1(C_{3v})		**13T-1(C_S)**	
BP86	B3LYP	BP86	B3LYP
59.8(e,0.0)	59.4 (e, 0.0)	56.9(a",0.0)	51.7 (a", 0.0)
59.8(e,0.0)	59.4 (e, 0.0)	63.2(a',0.1)	60.9 (a', 0.1)
76.7(e,0.0)	78.6 (e, 0.1)	69.9(a",0.1)	71.0 (a", 0.1)
76.7(e,0.0)	78.6 (e, 0.1)	76.4(a',0.2)	75.8 (a', 0.1)
84.7(a_1,0.0)	86.9 (a_1, 0.0)	88.2(a',0.1)	82.5 (a', 0.3)
292.3(e,0.0)	295.3 (e, 0.3)	203.3(a",0.0)	218.8 (a", 0.4)
292.3(e,0.0)	295.3 (e, 0.3)	242.6(a',0.7)	229.6 (a', 1.8)
322.2(a_2,0.0)	321.6 (a_2, 0.0)	301.1(a",0.2)	289.6 (a", 0.3)
425.1(a_1,0.2)	407.3 (a_1, 3.7)	333.3(a",1.4)	343.0 (a", 0.0)
474.5(e,3.4)	455.0 (e, 14.8)	373.5(a',1.0)	353.4 (a', 5.5)
474.5(e,3.4)	455.0 (e, 14.8)	423.7(a',0.7)	376.2 (a', 21.5)
490.4(a_1,54.4)	490.5 (a_1, 63.4)	426.5(a",0.0)	401.3 (a', 11.5)
509.0(e,20.5)	501.8 (e, 24.4)	440.6(a',20.2)	428.3 (a", 12.6)
509.0(e,20.5)	501.8 (e, 24.4)	463.9(a',31.3)	448.4 (a', 59.7)
591.3(e,60.6)	599.8 (e, 48.8)	486.8(a',14.2)	457.2 (a", 46.7)
591.3(e,60.6)	599.8 (e, 48.8)	491.4(a",43.0)	464.4 (a', 9.6)
620.2(a_1,8.8)	639.0 (a_1, 9.1)	565.1(a',14.1)	518.9 (a', 16.2)
1839.7(a_1,1014.9)	1897.2(a_1,1369.2)	1673.7(a',702.3)	1745.6 (a', 1031.2)
2005.9(e,868.5)	2095.5 (e, 974.2)	1989.9(a",1040.1)	2081.3(a", 1197.9)
2005.9(e,868.4)	2095.5 (e, 974.1)	1995.1(a',768.0)	2098.4 (a', 847.6)
2063.4(a_1,165.3)	2153.9(a_1, 205.4)	2046.4(a',261.6)	2146.5 (a', 334.3)

Table S3. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co(NO)(CO)_2$.

12S-1(C_s)		**12T-1(C_{2v})**	
BP86	B3LYP	BP86	B3LYP
65.1(a",0.3)	49.8 (a', 1.5)	52.0(b_2,0.0)	52.0 (b_2, 0.0)
65.3(a',0.9)	58.6 (a", 0.7)	69.9(a_1,0.0)	67.2 (a_1, 0.0)
73.6(a',0.3)	71.7 (a', 0.1)	76.7(b_1,0.9)	75.9 (b_1, 1.4)
274.6(a',1.7)	264.9 (a', 2.4)	263.3(b_1,0.0)	235.8 (b_1, 0.1)
281.0(a",0.6)	286.1 (a", 1.1)	288.0(a_2,0.0)	279.1 (a_2, 0.0)
308.6(a",1.1)	306.5 (a", 0.1)	299.7(b_2,0.0)	303.1 (b_2, 0.2)
457.1(a',0.4)	425.6 (a', 6.1)	423.5(a_1,5.0)	387.5 (a_1, 21.7)
493.4(a',13.0)	458.5 (a', 2.7)	475.9(a_1,27.6)	445.0 (b_2, 56.3)
500.2(a",31.4)	470.9 (a", 53.5)	479.3(b_2,29.4)	466.5 (a_1, 47.8)
518.1(a',24.7)	500.7 (a', 46.3)	498.9(b_1,7.9)	466.8 (b_1, 5.4)
588.0(a",38.3)	611.8 (a", 41.3)	534.6(b_2,27.0)	506.6 (a_1, 0.0)
643.6(a',2.9)	666.5 (a', 7.7)	541.3(a_1,0.0)	513.5 (b_2, 27.2)
1812.5(a',976.2)	1875.3(a',1342.2)	1770.5(a_1,963.0)	1807.1(a_1, 1176.9)
1976.4(a",1145.0)	2072.8(a",1332.1)	1984.6(b_2,1082.8)	2079.3(b_2, 1248.6)
2033.9(a',279.0)	2132.8 (a', 333.3)	2036.5(a_1,365.9)	2132.8 (a_1, 467.6)

Table S4. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of Co(NO)(CO)

11S-1(C_s)		**11T-1(C_s)**	
BP86	B3LYP	BP86	B3LYP
83.5(a',1.2)	79.3 (a', 1.5)	54.3(a',1.7)	53.3 (a', 2.3)
280.2(a",1.6)	275.1 (a", 3.6)	224.4(a",0.0)	181.9 (a", 2.2)
306.2(a',1.4)	304.0 (a', 1.7)	279.3(a',3.1)	264.0 (a', 4.9)
387.7(a",10.7)	382.1 (a", 9.1)	333.5(a",2.4)	331.0 (a", 7.0)
543.0(a',15.4)	514.7 (a', 37.1)	469.4(a',13.1)	417.1 (a', 25.9)
564.0(a',6.2)	564.8 (a', 4.5)	496.4(a',7.8)	434.5 (a', 30.0)
685.5(a',3.5)	711.9 (a', 4.1)	550.6(a',6.9)	507.5 (a', 28.8)
1799.5(a',874.7)	1858.2(a',1208.0)	1757.2(a',965.5)	1782.5(a',1480.5)
1990.8(a',555.7)	2088.7 (a', 707.3)	1997.9(a',721.9)	2102.4 (a', 983.1)

Table S5. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_5$.

25S-1(C_1)		**25S-2(C_2)**	
BP86	B3LYP	BP86	B3LYP
25.6(a,0.0)	21.0 (a, 0.0)	17.2(b,0.1)	-3.5 (b, 0.1)
27.3(a,0.0)	23.3 (a, 0.0)	28.6(a,0.0)	25.8 (a, 0.0)
54.3(a,0.1)	51.0 (a, 0.1)	52.8(a,0.0)	49.8 (a, 0.1)
60.4(a,0.0)	58.0 (a, 0.1)	54.7(b,0.1)	53.0 (b, 0.0)
63.0(a,0.0)	61.7 (a, 0.0)	58.2(a,0.0)	56.5 (a, 0.0)
69.6(a,0.0)	68.4 (a, 0.1)	60.4(b,0.0)	59.2 (b, 0.1)
74.1(a,0.3)	74.2 (a, 0.1)	68.7(a,0.1)	68.6 (a, 0.2)
75.8(a,0.3)	77.4 (a, 0.1)	70.7(b,0.2)	73.0 (b, 0.1)
79.4(a,0.0)	80.6 (a, 0.1)	82.5(a,0.0)	81.3 (a, 0.0)
83.8(a,0.1)	85.9 (a, 0.2)	83.7(b,0.2)	85.4 (b, 0.2)
91.5(a,0.0)	92.8 (a, 0.0)	95.2(b,0.0)	96.4 (b, 0.2)
100.4(a,0.1)	100.3 (a, 0.1)	97.5(a,0.0)	97.5 (a, 0.0)
178.4(a,0.9)	171.7 (a, 6.4)	170.2(a,0.2)	157.3 (a, 0.5)
239.4(a,1.7)	231.8 (a, 3.6)	241.6(b,1.9)	235.8 (b, 10.5)
279.1(a,0.6)	283.5 (a, 0.7)	279.8(b,1.7)	282.3 (b, 5.3)
308.3(a,2.4)	311.2 (a, 1.9)	291.0(a,0.1)	293.9 (a, 0.0)
320.6(a,1.7)	323.9 (a, 4.1)	320.4(b,1.8)	326.2 (b, 0.5)
341.7(a,0.3)	342.2 (a, 0.5)	350.4(b,2.8)	344.0 (b, 19.7)
355.3(a,1.4)	357.3 (a, 6.0)	351.5(a,0.4)	352.6 (a, 0.3)
391.4(a,10.3)	385.6 (a, 23.6)	379.9(a,0.0)	364.4 (a, 0.8)
427.3(a,1.7)	412.0 (a, 3.4)	420.6(a,0.0)	410.7 (b, 94.7)
454.9(a,6.2)	435.9 (a, 5.2)	436.3(b,54.2)	414.2 (a, 2.2)
458.9(a,55.8)	441.0 (a, 41.7)	452.9(b,20.3)	437.5 (a, 8.5)
464.6(a,3.8)	453.4 (a, 21.5)	462.2(a,8.2)	442.3 (b, 15.5)
474.4(a,9.4)	461.1 (a, 16.8)	478.7(b,58.6)	453.7 (b, 55.8)
479.5(a,9.7)	464.4 (a, 11.8)	500.0(a,16.1)	479.2 (a, 35.4)
492.4(a,12.5)	473.9 (a, 29.9)	508.0(b,66.3)	499.0 (b, 200.8)
505.4(a,36.6)	506.2 (a, 67.0)	515.2(a,2.6)	509.6 (b, 41.2)
514.8(a,21.8)	508.6 (a, 8.5)	519.1(b,179.2)	513.0 (a, 0.2)
526.5(a,57.3)	541.1 (a, 30.7)	561.5(a,71.5)	565.4 (a, 38.9)
541.6(a,74.2)	547.4(a,108.0)	573.5(a,2.8)	583.5 (b, 14.6)
548.1(a,38.9)	556.0 (a, 38.3)	575.1(b,30.6)	585.5 (a, 20.6)
563.7(a,32.9)	576.1 (a, 20.5)	605.3(b,52.3)	608.3 (b, 53.4)
617.7(a,24.4)	637.7 (a, 7.6)	614.0(b,17.2)	636.4 (a, 3.7)
664.5(a,218.2)	678.5(a,276.1)	616.8(a,2.3)	637.9 (b, 9.7)
1660.0(a,480.4)	1715.4(a,627.8)	1822.1(b,1968.7)	1882.4 (b, 2544.4)
1813.5(a,1063.8)	1878.0(a,1457.1)	1826.2(a,39.3)	1885.5 (a, 47.1)
1989.8(a,44.0)	2075.8(a,139.3)	1880.9(a,385.2)	1968.2 (a, 446.6)
1999.7(a,769.9)	2092.0(a,796.4)	1989.4(b,107.5)	2083.1 (b, 140.2)
2007.4(a,907.7)	2098.8(a,1048.3)	2005.7(a,1121.2)	2098.1 (a, 1282.3)
2022.9(a,1375.0)	2112.1(a,1606.2)	2023.8(b,1403.2)	2114.6 (b, 1607.0)
2060.4(a,266.2)	2152.4(a,310.9)	2051.1(a,4.2)	2143.5 (a, 3.8)

Table S6. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_5$.

