Binuclear Cyclopentadienylmolybdenum Carbonyl Derivatives: Where is the Missing Mo=Mo Double Bonded Species $Cp_2Mo_2(CO)_5$?

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Complete Gaussian 03 reference (Reference 38)

Table S1. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Cp_2Mo_2(CO)_6$ by BP86/SDD method (infrared intensities in parentheses are in km/mol).

6S-1(C_{2h})	**6S-2(C_2)**
47.1(b_u, 0.7)	41.1(a, 0.1)
57.1(a_u, 1.6)	51.2(a, 0.4)
60.6(b_g, 0.0)	61.5(b, 0.1)
72.6(a_u, 0.2)	65.7(a, 0.1)
75.0(a_g, 0.0)	66.6(b, 0.0)
75.0(bg, 0.0)	72.6(a, 0.1)
78.4(a_u, 0.1)	78.7(b, 0.1)
93.7(b_g, 0.0)	86.2(a, 0.0)
95.4(a_g, 0.0)	90.5(b, 1.0)
96.5(a_g, 0.0)	96.9(a, 0.2)
97.3(b_u, 1.2)	99.1(b, 0.0)
100.9(a_u, 0.1)	101.0(a, 0.3)
111.2(b_u, 0.1)	106.3(b, 0.0)
116.5(a_g, 0.0)	107.8(a, 0.1)
119.0(b_g, 0.0)	122.9(a, 0.3)
123.5(a_u, 0.5)	126.6(b, 2.0)
124.5(b_u, 8.7)	130.5(b, 5.2)
142.5(a_g, 0.0)	151.2(a, 0.0)
314.9(b_u, 2.5)	311.7(b, 2.9)
315.2(a_g, 0.0)	312.4(a, 0.1)
318.4(b_g, 0.0)	316.4(a, 1.7)
319.3(a_u, 9.6)	318.6(b, 5.9)
342.0(b_u, 0.7)	342.0(b, 1.2)
345.4(a_g, 0.0)	348.7(a, 0.1)
401.3(b_g, 0.0)	399.5(a, 0.7)
426.2(b_u, 23.2)	406.0(b, 27.5)
429.8(a_g, 0.0)	425.6(a, 2.4)
441.5(a_u, 0.3)	425.9(b, 8.7)
454.1(b_u, 78.7)	454.2(b, 62.4)
460.3(b_g, 0.0)	458.9(a, 0.0)
460.4(a_u, 0.4)	460.9(b, 23.3)
463.8(a_g, 0.0)	463.2(a, 0.0)
494.6(b_u, 56.2)	491.8(a, 9.1)
497.6(a_g, 0.0)	494.1(b, 29.4)
501.9(b_g, 0.0)	498.6(a, 12.9)
508.2(a_u, 57.0)	499.0(b, 55.4)
544.3(b_u, 223.6)	538.8(b, 212.9)
557.9(a_g, 0.0)	549.9(a, 1.5)
567.4(b_g, 0.0)	567.9(a, 9.3)
573.1(a_u, 6.6)	568.5(b, 19.9)
578.9(a_u, 4.6)	579.0(b, 3.2)
579.7(b_g, 0.0)	580.2(a, 0.1)
581.6(b_u, 47.4)	583.2(a, 27.3)
584.1(a_g, 0.0)	583.4(b, 5.3)
587.1(b_u, 27.3)	587.6(b, 3.2)
588.0(a_g, 0.0)	587.9(a, 6.1)
782.9(a_g, 0.0)	778.7(b, 68.6)
783.4(b_u, 134.3)	793.7(a, 58.8)
805.4(b_u, 58.1)	799.7(b, 26.1)
807.3(a_g, 0.0)	806.1(a, 20.9)
808.2(a_u, 10.6)	807.9(b, 18.8)

808.9(b_g, 0.0)	808.1(a, 10.4)
812.4(a_u, 0.0)	809.8(b, 0.6)
812.9(b_g, 0.0)	810.9(a, 0.8)
815.3(b_u, 3.6)	814.4(a, 3.8)
815.8(a_g, 0.0)	816.8(b, 2.0)
871.0(a_u, 2.1)	868.6(b, 2.1)
871.4(b_g, 0.0)	869.3(a, 0.0)
875.6(b_u, 3.1)	874.9(a, 0.1)
876.6(a_g, 0.0)	884.0(b, 0.2)
989.4(b_u, 6.9)	988.0(b, 8.6)
989.7(a_g, 0.0)	988.8(a, 0.0)
999.7(b_g, 0.0)	997.2(b, 9.3)
999.7(a_u, 12.7)	997.7(a, 3.5)
1045.6(a_u, 3.2)	1036.4(b, 1.6)
1045.8(b_u, 4.7)	1044.5(a, 0.1)
1046.1(b_g, 0.0)	1045.1(b, 2.9)
1046.2(a_g, 0.0)	1047.5(a, 0.4)
1101.5(b_u, 1.3)	1102.7(b, 0.6)
1101.7(a_g, 0.0)	1103.1(a, 2.6)
1230.2(a_u, 0.1)	1225.2(a, 0.0)
1230.2(b_g, 0.0)	1227.0(b, 0.1)
1357.2(a_u, 3.6)	1358.6(b, 4.0)
1359.5(b_g, 0.0)	1360.4(a, 0.5)
1360.6(b_u, 5.2)	1362.3(b, 1.1)
1361.5(ag, 0.0)	1363.0(a, 0.7)
1404.1(bu, 10.2)	1404.6(b, 9.3)
1404.4(ag, 0.0)	1405.0(a, 0.7)
1414.8(bg, 0.0)	1411.5(a, 1.8)
1414.8(au, 6.0)	1411.9(b, 3.9)
1880.9(bg, 0.0)	1886.5(a, 380.6)
1901.9(b_u, 396.8)	1892.1(b, 711.4)
1911.7(a_u, 1831.1)	1924.5(b, 1038.1)
1915.2(a_g, 0.0)	1927.7(a, 4.0)
1955.4(b_u, 2265.8)	1957.2(b, 1348.1)
1986.3(a_g, 0.0)	2000.8(a, 977.7)
3173.8(b_g, 0.0)	3171.6(b, 0.1)
3173.8(a_u, 0.7)	3171.7(a, 0.3)
3179.5(a_g, 0.0)	3177.4(b, 0.9)
3179.6(b_u, 0.2)	3177.5(a, 0.3)
3188.6(a_g, 0.0)	3187.8(b, 0.2)
3188.6(b_u, 2.5)	3187.8(a, 0.4)
3190.7(a_u, 0.5)	3191.1(b, 2.3)
3190.8(b_g, 0.0)	3191.3(a, 0.0)
3200.5(b_u, 0.2)	3202.6(b, 1.1)
3200.5(a_g, 0.0)	3202.7(a, 2.1)

Table S2. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