25S-3(C_{2v})		**25S-4(C_s)**	
BP86	B3LYP	BP86	B3LYP
5.9(b_1,0.0)	6.0 (b_1, 0.0)	-19.4(a",0.0)	-26.0 (a", 0.0)
9.3(a_2,0.0)	11.8 (a_2, 0.0)	14.8(a",0.0)	9.6 (a", 0.0)
61.3(b_2,0.2)	61.5 (b_2, 0.0)	57.0(a',0.0)	56.4 (a', 0.0)
62.3(b_1,0.0)	62.1 (b_1, 0.1)	57.2(a',0.0)	59.1 (a", 0.1)
62.3(a_1,0.0)	62.9 (a_1, 0.1)	60.3(a",0.0)	59.2 (a', 0.0)
63.7(a_2,0.0)	64.5 (a_2, 0.0)	66.5(a",0.0)	65.8 (a", 0.0)
77.4(a_1,0.1)	78.8 (a_1, 0.1)	69.1(a',0.0)	68.7 (a', 0.1)
84.9(a_1,0.0)	89.2 (b_1, 0.1)	73.4(a',0.1)	73.7 (a', 0.3)
86.7(b_1,0.0)	89.4 (b_2, 1.1)	79.9(a",0.0)	81.5 (a", 0.1)
88.9(b_2,0.1)	91.9 (a_1, 0.1)	80.9(a',0.0)	82.6 (a', 0.1)
91.6(a_2,0.0)	92.0 (b_2, 0.1)	91.3(a',0.2)	92.0 (a', 0.4)
92.0(b_2,0.2)	92.3 (a_2, 0.0)	92.7(a",0.1)	94.7 (a", 0.1)
173.5(a_1,0.0)	162.2 (a_1, 0.5)	186.9(a',0.9)	179.6 (a', 5.7)
239.8(b_2,9.7)	229.8 (b_2, 20.2)	235.0(a',13.0)	225.7 (a', 10.9)
294.7(a_2,0.0)	302.1 (b_1, 0.2)	282.7(a",0.0)	291.3 (a", 0.0)
295.8(b_1,0.0)	302.2 (a_2, 0.0)	310.9(a",1.2)	307.8 (a", 2.5)
338.3(b_2,24.9)	327.9 (b_2, 46.4)	333.6(a",0.0)	334.3 (a", 0.0)
345.6(b_1,0.1)	345.8 (b_1, 0.4)	342.9(a',4.0)	345.4 (a', 7.8)
361.0(a_1,0.0)	347.7 (a_1, 1.1)	370.1(a",0.1)	372.3 (a", 0.1)
378.7(a_2,0.0)	380.3 (a_2, 0.0)	378.7(a',14.2)	374.1 (a', 23.1)
417.7(a_1,11.2)	416.9 (a_1, 12.4)	421.3(a',16.5)	403.3 (a', 11.0)
450.7(b_2,48.0)	431.5 (b_2, 43.3)	432.4(a",3.9)	414.7 (a", 4.7)
459.7(a_1,1.0)	441.7 (a_1, 2.4)	438.5(a',48.5)	418.3 (a', 26.5)
460.1(b_1,3.6)	443.4 (b_1, 26.4)	447.3(a',42.7)	442.2 (a', 48.4)
478.0(b_2,89.2)	464.8 (b_2, 137.0)	469.1(a',12.0)	444.9 (a", 46.7)
492.7(a_1,32.9)	467.5 (a_2, 0.0)	471.1(a",31.1)	456.9 (a', 8.6)
494.4(a_2,0.0)	490.7 (a_1, 40.0)	481.0(a',18.9)	467.2 (a", 0.0)
505.2(b_2,243.4)	498.8 (b_2, 149.8)	485.7(a",1.1)	482.0 (a', 26.6)
524.9(b_1,76.2)	524.6 (b_1, 62.4)	513.2(a',9.1)	500.9 (a', 34.3)
551.0(a_1,15.5)	556.9 (a_1, 25.0)	536.6(a',142.8)	543.5 (a', 61.1)
566.7(b_1,30.3)	581.9 (b_1, 34.9)	539.5(a',28.9)	552.6 (a', 82.8)
570.1(a_2,0.0)	583.2 (b_2, 3.8)	548.9(a",70.5)	554.9 (a", 51.3)
578.7(b_2,0.0)	586.3 (a_2, 0.0)	560.9(a",0.1)	578.9 (a", 10.2)
588.8(a_1,12.0)	607.5 (a_1, 14.1)	588.1(a',10.3)	614.1 (a', 13.2)
600.4(b_2,19.9)	620.5 (b_2, 7.0)	656.2(a',195.3)	669.1 (a', 203.3)
1790.5(b_2,97.5)	1840.8 (b_2, 94.5)	1666.6(a',479.3)	1716.1 (a', 617.2)
1846.6(a_1,1649.5)	1912.4(a_1,2171.8)	1818.8(a',659.0)	1865.7 (a', 931.2)
1882.0(a_1,20.0)	1966.3 (a_1, 56.4)	1994.6(a",17.8)	2087.2 (a", 241.0)
1998.3(a_2,0.0)	2088.0 (a_2, 0.0)	2003.1(a",1606.9)	2098.4 (a', 725.5)
2004.9(b_1,1628.4)	2093.8(b_1,1874.2)	2003.4(a',627.0)	2098.5 (a", 1570.7)
2028.1(b_2,1066.5)	2117.5(b_2,1202.8)	2025.3(a',1355.6)	2116.0 (a', 1539.5)
2055.2(a_1,202.6)	2147.2 (a_1, 258.9)	2058.5(a',56.3)	2152.5 (a', 72.1)

Table S7. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_5$.

25S-5(C_s)		**25S-6(C_s)**	
BP86	B3LYP	BP86	B3LYP
-14.9(a",0.0)	-11.7 (a", 0.0)	19.6(a",0.1)	21.9 (a", 0.0)
11.3(a",0.0)	21.0 (a", 0.0)	36.3(a",0.0)	39.8 (a', 0.0)
54.8(a',0.0)	53.5 (a', 0.1)	52.2(a',0.1)	41.4 (a", 0.0)
62.2(a",0.0)	61.9 (a", 0.1)	55.3(a',0.0)	47.7 (a", 0.0)
63.3(a',0.0)	63.6 (a', 0.0)	61.1(a",0.0)	49.5 (a', 0.1)
73.1(a',0.2)	73.6 (a', 0.2)	65.4(a',0.2)	61.6 (a', 0.2)
74.0(a",0.0)	77.3 (a", 0.1)	81.8(a",0.0)	72.2 (a', 0.9)
85.8(a',0.0)	86.2 (a', 0.0)	86.3(a',0.0)	75.0 (a", 0.0)
87.7(a",0.0)	90.5 (a', 0.2)	89.1(a",0.0)	80.7 (a", 0.1)
90.3(a',0.1)	91.7 (a", 0.1)	94.9(a',0.3)	81.6 (a', 0.1)
93.0(a',0.0)	94.3 (a', 0.5)	108.5(a",0.2)	92.3 (a', 0.0)
97.6(a",0.0)	99.3 (a", 0.0)	179.4(a',6.8)	92.4 (a", 0.1)
178.7(a',1.9)	176.0 (a', 4.8)	212.8(a',0.4)	104.1 (a', 1.1)
249.9(a',10.6)	248.1 (a', 8.0)	222.6(a',0.3)	171.6 (a', 0.2)
282.9(a",0.0)	291.6 (a", 0.0)	266.8(a",1.7)	285.1 (a", 0.7)
308.4(a",0.0)	313.7 (a", 0.0)	271.9(a',0.6)	336.5 (a", 0.0)
325.5(a",0.1)	329.6 (a", 0.9)	325.1(a",0.1)	346.0 (a', 2.5)
330.5(a',9.5)	334.1 (a', 10.2)	347.2(a",0.2)	350.0 (a", 5.9)
369.1(a",0.0)	373.9 (a", 0.0)	361.9(a",0.7)	382.7 (a', 9.4)
372.5(a',13.5)	376.6 (a', 11.2)	384.3(a',20.3)	389.3 (a", 6.2)
437.8(a',8.2)	416.3 (a', 11.5)	408.6(a',6.9)	408.0 (a', 31.1)
446.6(a',27.6)	427.2 (a', 26.3)	432.5(a',17.1)	435.1 (a', 19.4)
458.0(a',2.1)	440.1 (a", 22.3)	438.0(a",2.6)	464.5 (a', 20.4)
460.5(a",2.6)	440.7 (a', 0.6)	453.4(a',3.0)	466.9 (a", 15.2)
478.1(a',5.4)	453.4 (a", 11.4)	461.4(a",2.0)	473.0 (a", 29.3)
478.3(a",15.2)	465.3 (a', 3.7)	474.9(a',2.0)	474.4 (a', 14.4)
486.9(a',32.9)	485.1 (a', 28.3)	516.9(a",7.0)	496.4 (a', 1.2)
499.8(a',49.9)	504.6 (a', 56.9)	525.7(a',117.1)	500.5 (a", 1.5)
518.8(a",6.3)	522.3 (a", 9.9)	540.2(a",56.4)	548.8 (a', 214.5)
529.7(a',42.0)	530.9 (a', 37.5)	547.4(a',89.0)	555.9 (a', 51.8)
542.7(a',131.8)	559.5 (a', 107.7)	555.2(a',10.0)	557.2 (a", 40.5)
555.5(a",80.1)	563.0 (a", 39.6)	591.2(a',8.2)	568.3 (a', 4.4)
558.9(a",6.1)	575.2 (a", 37.5)	610.1(a',309.1)	598.8 (a', 44.1)
592.3(a',5.4)	615.9 (a', 1.9)	624.3(a",0.0)	654.0 (a", 1.9)
665.3(a',236.3)	679.9 (a', 249.9)	636.5(a',3.3)	655.8 (a', 47.7)
1657.4(a',450.8)	1702.9 (a', 538.4)	1812.2(a",1071.3)	1884.6(a", 1345.7)
1816.3(a',618.5)	1858.3 (a', 869.2)	1839.7(a',751.0)	1918.2 (a', 972.2)
1995.8(a",107.1)	2085.6 (a", 214.8)	1875.1(a',902.8)	2058.8 (a', 807.4)
2001.1(a',704.2)	2092.1(a", 1725.4)	1904.6(a',373.5)	2058.9(a", 1190.3)
2002.0(a",1539.3)	2098.9 (a', 748.8)	2001.2(a",921.8)	2075.6 (a', 268.9)
2025.8(a',1411.0)	2116.6 (a', 1579.5)	2011.7(a',547.0)	2111.9 (a', 1425.9)
2057.1(a',23.7)	2151.4 (a', 43.9)	2057.9(a',538.4)	2148.1 (a', 286.9)

Table S8. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_5$.

25S-7(C_s)		**25T-1(C_1)**	
BP86	B3LYP	BP86	B3LYP
11.6(a",0.0)	9.7 (a", 0.0)	15.8(a,0.1)	19.2 (a, 0.1)
12.3(a',0.0)	20.9 (a', 0.0)	28.0(a,0.1)	26.9 (a, 0.0)
44.5(a",0.0)	50.8 (a", 0.1)	52.3(a,0.1)	51.3 (a, 0.1)
51.7(a',0.1)	52.1 (a', 0.2)	58.7(a,0.4)	57.1 (a, 0.8)
61.4(a',1.2)	58.9 (a', 1.1)	63.2(a,0.1)	59.3 (a, 0.3)
66.8(a',0.2)	68.0 (a', 0.3)	66.2(a,0.1)	62.6 (a, 0.1)
70.8(a",0.3)	75.4 (a", 0.6)	68.0(a,0.0)	67.8 (a, 0.0)
75.3(a",0.1)	79.3 (a", 0.3)	73.2(a,0.1)	69.9 (a, 0.1)
78.9(a',0.6)	85.5 (a", 0.1)	74.6(a,0.1)	70.8 (a, 0.3)
80.1(a",0.0)	86.4 (a', 0.8)	82.3(a,0.3)	81.7 (a, 1.0)
90.9(a',0.5)	96.5 (a', 0.4)	88.6(a,0.1)	85.9 (a, 0.1)
100.5(a",0.0)	105.6 (a", 0.1)	96.1(a,0.4)	95.7 (a, 0.1)
124.4(a',3.4)	128.9 (a', 4.3)	160.7(a,0.1)	141.1 (a, 3.9)
166.3(a',0.0)	165.3 (a', 0.0)	236.2(a,1.2)	234.5 (a, 0.8)
274.1(a",0.6)	294.5 (a", 0.0)	249.2(a,0.4)	252.3 (a, 6.7)
316.2(a',0.0)	324.7 (a', 0.3)	279.8(a,0.2)	270.1 (a, 0.8)
333.7(a",3.2)	345.2 (a", 0.1)	295.4(a,0.2)	273.4 (a, 1.5)
343.1(a",0.1)	351.8 (a", 4.0)	323.0(a,2.0)	315.7 (a, 3.9)
363.7(a',13.1)	374.1 (a', 16.0)	347.0(a,5.3)	331.4 (a, 35.7)
386.3(a",7.6)	400.1 (a", 8.3)	368.6(a,1.6)	346.2 (a, 26.5)
436.9(a',23.4)	419.2 (a', 50.5)	390.3(a,9.2)	365.1 (a, 31.1)
459.8(a',16.1)	441.2 (a', 11.4)	413.1(a,3.5)	369.9 (a, 8.4)
465.0(a',1.4)	449.0 (a', 12.9)	415.8(a,4.3)	392.5 (a, 12.2)
470.5(a',5.1)	454.5 (a', 1.0)	432.6(a,20.6)	399.7 (a, 4.1)
480.5(a",16.9)	481.1 (a", 24.6)	435.9(a,1.8)	408.7 (a, 9.5)
498.5(a',9.0)	488.9 (a', 18.3)	446.6(a,8.3)	425.0 (a, 5.0)
515.0(a",7.3)	516.7 (a", 0.1)	453.8(a,3.3)	435.5 (a, 7.1)
526.1(a",0.1)	537.6 (a", 0.1)	467.0(a,13.0)	444.4 (a, 43.9)
552.9(a',83.3)	550.1 (a", 50.6)	473.3(a,6.9)	450.5 (a, 5.0)
555.6(a",39.7)	559.4 (a', 169.0)	474.2(a,35.2)	456.7 (a, 1.5)
560.2(a',76.2)	571.3 (a', 70.8)	484.4(a,36.8)	466.3 (a, 26.0)
563.5(a',99.8)	573.5 (a', 21.2)	502.6(a,34.8)	474.1 (a, 40.5)
591.8(a',43.8)	601.6 (a', 78.9)	514.0(a,41.0)	499.7 (a, 50.4)
629.3(a',47.5)	650.0 (a', 63.8)	535.0(a,57.0)	525.2 (a, 50.3)
636.0(a",0.1)	656.1 (a", 0.6)	603.5(a,79.2)	606.4 (a, 136.5)
1822.2(a",727.4)	1873.4(a", 1056.2)	1610.9(a,540.3)	1628.0 (a, 617.1)
1849.3(a',891.1)	1907.2 (a', 1233.6)	1729.0(a,760.0)	1783.8 (a, 983.3)
1973.0(a",1232.2)	2060.5(a", 1464.7)	1992.6(a,5.1)	2075.4 (a, 429.5)
1986.5(a',97.4)	2073.0 (a', 18.8)	1999.6(a,732.7)	2098.5 (a, 1041.7)
1992.6(a',728.4)	2076.9 (a', 871.8)	2005.6(a,1180.1)	2106.8 (a, 956.4)
2018.6(a',1040.3)	2102.2 (a', 1372.3)	2023.3(a,1681.0)	2114.5 (a, 1680.4)
2056.7(a',252.3)	2146.0 (a', 306.1)	2054.6(a,109.4)	2152.8 (a, 242.9)

Table S9. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_4$.

24S-1(C_s)		**24S-2(C_1)**	
BP86	B3LYP	BP86	B3LYP
22.9(a',0.2)	17.4 (a', 0.1)	17.5(a,0.2)	16.2 (a, 0.1)
26.0(a',0.2)	23.7 (a", 1.3)	39.7(a,1.0)	34.3 (a, 0.1)
45.7(a",0.0)	43.7 (a", 0.0)	44.1(a,0.0)	44.1 (a, 0.9)
54.4(a',0.1)	53.5 (a', 0.3)	54.6(a,0.2)	56.5 (a, 0.2)
58.0(a',0.1)	54.0 (a", 0.3)	61.8(a,0.0)	58.5 (a, 0.2)
61.1(a",0.5)	62.2 (a', 0.3)	62.7(a,0.2)	63.3 (a, 0.4)
67.5(a",0.1)	72.1 (a", 0.0)	74.9(a,0.1)	74.7 (a, 0.3)
74.2(a',0.3)	72.6 (a', 0.2)	78.9(a,0.2)	80.7 (a, 0.1)
89.8(a",0.3)	86.1 (a', 0.1)	92.9(a,0.1)	92.3 (a, 0.0)
156.3(a",0.7)	138.2 (a", 3.0)	158.2(a,0.7)	131.4 (a, 0.3)
210.0(a",0.1)	139.6 (a', 1.3)	203.1(a,0.6)	181.3 (a, 0.9)
214.1(a',0.4)	203.1 (a', 0.9)	207.3(a,0.2)	211.6 (a, 0.4)
247.0(a',2.4)	209.4 (a", 0.0)	241.0(a,0.9)	216.6 (a, 5.2)
252.5(a",0.0)	213.3 (a', 20.5)	263.4(a,1.9)	265.8 (a, 4.0)
288.9(a",0.3)	253.8 (a", 3.1)	283.0(a,0.2)	297.5 (a, 20.2)
291.9(a',0.1)	298.6 (a', 0.1)	296.0(a,0.3)	304.9 (a, 1.8)
353.7(a",0.9)	333.6 (a', 6.0)	341.4(a,0.7)	336.0 (a, 40.2)
375.3(a',2.1)	349.5 (a", 0.1)	374.5(a,8.8)	358.6 (a, 0.4)
386.6(a",2.4)	370.3 (a', 0.5)	399.3(a,3.9)	382.3 (a, 24.2)
388.2(a',2.3)	376.0 (a", 9.2)	415.9(a,2.2)	416.0 (a, 5.0)
399.9(a',2.8)	427.4 (a", 0.4)	442.2(a,5.8)	436.6 (a, 5.2)
445.2(a',1.3)	437.8 (a', 0.4)	455.2(a,16.8)	444.1 (a, 32.2)
446.6(a",0.4)	439.0 (a", 3.9)	466.5(a,5.5)	466.5 (a, 22.9)
469.3(a",36.5)	447.0 (a', 30.4)	490.3(a,27.8)	475.2 (a, 40.9)
489.6(a',40.9)	471.6 (a', 67.3)	500.9(a,32.6)	497.9 (a, 23.9)
524.1(a',8.0)	562.4 (a", 15.5)	532.7(a,16.6)	572.7 (a, 15.6)
563.6(a",12.1)	579.6 (a', 13.3)	553.5(a,27.9)	580.7 (a, 44.2)
585.5(a',1.7)	600.1 (a', 1.0)	566.8(a,0.6)	591.3 (a, 1.0)
615.2(a",2.1)	640.9 (a', 1.9)	619.6(a,9.2)	645.5 (a, 9.2)
625.6(a',11.0)	652.8 (a', 10.9)	625.4(a,0.1)	649.9 (a, 0.4)
1812.8(a",1591.4)	1873.8 (a', 1805.6)	1805.0(a,2221.9)	1867.1 (a, 2129.3)
1824.2(a',706.9)	1891.4 (a', 1170.5)	1814.1(a,63.5)	1885.7 (a, 746.0)
1899.5(a',968.9)	2009.2(a", 1159.6)	1902.4(a,870.4)	2000.3 (a, 677.0)
1909.5(a',449.8)	2017.2 (a', 428.7)	1913.5(a,115.2)	2031.9 (a, 509.1)
1994.9(a",764.8)	2090.0 (a', 755.0)	2003.0(a,1808.5)	2099.7 (a, 1814.9)
2030.9(a',707.1)	2126.5 (a', 795.9)	2029.0(a,9.7)	2125.9 (a, 46.3)

Table S10. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_4$.

24S-3(C_1)		**24S-4**	
BP86	B3LYP	BP86	B3LYP
29.0(a,0.1)	21.8 (a, 0.2)	29.8(b_u,0.1)	12.9 (a_2, 0.0)
43.2(a,0.3)	25.2 (a, 0.1)	34.9(a_u,0.4)	31.7 (b_1, 0.1)
52.3(a,0.4)	50.4 (a, 0.1)	60.6(b_u,0.5)	54.0 (b_2, 1.4)
64.5(a,0.2)	58.4 (a, 1.0)	67.8(a_g,0.0)	57.3 (a_2, 0.0)
67.9(a,0.1)	62.8 (a, 0.8)	78.2(a_g,0.0)	74.2 (a_1, 0.0)
76.1(a,0.2)	74.7 (a, 0.1)	81.7(a_u,0.2)	84.6 (b_1, 0.8)
77.0(a,0.1)	79.6 (a, 0.1)	94.3(b_g,0.0)	86.0 (b_2, 0.6)
88.0(a,0.2)	90.6 (a, 0.3)	97.3(b_u,0.7)	95.2 (a_1, 0.1)
93.9(a,0.1)	94.2 (a, 0.1)	101.8(b_g,0.0)	114.5 (b_1, 1.1)
199.0(a,0.3)	98.2 (a, 0.0)	221.0(a_g,0.0)	158.4 (b_2, 5.8)
214.7(a,3.4)	190.0 (a, 6.2)	221.6(a_u,0.8)	211.6 (a_1, 2.6)
231.4(a,0.3)	247.6 (a, 0.4)	270.2(b_g,0.0)	234.9 (a_1, 0.1)
273.7(a,0.2)	291.3 (a, 1.2)	275.4(a_u,0.5)	293.0 (a_2, 0.0)
316.2(a,4.3)	315.9 (a, 0.5)	323.8(b_u,0.9)	314.5 (b_2, 0.0)
321.4(a,0.4)	326.1 (a, 5.8)	331.7(a_g,0.0)	342.1 (b_1, 0.1)
334.3(a,2.2)	339.3 (a, 1.0)	347.6(b_g,0.0)	378.6 (a_2, 0.0)
387.8(a,1.0)	405.3 (a, 3.1)	410.2(b_u,7.8)	437.0 (a_1, 42.4)
397.2(a,1.1)	413.2 (a, 22.2)	429.5(b_g,0.0)	448.3 (b_2, 1.1)
434.8(a,7.1)	427.9 (a, 5.2)	441.5(a_g,0.0)	455.8 (b_1, 3.8)
440.9(a,1.3)	434.8 (a, 22.2)	456.3(a_u,0.6)	462.5 (b_2, 44.8)
447.0(a,12.9)	468.5 (a, 15.6)	464.6(b_u,6.9)	474.0 (a_1, 15.1)
458.3(a,13.7)	478.0 (a, 10.2)	468.9(a_g,0.0)	482.6 (b_1, 19.1)
476.1(a,19.6)	478.9 (a, 13.9)	477.7(b_g,0.0)	488.8 (a_1, 28.2)
480.3(a,10.3)	489.2 (a, 15.0)	484.7(b_u,34.3)	503.2 (a_1, 3.3)
528.4(a,28.7)	533.4 (a, 16.9)	515.7(a_u,59.6)	538.7 (a_2, 0.0)
532.5(a,11.0)	561.1 (a, 76.9)	524.1(a_g,0.0)	556.9 (b_1, 53.3)
541.1(a,33.3)	580.8 (a, 62.4)	548.9(b_u,87.6)	562.7 (b_2, 58.7)
550.1(a,34.8)	593.9 (a, 47.3)	564.6(a_g,0.0)	592.9 (a_1, 36.0)
606.5(a,39.9)	636.8 (a, 19.2)	577.2(b_g,0.0)	625.1 (b_2, 0.2)
644.3(a,8.4)	708.4 (a, 190.9)	601.9(a_u,90.2)	667.8 (a_1, 182.1)
1649.1(a,591.3)	1696.8 (a, 595.4)	1640.5(b_u,1059.2)	1693.1(b_2, 239.8)
1826.2(a,1193.8)	1899.7 (a, 1685.8)	1671.4(a_g,0.0)	1729.7 (a_1, 0.5)
1912.9(a,569.1)	2051.7 (a, 674.7)	1987.6(b_g,0.0)	2093.5 (b_2, 784.8)
1987.7(a,459.4)	2083.4 (a, 750.6)	1996.4(b_u,1550.2)	2097.5 (b_1, 931.9)
2007.7(a,1591.6)	2100.5 (a, 1404.5)	2014.9(a_u,1984.1)	2116.4(a_1, 217.4)
2041.7(a,405.2)	2140.4 (a, 579.0)	2044.5(a_g,0.0)	2148.3 (a_1, 0.2)

Table S11. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_4$.

24S-5(C_{2v})	
BP86	B3LYP
27.6(b_2,0.2)	25.0 (b_2, 0.2)
40.9(a_2,0.0)	38.1 (a_2, 0.0)
48.6(b_1,0.7)	43.1 (b_1, 1.4)
53.0(a_1,0.1)	51.5 (a_1, 0.3)
59.9(a_2,0.0)	56.1 (a_2, 0.0)
65.5(a_1,0.0)	65.6 (a_1, 0.1)
70.4(b_1,0.4)	68.7 (b_1, 1.1)
74.0(b_2,0.4)	78.5 (b_2, 0.5)
90.4(b_2,0.3)	91.5 (b_2, 0.6)
186.2(a_1,0.6)	179.4 (b_1, 5.7)
206.5(b_1,1.5)	195.2 (a_1, 2.6)
225.9(a_1,2.8)	224.8 (a_1, 6.5)
226.5(b_2,1.6)	238.5 (a_2, 0.0)
238.3(a_2,0.0)	265.8 (b_2, 3.6)
310.2(b_1,2.9)	280.9 (b_1, 3.9)
333.6(b_2,0.0)	340.1 (b_2, 0.0)
339.4(a_2,0.0)	350.7 (b_1, 4.6)
364.1(b_1,1.8)	353.4 (a_2, 0.0)
393.3(a_1,1.5)	388.8 (a_1, 7.4)
408.8(a_2,0.0)	410.2 (b_2, 0.6)
420.5(b_2,0.2)	418.1 (a_1, 21.4)
432.2(b_1,3.7)	421.5 (a_2, 0.0)
434.2(a_1,8.0)	424.3 (b_1, 7.6)
483.9(a_1,22.1)	479.6 (a_1, 18.8)
514.1(b_2,49.5)	502.9 (b_2, 64.3)
568.1(a_1,20.8)	583.8 (a_1, 0.0)
571.6(a_1,37.1)	593.9 (a_1, 95.9)
576.8(b_1,28.1)	605.2 (b_1, 46.3)
623.8(b_2,0.0)	648.6 (b_2, 3.0)
658.3(a_1,7.8)	674.2 (a_1, 13.6)
1823.2(b_2,1040.2)	1887.8 (b_2, 1516.3)
1850.0(a_1,879.2)	1928.4 (a_1, 1112.2)
1869.4(b_1,935.9)	1945.0 (b_1, 1198.1)
1886.6(a_1,671.3)	1964.0 (a_1, 888.2)
1983.3(b_2,1084.2)	2072.2 (b_2, 1300.4)
2027.6(a_1,585.0)	2121.0 (a_1, 609.8)

Table S12. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_3$.

23S-1(D_{3h})		**23S-2(C_s)**	
BP86	B3LYP	BP86	B3LYP
50.6(e',0.1)	50.6 (e', 0.4)	18.7(a",0.1)	18.4 (a", 0.0)
50.6(e',0.1)	50.6 (e', 0.4)	48.0(a",0.5)	49.8 (a", 0.1)
69.3(e",0.0)	68.2 (e", 0.0)	54.6(a',0.7)	56.6 (a', 0.5)
69.3(e",0.0)	68.2 (e", 0.0)	57.8(a",0.3)	65.5 (a', 0.1)
85.3(e',0.6)	86.1 (e', 0.7)	64.5(a',0.1)	69.0 (a", 0.5)
85.3(e',0.6)	86.1 (e', 0.7)	69.8(a',0.1)	74.4 (a', 0.1)
161.0(a_2",0.0)	136.0 (e", 0.0)	97.1(a",0.3)	98.7 (a", 0.6)
196.3(e",0.0)	136.0 (e", 0.0)	159.5(a',0.2)	127.3 (a', 0.2)
196.3(e",0.0)	154.8 (a_2", 1.1)	226.1(a',2.4)	222.1 (a', 2.5)
268.1(e",0.0)	246.7 (e", 0.0)	237.1(a',0.9)	238.8 (a', 2.0)
268.1(e",0.0)	246.7 (e", 0.0)	275.6(a',1.6)	295.1 (a", 0.1)
293.9(a_1',0.0)	287.9 (a_1', 0.0)	297.0(a",0.0)	304.8 (a', 11.4)
339.2(a_2',0.0)	316.0 (a_2", 24.8)	321.6(a",0.9)	324.9 (a", 0.9)
383.6(a_2",6.7)	338.3 (a_2', 0.0)	371.6(a",0.0)	371.4 (a", 0.6)
393.5(e',9.6)	374.0 (e', 18.2)	390.9(a',3.5)	381.1 (a', 5.5)
393.5(e',9.6)	374.0 (e', 18.2)	425.2(a',4.7)	428.4 (a', 3.3)
406.0(a_1',0.0)	385.9 (a_1', 0.0)	433.1(a",0.0)	441.2 (a", 14.2)
484.4(e',0.7)	479.3 (e', 2.2)	441.0(a',0.1)	452.9 (a', 7.0)
484.4(e',0.7)	479.3 (e', 2.2)	448.7(a",1.9)	461.6 (a", 3.3)
576.6(e",0.0)	588.3 (e', 11.3)	464.2(a',5.6)	468.8 (a', 8.2)
576.6(e",0.0)	588.3 (e', 11.3)	493.1(a',28.6)	474.3 (a', 28.4)
580.5(e',10.7)	592.6 (e", 0.0)	508.5(a",36.8)	510.8 (a", 33.9)
580.5(e',10.7)	592.7 (e", 0.0)	557.7(a',57.2)	589.1 (a', 117.1)
643.3(a_2",0.1)	670.5 (a_2", 1.5)	627.1(a',29.8)	666.9 (a', 39.7)
680.1(a_1',0.0)	702.1 (a_1', 0.0)	665.9(a',2.8)	698.9 (a', 26.5)
1845.4(a_2",2361.4)	1907.3(a_2",3149.2)	1667.4(a',494.8)	1717.5 (a', 615.1)
1853.9(a_1',0.0)	1917.4 (a_1', 0.0)	1836.5(a',1361.1)	1899.5 (a', 1838.6)
1921.1(e',969.4)	2025.8 (e', 1137.3)	1897.5(a',679.1)	2004.3 (a', 754.8)
1921.1(e',969.4)	2025.8 (e', 1137.3)	1995.7(a",945.3)	2093.7(a", 1067.3)
1966.8(a_1',0.0)	2070.9 (a_1', 0.0)	2037.3(a',679.0)	2135.3 (a', 777.5)

Table S13. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_3$.

23S-3(C_1)		**23S-4(C_s)**	
BP86	B3LYP	BP86	B3LYP
33.0(a,0.0)	31.5 (a, 0.1)	33.6(a",0.1)	36.1 (a", 0.0)
47.8(a,0.1)	44.0 (a, 0.2)	43.0(a",0.1)	52.5 (a", 0.2)
54.6(a,0.5)	51.7 (a, 1.4)	67.2(a',0.3)	69.1 (a', 0.2)
64.5(a,0.0)	57.6 (a, 1.2)	75.1(a',0.0)	75.6 (a', 0.0)
69.9(a,1.5)	64.9 (a, 0.0)	76.3(a",0.8)	78.3 (a", 1.7)
78.2(a,0.0)	78.3 (a, 0.0)	91.1(a',0.4)	93.6 (a', 0.2)
90.7(a,0.0)	89.9 (a, 0.2)	101.2(a",0.6)	101.9 (a", 0.5)
189.1(a,0.4)	151.1 (a, 0.7)	198.1(a',3.0)	222.9 (a', 1.4)
219.9(a,0.5)	182.2 (a, 2.1)	241.2(a',3.1)	238.0 (a', 0.7)
234.0(a,1.9)	226.1 (a, 0.2)	245.7(a',1.0)	246.0 (a', 7.9)
244.1(a,0.2)	237.5 (a, 0.5)	263.7(a",0.6)	282.3 (a", 0.0)
299.7(a,1.1)	238.8 (a, 8.6)	319.2(a',0.7)	324.2 (a', 2.1)
323.0(a,0.9)	304.4 (a, 0.4)	350.8(a",0.4)	358.8 (a", 2.2)
358.9(a,3.2)	341.1 (a, 0.8)	426.8(a',14.3)	429.3 (a', 25.6)
399.8(a,8.5)	379.3 (a, 20.6)	440.7(a",0.0)	432.3 (a", 10.0)
424.6(a,10.1)	403.6 (a, 14.9)	462.0(a',4.7)	438.9 (a', 6.3)
455.6(a,9.9)	453.6 (a, 14.0)	465.1(a",0.1)	457.2 (a", 7.8)
462.4(a,0.0)	459.8 (a, 0.7)	486.6(a',17.6)	486.2 (a", 23.3)
483.7(a,38.4)	463.9 (a, 48.1)	498.1(a",39.9)	489.0 (a', 28.7)
492.6(a,25.0)	472.5 (a, 24.2)	504.8(a',85.7)	495.5 (a', 96.9)
513.6(a,2.3)	533.0 (a, 17.0)	520.5(a",15.3)	535.0 (a', 18.7)
544.4(a,24.9)	547.4 (a, 11.8)	536.1(a',36.8)	543.2 (a", 20.7)
553.4(a,36.5)	574.9 (a, 30.9)	568.4(a',6.8)	586.6 (a', 8.2)
616.0(a,5.8)	642.8 (a, 7.5)	623.7(a',13.9)	649.3 (a', 5.5)
654.0(a,0.3)	682.9 (a, 0.7)	654.4(a',151.8)	670.5 (a', 175.7)
1823.1(a,1906.1)	1885.8 (a, 2502.9)	1497.3(a',434.8)	1529.1 (a', 541.2)
1832.7(a,487.0)	1899.6 (a, 725.6)	1693.3(a',352.6)	1739.2 (a', 483.0)
1898.6(a,1032.8)	2005.8 (a, 1269.2)	2001.8(a",825.7)	2100.2 (a', 2017.7)
1923.7(a,120.4)	2031.0 (a, 113.5)	2008.8(a',1759.5)	2100.6 (a", 937.1)
2024.6(a,764.7)	2119.8 (a, 879.2)	2044.7(a',215.7)	2142.1 (a', 268.3)

Table S14. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_3$.

23S-5(C_1)		**23S-6(C_1)**	
BP86	B3LYP	BP86	B3LYP
34.7(a,0.0)	35.4 (a, 0.1)	24.3(a,0.2)	19.5 (a, 0.0)
47.1(a,1.3)	51.2 (a, 0.4)	27.0(a,0.0)	26.1 (a, 0.1)
54.2(a,0.3)	62.2 (a, 0.3)	51.6(a,0.2)	45.1 (a, 3.0)
63.8(a,0.1)	64.5 (a, 0.8)	56.1(a,1.6)	53.5 (a, 0.1)
70.2(a,0.5)	72.3 (a, 0.9)	66.7(a,0.1)	64.2 (a, 0.1)
76.7(a,0.3)	74.5 (a, 0.4)	69.9(a,0.1)	71.3 (a, 0.1)
95.7(a,0.1)	96.5 (a, 0.1)	84.4(a,0.2)	78.0 (a, 0.4)
135.9(a,0.2)	124.9 (a, 0.3)	90.1(a,0.0)	91.6 (a, 0.2)
232.0(a,0.5)	222.9 (a, 2.9)	204.5(a,0.1)	201.8 (a, 1.5)
237.2(a,2.5)	235.2 (a, 0.2)	257.6(a,1.6)	259.0 (a, 3.1)
282.0(a,3.2)	285.5 (a, 4.1)	283.9(a,0.3)	283.2 (a, 0.1)
294.7(a,0.5)	304.0 (a, 0.7)	310.4(a,1.0)	319.0 (a, 2.5)
314.9(a,9.0)	314.0 (a, 2.5)	337.2(a,1.6)	356.4 (a, 2.7)
395.7(a,0.7)	408.1 (a, 7.3)	378.6(a,1.0)	388.8 (a, 2.6)
398.6(a,1.4)	413.2 (a, 3.5)	398.8(a,1.9)	391.2 (a, 3.9)
413.9(a,6.9)	425.3 (a, 6.6)	439.6(a,12.6)	425.0 (a, 22.2)
445.2(a,0.6)	443.2 (a, 13.4)	448.1(a,1.9)	431.7 (a, 21.8)
475.9(a,27.1)	469.8 (a, 37.4)	473.3(a,75.1)	452.8 (a, 37.2)
494.8(a,7.0)	487.7 (a, 13.9)	491.1(a,13.5)	465.6 (a, 28.1)
497.5(a,11.4)	503.5 (a, 19.1)	495.7(a,5.1)	495.3 (a, 2.8)
531.7(a,28.1)	546.1 (a, 34.2)	504.1(a,2.6)	507.7 (a, 41.4)
555.1(a,44.4)	573.1 (a, 45.1)	528.3(a,32.5)	542.1 (a, 41.3)
586.0(a,60.8)	603.6 (a, 67.1)	563.2(a,22.5)	569.8 (a, 28.8)
620.3(a,12.4)	644.2 (a, 8.9)	630.0(a,41.9)	668.5 (a, 12.0)
690.9(a,93.5)	719.1 (a, 129.6)	644.1(a,49.5)	693.2 (a, 182.2)
1667.4(a,415.3)	1723.8 (a, 509.5)	1637.6(a,489.8)	1674.7 (a, 611.6)
1829.2(a,1193.6)	1892.3 (a, 1630.7)	1794.8(a,908.7)	1856.0 (a, 1103.3)
1886.8(a,562.9)	1982.8 (a, 654.4)	1970.7(a,863.9)	2076.9 (a, 1063.5)
1999.0(a,1678.6)	2094.1 (a, 1844.3)	2003.9(a,1840.7)	2101.7 (a, 2208.0)
2030.0(a,290.2)	2125.2 (a, 332.3)	2033.0(a,128.7)	2133.2 (a, 71.4)

Table S15. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_3$.

23S-7(C_2)		**23S-8(C_s)**	
BP86	B3LYP	BP86	B3LYP
21.9(b,0.0)	19.2 (b, 0.1)	24.9(a',0.1)	26.9 (a', 0.2)
30.9(a,0.0)	33.1 (a, 0.0)	54.3(a",0.0)	50.1 (a", 0.1)
56.3(a,0.2)	53.1 (b, 1.2)	54.7(a",0.4)	53.6 (a", 0.6)
59.2(b,0.9)	55.3 (a, 0.5)	58.2(a',0.3)	58.7 (a', 0.5)
64.2(a,0.2)	64.0 (a, 0.2)	73.8(a',0.8)	74.1 (a', 0.5)
70.3(b,0.2)	68.3 (b, 0.6)	77.9(a",0.3)	76.6 (a", 0.3)
76.4(a,0.2)	74.6 (a, 0.2)	90.1(a',0.5)	89.1 (a', 1.0)
90.6(b,0.3)	88.8 (b, 0.7)	191.7(a',1.1)	191.0 (a', 3.3)
188.9(a,0.0)	180.6 (a, 0.1)	223.7(a',4.1)	193.1 (a", 0.1)
243.2(b,1.5)	233.8 (b, 3.9)	228.0(a",0.0)	224.0 (a', 4.6)
281.5(b,3.3)	272.0 (b, 21.3)	270.7(a",0.2)	247.3 (a", 0.1)
296.1(a,0.0)	299.1 (a, 0.0)	297.0(a',6.5)	312.1 (a', 6.4)
321.5(b,3.2)	325.6 (b, 7.2)	308.9(a",0.8)	317.5 (a", 0.4)
356.9(a,0.7)	351.0 (b, 66.4)	360.4(a',0.3)	343.5 (a', 1.4)
366.6(b,32.7)	354.5 (a, 0.0)	408.6(a",4.3)	405.9 (a", 8.4)
434.1(a,3.1)	423.3 (a, 7.1)	426.7(a",0.3)	427.5 (a", 0.4)
460.4(b,0.2)	444.9 (b, 9.8)	442.5(a',3.7)	442.0 (a', 5.4)
475.3(a,2.1)	451.3 (a, 3.6)	483.1(a",1.4)	483.3 (a", 2.7)
492.9(b,72.4)	466.3 (b, 113.1)	486.1(a',16.2)	491.2 (a', 30.7)
494.4(a,2.3)	472.6 (a, 6.5)	506.9(a',0.7)	499.7 (a', 2.3)
496.4(b,68.4)	482.7 (b, 46.8)	547.3(a',2.8)	553.1 (a', 101.1)
538.6(a,6.4)	556.3 (a, 8.9)	566.4(a',87.6)	565.8 (a', 8.9)
564.4(b,9.8)	576.6 (b, 7.0)	573.5(a",25.4)	594.6 (a", 32.3)
640.6(a,6.3)	669.8 (a, 7.2)	628.6(a',0.7)	652.0 (a', 2.9)
646.8(b,23.2)	674.9 (b, 12.9)	636.7(a',18.6)	658.9 (a', 32.0)
1795.0(b,1572.8)	1854.1 (b, 1990.7)	1814.7(a',1212.5)	1873.4 (a', 1662.5)
1806.8(a,519.0)	1869.0 (a, 748.1)	1844.3(a',828.3)	1916.7 (a', 1203.7)
1873.8(a,207.2)	1968.9 (a, 298.3)	1878.8(a",954.2)	1962.0(a", 1189.1)
2000.0(b,1854.6)	2096.8 (b, 2061.8)	1899.7(a',667.9)	1986.0 (a', 877.9)
2025.7(a,172.0)	2123.6 (a, 208.7)	2000.7(a',833.6)	2096.9 (a', 1022.9)

Table S16. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_2$.

22S-1(C_1)		**22S-2**	
BP86	B3LYP	BP86	B3LYP
12.4(a,1.3)	21.8 (a, 0.2)	25.3(a',0.8)	37.8 (a_1, 0.3)
43.5(a,0.7)	29.0 (a, 0.5)	43.5(a",0.2)	40.4 (b_2, 0.1)
63.2(a,0.1)	49.9 (a, 0.3)	53.2(a",0.4)	51.0 (b_1, 0.7)
69.1(a,1.4)	65.9 (a, 0.7)	61.8(a',1.7)	56.6 (a_2, 0.0)
91.5(a,1.3)	79.2 (a, 3.4)	83.4(a',0.4)	79.7 (a_1, 2.0)
145.2(a,1.9)	112.0 (a, 0.3)	177.4(a',0.2)	187.2 (a_2, 0.0)
206.6(a,2.4)	234.8 (a, 1.8)	195.6(a",2.6)	195.8 (b_2, 0.7)
259.4(a,0.9)	239.2 (a, 1.0)	230.2(a",0.1)	228.9 (a_1, 1.0)
300.7(a,2.5)	316.0 (a, 0.8)	250.8(a',2.5)	248.4 (a_2, 0.0)
317.6(a,6.7)	339.6 (a, 0.1)	304.9(a",0.1)	310.0 (b_2, 9.8)
331.3(a,4.0)	343.9 (a, 27.4)	309.8(a',13.0)	328.0 (b_1, 3.9)
375.6(a,3.0)	373.1 (a, 0.7)	394.2(a',6.0)	355.9 (a_1, 0.7)
431.3(a,2.2)	419.3 (a, 4.9)	416.7(a",8.7)	403.6 (b_1, 21.2)
438.7(a,1.4)	422.4 (a, 1.6)	418.5(a',0.4)	428.5 (b_2, 47.2)
448.9(a,2.0)	456.1 (a, 39.6)	461.2(a',12.3)	433.4 (a_1, 0.5)
488.3(a,15.2)	490.1 (a, 3.8)	507.7(a',6.0)	468.9 (a_1, 1.0)
506.5(a,2.4)	535.8 (a, 7.0)	507.8(a",0.1)	546.2 (a_2, 0.0)
601.0(a,51.5)	647.4 (a, 72.7)	569.3(a",12.6)	572.7 (b_1, 4.3)
651.1(a,21.2)	673.6 (a, 44.0)	635.8(a',0.9)	666.0 (b_2, 4.6)
669.4(a,29.2)	723.5 (a, 79.9)	653.0(a',0.9)	677.8 (a_1, 0.0)
1636.4(a,490.6)	1697.7 (a, 512.6)	1812.0(a',2449.6)	1879.4 (b_2, 3102.0)
1826.4(a,1282.2)	1889.5 (a, 1851.9)	1824.2(a',67.7)	1893.3 (a_1, 49.4)
1867.6(a,744.5)	1976.7 (a, 717.5)	1883.8(a",1149.7)	1980.7 (b_1, 1381.1)
2006.9(a,920.7)	2111.5 (a, 1158.1)	1918.7(a',44.6)	2017.1 (a_1, 119.5)

Table S17. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Co_2(NO)_2(CO)_2$.

22T-1(C_s)	
BP86	B3LYP
27.7(a",0.5)	36.2 (a", 0.0)
54.3(a',0.2)	54.2 (a', 0.2)
65.7(a",2.0)	66.7 (a", 2.5)
71.7(a',0.3)	69.1 (a', 0.3)
95.6(a",0.3)	85.6 (a", 0.6)
131.0(a',0.8)	115.7 (a', 0.7)
228.7(a',0.8)	208.8 (a', 4.3)
241.4(a',6.5)	218.7 (a', 5.6)
288.3(a",0.0)	257.6 (a", 0.0)
319.8(a',7.6)	290.3 (a', 12.7)
332.9(a",0.4)	316.9 (a", 0.0)
390.6(a",0.1)	384.4 (a", 0.3)
416.7(a',1.4)	386.9 (a', 6.3)
446.3(a",0.5)	433.3 (a', 9.0)
463.1(a',16.6)	452.3 (a', 13.0)
470.9(a',5.6)	462.5 (a", 1.3)
483.2(a',2.5)	482.5 (a', 26.7)
543.3(a',13.6)	528.6 (a', 77.7)
608.0(a',9.2)	552.0 (a', 2.0)
644.2(a',15.4)	601.7 (a', 26.9)
1617.7(a',497.8)	1646.6 (a', 558.5)
1816.8(a',1416.2)	1848.6 (a', 1267.9)
1884.8(a',735.3)	1982.9 (a', 809.4)
2016.8(a',1071.7)	2122.4 (a', 1225.2)

Table S18. Theoretical Cartesian coordinates (in Å) for the structure 14**S-1** using the BP86/DZP method

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	6	0	0.018106	-0.846972	1.549893
2	6	0	0.115384	1.913188	0.000000

3	6	0	-1.893861	0.190082	0.000000
4	27	0	-0.060834	0.079536	0.000000
5	8	0	0.018106	-1.458150	-2.545896
6	8	0	-3.059094	0.229211	0.000000
7	8	0	0.018106	-1.458150	2.545896
8	8	0	0.159074	3.078332	0.000000
9	8	0	2.602714	-1.000435	0.000000
10	6	0	0.018106	-0.846972	-1.549893
11	7	0	2.026410	0.038586	0.000000

Table S19. Theoretical Cartesian coordinates (in Å) for the structure **14T-1** using the BP86/DZP method

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	6	0	-0.072575	-0.745352	1.617189
2	6	0	0.289987	1.905110	0.000000
3	6	0	-1.881545	0.314760	0.000000
4	27	0	-0.091712	0.102326	0.000000
5	8	0	-0.072575	-1.281910	-2.652697
6	8	0	-3.042151	0.428020	0.000000
7	8	0	-0.072575	-1.281910	2.652697
8	8	0	0.463550	3.056976	0.000000
9	8	0	2.602662	-1.449527	0.000000
10	6	0	-0.072575	-0.745352	-1.617189
11	7	0	1.980739	-0.415856	0.000000

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

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	6	0	0.000000	1.628571	-0.665602
2	6	0	-1.410384	-0.814285	-0.665602
3	6	0	1.410384	-0.814285	-0.665602
4	27	0	0.000000	0.000000	0.118923
5	7	0	0.000000	0.000000	1.785627
6	8	0	0.000000	0.000000	2.968560
7	8	0	0.000000	2.693122	-1.144915
8	8	0	2.332312	-1.346561	-1.144915
9	8	0	-2.332312	-1.346561	-1.144915

Table S21. Theoretical Cartesian coordinates (in Å) for the structure 13T**-1** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z

1	6	0	-1.627052	0.553949	0.000000
2	6	0	0.122270	-0.974697	1.511600
3	6	0	0.122270	-0.974697	-1.511600
4	27	0	0.126821	0.041327	0.000000
5	7	0	1.049264	1.610147	0.000000
6	8	0	2.211099	1.925539	0.000000
7	8	0	-2.764883	0.812777	0.000000
8	8	0	0.122270	-1.620044	-2.485238
9	8	0	0.122270	-1.620044	2.485238

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

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	6	0	0.548210	-0.720064	1.454729
2	27	0	0.306358	0.299386	0.000000
3	8	0	0.548210	-1.429374	-2.386343
4	8	0	0.548210	-1.429374	2.386343
5	8	0	-2.089742	1.766905	0.000000
6	6	0	0.548210	-0.720064	-1.454729
7	7	0	-0.986230	1.327443	0.000000

Table S23. Theoretical Cartesian coordinates (in Å) for the structure 12**T-1** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	6	0	0.000000	-1.479026	-0.979984
2	27	0	0.000000	0.000000	0.074904
3	8	0	0.000000	2.422744	-1.671388
4	8	0	0.000000	-2.422744	-1.671388
5	8	0	0.000000	0.000000	2.990166
6	6	0	0.000000	1.479026	-0.979984
7	7	0	0.000000	0.000000	1.794044

Table S24. 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	6	0	1.474665	-0.241128	0.000000
2	27	0	0.000000	0.688270	0.000000
3	7	0	-1.430696	-0.086228	0.000000
4	8	0	-2.181323	-1.013084	0.000000
5	8	0	2.327183	-1.053530	0.000000

Table S25. Theoretical Cartesian coordinates (in Å) for the structure 11**T-1** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	6	0	1.706737	-0.100525	0.000000
2	27	0	0.000000	0.410694	0.000000
3	7	0	-1.613914	-0.137872	0.000000
4	8	0	-2.680027	-0.691802	0.000000
5	8	0	2.812149	-0.498259	0.000000

Table S26. 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	8	0	-1.958074	1.489195	2.421700
2	8	0	-1.535648	1.725932	-2.370370
3	8	0	-0.007390	-2.607354	0.278565
4	8	0	-3.760232	-1.632325	-0.343553
5	8	0	3.087444	-0.535677	-2.236626
6	8	0	2.904118	-0.719498	2.333850
7	8	0	1.128899	2.859611	0.350671
8	27	0	1.317337	-0.075277	-0.079067
9	27	0	-1.262908	-0.090205	-0.015692
10	6	0	1.147844	1.704206	0.177803
11	6	0	2.234126	-0.498005	1.403067
12	6	0	-1.423093	1.041122	-1.431154
13	7	0	-0.122424	-1.412978	0.149594
14	6	0	-1.664664	0.904977	1.454700
15	6	0	-2.765096	-1.035698	-0.216197
16	7	0	2.191394	-0.425692	-1.470265

Table S27. 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	8	0	-1.728670	-3.182358	1.517142
2	8	0	-1.722920	-1.072074	-2.446680
3	8	0	0.000000	0.000000	2.586888
4	8	0	2.515343	-2.604442	-0.217155
5	8	0	1.722920	1.072074	-2.446680
6	8	0	1.728670	3.182358	1.517142
7	8	0	-2.515343	2.604442	-0.217155
8	27	0	0.000000	1.350858	-0.024262
9	27	0	0.000000	-1.350858	-0.024262
10	6	0	1.075161	2.434174	0.933550
11	6	0	-1.063769	-1.136560	-1.503550
12	6	0	-1.075161	-2.434174	0.933550
13	6	0	0.000000	0.000000	1.417280
14	7	0	1.517310	-1.992445	-0.192966
15	7	0	-1.517310	1.992445	-0.192966
16	6	0	1.063769	1.136560	-1.503550

Table S28. 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	-1.428914	2.161654	0.617454
2	6	0	-1.428914	-2.161654	0.617454
3	6	0	1.428914	-2.161654	0.617454
4	8	0	2.333256	2.788169	1.008912
5	8	0	0.000000	1.513594	-2.934060
6	8	0	0.000000	0.000000	2.561579
7	8	0	-2.333256	2.788169	1.008912
8	8	0	-2.333256	-2.788169	1.008912
9	8	0	2.333256	-2.788169	1.008912
10	8	0	0.000000	-1.513594	-2.934060
11	27	0	0.000000	-1.324974	-0.079478
12	27	0	0.000000	1.324974	-0.079478

13	7	0	0.000000	1.383636	-1.758368
14	6	0	1.428914	2.161654	0.617454
15	6	0	0.000000	0.000000	1.376197
16	7	0	0.000000	-1.383636	-1.758368

Table S29. 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	1.557369	1.794569	2.423795
2	8	0	1.557369	1.794569	-2.423795
3	8	0	-2.566126	-0.137295	0.000000
4	8	0	-1.780707	3.684795	0.000000
5	8	0	-0.841905	-2.916688	-2.329206
6	8	0	-0.841905	-2.916688	2.329206
7	8	0	2.935604	-1.117504	0.000000
8	27	0	0.083937	-1.320919	0.000000
9	27	0	-0.112157	1.254996	0.000000
10	6	0	0.932888	1.577998	1.461766
11	6	0	0.932888	1.577998	-1.461766
12	6	0	-1.134157	2.712660	0.000000
13	6	0	-0.537287	-2.238581	1.428681
14	6	0	-0.537287	-2.238581	-1.428681
15	7	0	1.754377	-1.187303	0.000000
16	7	0	-1.374075	0.036574	0.000000

Table S30. Theoretical Cartesian coordinates (in Å) for the structure 25**S-5** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	6	0	0.389011	-2.298116	1.423770
2	6	0	0.389011	-2.298116	-1.423770
3	6	0	0.665649	2.162635	-1.479580
4	6	0	0.665649	2.162635	1.479580
5	6	0	-1.600859	1.727859	0.000000
6	8	0	0.665649	-2.995141	-2.318562
7	8	0	2.501796	-0.267384	0.000000
8	8	0	-3.023061	-1.196279	0.000000
9	8	0	0.665649	-2.995141	2.318562
10	8	0	1.023762	2.811997	2.382454
11	8	0	-2.729314	2.028008	0.000000
12	8	0	1.023762	2.811997	-2.382454

13	27	0	0.156301	1.277407	0.000000
14	27	0	-0.170961	-1.340011	0.000000
15	7	0	1.314211	-0.062072	0.000000
16	7	0	-1.840054	-1.171573	0.000000

Table S31. Theoretical Cartesian coordinates (in Å) for the structure 25S-**6** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	8	0	1.367762	1.995214	2.550282
2	8	0	1.367762	1.995214	-2.550282
3	8	0	-2.692565	0.053285	0.000000
4	8	0	-1.739519	3.430046	0.000000
5	8	0	-0.298181	-2.934413	-2.424052
6	8	0	-0.298181	-2.934413	2.424052
7	8	0	2.604944	-0.570149	0.000000
8	27	0	-0.188068	-1.438599	0.000000
9	27	0	0.104148	1.121726	0.000000
10	6	0	0.891295	1.608182	1.557003
11	6	0	-1.506881	0.021099	0.000000
12	6	0	0.891295	1.608182	-1.557003
13	7	0	-0.298181	-2.241778	-1.463234
14	6	0	-1.043852	2.494237	0.000000
15	6	0	1.425509	-0.454667	0.000000
16	7	0	-0.298181	-2.241778	1.463234

Table S32. Theoretical Cartesian coordinates (in Å) for the structure 25S-**7** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	6	0	1.329577	2.273168	0.000000
2	6	0	-1.681091	2.021351	0.000000
3	6	0	1.765247	-1.342645	0.000000
4	8	0	-2.682325	2.626237	0.000000
5	8	0	-0.034511	0.703217	2.914538
6	8	0	-0.034511	0.703217	-2.914538
7	8	0	2.214624	3.038330	0.000000
8	8	0	2.931055	-1.323077	0.000000
9	8	0	-0.935355	-2.410080	-2.529754
10	8	0	-0.935355	-2.410080	2.529754
11	27	0	-0.034855	-1.458400	0.000000
12	27	0	-0.093533	1.189525	0.000000

13	7	0	-0.603874	-1.960503	1.488952
14	7	0	-0.603874	-1.960503	-1.488952
15	6	0	-0.062555	0.797775	1.745895
16	6	0	-0.062555	0.797775	-1.745895

Table S33. Theoretical Cartesian coordinates (in Å) for the structure 25**T-1** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	8	0	-2.534606	-0.691177	2.476073
2	8	0	-1.354984	3.010041	-0.084118
3	8	0	-0.083958	-2.568318	-0.555899
4	8	0	-3.600309	-0.778733	-1.842528
5	8	0	2.443495	2.060401	-1.569023
6	8	0	3.685329	-1.748788	-0.280317
7	8	0	1.541656	0.778645	2.741324
8	27	0	1.257202	-0.080691	-0.084316
9	27	0	-1.281697	0.017482	-0.131822
10	6	0	1.402853	0.451802	1.628747
11	6	0	2.716326	-1.100719	-0.227834
12	6	0	-1.305887	1.844821	-0.121662
13	7	0	-0.021352	-1.367691	-0.378885
14	6	0	-2.024251	-0.427198	1.460230
15	6	0	-2.686900	-0.486504	-1.178664
16	7	0	1.632143	1.298672	-1.137296

Table S34. Theoretical Cartesian coordinates (in Å) for the structure 24**S-1** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	27	0	-0.069963	0.031421	1.254178
2	27	0	-0.069963	0.031421	-1.254178
3	8	0	2.712342	0.084473	2.285919
4	8	0	-0.255696	-2.609311	0.000000
5	8	0	-0.724924	2.600881	0.000000
6	8	0	2.712342	0.084473	-2.285919
7	8	0	-1.934999	-0.195691	3.379327
8	8	0	-1.934999	-0.195691	-3.379327
9	6	0	1.634499	0.064528	-1.834871
10	6	0	-0.121599	-1.434965	0.000000
11	6	0	-0.367325	1.474678	0.000000
12	6	0	1.634499	0.064528	1.834871

13	7	0	-1.249641	-0.061603	2.421870
14	7	0	-1.249641	-0.061603	-2.421870

Table S35. Theoretical Cartesian coordinates (in Å) for the structure 24**S-2** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	27	0	-1.223139	0.038687	-0.006485
2	27	0	1.258599	-0.010181	-0.127390
3	8	0	-2.753529	-2.427249	0.539152
4	8	0	-0.055150	-0.965513	-2.542846
5	8	0	0.208385	0.394026	2.558709
6	8	0	3.285304	-1.887916	0.439803
7	8	0	-3.164066	2.088201	-0.251131
8	8	0	2.437524	2.704637	-0.285217
9	6	0	-0.206175	-0.525110	-1.457281
10	6	0	0.129079	0.198803	1.395698
11	6	0	-2.119079	-1.467658	0.330154
12	7	0	-2.245271	1.356252	-0.089940
13	7	0	2.375675	-1.234427	0.051801
14	6	0	1.939840	1.648647	-0.232931

Table S36. 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	27	0	-1.163478	-0.081123	-0.102462
2	27	0	1.248581	-0.091261	-0.151524
3	8	0	-3.513357	-1.748495	0.505818
4	8	0	0.011432	-2.205971	-1.611897
5	8	0	0.064108	0.683309	2.465398
6	8	0	3.617766	-1.313419	0.797044
7	8	0	-2.557321	2.529222	-0.357020
8	8	0	1.972712	2.692672	-0.914893
9	6	0	1.666229	1.612634	-0.596329
10	6	0	0.055448	0.337266	1.336085
11	6	0	-2.577726	-1.103397	0.228348
12	6	0	-1.971710	1.531546	-0.189426
13	7	0	-0.052999	-1.165286	-0.999116
14	7	0	2.611005	-0.936493	0.300540

Table S37. 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	0.000000	0.000000	1.191013
2	27	0	0.000000	0.000000	-1.191013
3	8	0	0.000000	2.181329	3.182153
4	8	0	2.322917	1.192795	0.000000
5	8	0	-2.322917	-1.192795	0.000000
6	8	0	0.000000	-2.181329	-3.182153
7	8	0	0.000000	-2.181329	3.182153
8	8	0	0.000000	2.181329	-3.182153
9	6	0	-0.074175	-1.337495	-2.376700
10	6	0	0.074175	1.337495	-2.376700
11	7	0	-1.301585	-0.550281	0.000000
12	7	0	1.301585	0.550281	0.000000
13	6	0	0.074175	1.337495	2.376700
14	6	0	-0.074175	-1.337495	2.376700

Table S38. 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	0.000000	0.000000	-1.262678
2	27	0	0.000000	0.000000	1.278429
3	8	0	0.000000	2.381986	-2.815085
4	8	0	-2.612778	0.000000	0.188627
5	8	0	2.612778	0.000000	0.188627
6	8	0	0.000000	2.603943	2.733473
7	8	0	0.000000	-2.381986	-2.815085
8	8	0	0.000000	-2.603943	2.733473
9	6	0	0.000000	1.585889	2.158251
10	6	0	0.000000	-1.585889	2.158251
11	7	0	0.000000	-1.447652	-2.090453
12	7	0	0.000000	1.447652	-2.090453
13	6	0	-1.428705	0.000000	0.102486
14	6	0	1.428705	0.000000	0.102486

Table S39. 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	0.000000	0.000000	1.091150
2	27	0	0.000000	0.000000	-1.091150
3	8	0	0.000000	0.000000	3.915658
4	8	0	0.000000	2.801844	0.000000
5	8	0	2.426468	-1.400922	0.000000
6	8	0	-2.426468	-1.400922	0.000000
7	8	0	0.000000	0.000000	-3.915658
8	6	0	0.000000	1.622029	0.000000
9	6	0	-1.404718	-0.811015	0.000000
10	7	0	0.000000	0.000000	2.731206
11	7	0	0.000000	0.000000	-2.731206
12	6	0	1.404718	-0.811015	0.000000

Table S40. 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	27	0	-0.200972	1.354409	0.000000
2	27	0	0.240838	-0.961602	0.000000
3	8	0	-0.881682	4.092841	0.000000
4	8	0	0.317233	-2.703196	2.409546
5	8	0	-2.460525	-0.429820	0.000000
6	8	0	2.667641	0.458351	0.000000
7	8	0	0.317233	-2.703196	-2.409546
8	6	0	0.317233	-2.021002	1.462339
9	7	0	-1.317133	-0.046818	0.000000
10	6	0	1.494002	0.618087	0.000000
11	6	0	0.317233	-2.021002	-1.462339
12	7	0	-0.615210	2.935087	0.000000

Table S41. 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	1.272818	-0.417314	-0.038945
2	27	0	-1.008277	-0.093998	-0.011822
3	8	0	0.380645	0.952106	-2.460244
4	8	0	-2.592858	2.392743	0.226383
5	8	0	4.018423	0.178064	0.024341
6	8	0	0.368726	0.453244	2.599518
7	8	0	-2.757867	-2.325139	-0.225289
8	6	0	-1.943130	1.426099	0.133555
9	6	0	0.229380	0.146109	1.465517
10	7	0	-1.980489	-1.435611	-0.141000
11	6	0	0.236221	0.428284	-1.409292
12	7	0	2.892778	-0.193773	-0.014091

Table S42. 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	-0.192599	1.351418	0.000000
2	27	0	0.581755	-0.910357	0.000000
3	8	0	-2.073982	3.603753	0.000000
4	8	0	0.509866	-2.827414	2.259186
5	8	0	-2.284751	-0.504458	0.000000
6	8	0	1.923418	1.719082	0.000000
7	8	0	0.509866	-2.827414	-2.259186
8	6	0	-1.324388	2.704328	0.000000
9	6	0	0.509866	-2.058923	-1.379882
10	6	0	0.509866	-2.058923	1.379882
11	7	0	1.540787	0.536912	0.000000
12	7	0	-1.162879	-0.070620	0.000000

Table S43. Theoretical Cartesian coordinates (in Å) for the structure 23**S-5** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	27	0	-1.361169	0.299342	-0.058463
2	27	0	1.051521	-0.032943	-0.072727
3	8	0	-4.219115	-0.407260	-0.059250
4	8	0	2.319676	0.084962	2.604515
5	8	0	-0.723833	-2.347665	0.214922
6	8	0	-0.094225	2.713752	-0.388798
7	8	0	3.117210	-0.658140	-1.917352
8	6	0	-3.087592	-0.104114	-0.051919
9	6	0	1.780240	0.026465	1.570514
10	7	0	-0.502054	-1.164332	0.116807
11	7	0	2.182451	-0.444126	-1.222368
12	6	0	0.207355	1.574524	-0.243804

Table S44. Theoretical Cartesian coordinates (in Å) for the structure 23**S-6** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	27	0	-1.158427	-0.154853	0.069614
2	27	0	1.196081	-0.129098	-0.144284
3	8	0	-3.566241	1.241722	1.101104
4	8	0	1.400566	-1.982484	2.137445
5	8	0	-1.766465	-1.651808	-2.198569
6	8	0	0.017472	2.437724	-0.113771
7	8	0	3.869479	1.016189	-0.639959
8	7	0	-1.511698	-1.274486	-1.102081
9	6	0	1.335511	-1.345406	1.155033
10	6	0	2.806647	0.554354	-0.473574
11	6	0	-2.593470	0.707492	0.738476
12	7	0	0.090661	1.228385	-0.154138

Table S45. Theoretical Cartesian coordinates (in Å) for the structure 23**S-7** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	27	0	0.000000	1.193050	-0.287512
2	27	0	0.000000	-1.193050	-0.287512
3	8	0	-2.587537	1.870891	-1.098055
4	8	0	-1.366847	-3.500706	0.957179
5	8	0	1.366847	3.500706	0.957179
6	8	0	0.000000	0.000000	2.389149
7	8	0	2.587537	-1.870891	-1.098055
8	6	0	-0.879048	-2.566713	0.449638
9	6	0	0.000000	0.000000	1.201047
10	7	0	-1.447096	1.556180	-0.995391
11	7	0	1.447096	-1.556180	-0.995391
12	6	0	0.879048	2.566713	0.449638

Table S46. Theoretical Cartesian coordinates (in Å) for the structure 23**S-8** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	27	0	1.291155	0.237135	0.000000
2	27	0	-1.095361	0.223567	0.000000
3	8	0	0.254762	-0.881525	2.448713
4	8	0	-1.508365	3.052530	0.000000
5	8	0	0.254762	-0.881525	-2.448713
6	8	0	3.975104	-0.938721	0.000000
7	8	0	-3.086297	-1.814932	0.000000
8	6	0	2.932784	-0.398169	0.000000
9	6	0	0.254762	-0.394024	-1.366882
10	6	0	0.254762	-0.394024	1.366882
11	7	0	-2.258620	-0.969269	0.000000
12	7	0	-1.321384	1.882375	0.000000

Table S47. Theoretical Cartesian coordinates (in Å) for the structure 22**S-1** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	27	0	1.147313	0.157707	-0.421438
2	27	0	-1.109466	-0.001990	0.184792
3	7	0	-2.730007	-0.194316	0.320977
4	8	0	3.681610	-0.333876	1.010435
5	8	0	-3.915164	-0.283849	0.292871
6	8	0	0.339397	-2.425245	-0.510591
7	7	0	0.110186	-1.260785	-0.259112
8	6	0	2.735166	-0.099140	0.362833
9	6	0	-0.194070	1.565708	-0.077342
10	8	0	0.152944	2.690712	-0.262286

Table S48. Theoretical Cartesian coordinates (in Å) for the structure 22**S-2** using the BP86/DZP method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	27	0	-1.079615	-0.219584	0.000000
2	27	0	1.052256	0.478992	0.000000
3	8	0	-3.036496	-2.239474	0.000000
4	8	0	2.736754	2.746095	0.000000
5	8	0	0.163744	-0.676787	2.605623
6	8	0	0.163744	-0.676787	-2.605623
7	7	0	2.117369	1.731676	0.000000
8	7	0	-2.324251	-1.289505	0.000000
9	6	0	0.163744	-0.276965	1.489095
10	6	0	0.163744	-0.276965	-1.489095

Table S49. 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	0.218584	-1.168007	0.000000
2	27	0	0.000000	1.158330	0.000000
3	7	0	-0.200621	2.798531	0.000000
4	8	0	-0.551140	-4.035056	0.000000
5	8	0	-0.244166	3.987721	0.000000
6	8	0	-2.452961	-0.408658	0.000000
7	7	0	-1.267019	-0.135432	0.000000
8	6	0	-0.226538	-2.912187	0.000000
9	6	0	1.616772	0.398341	0.000000
10	8	0	2.752055	0.043824	0.000000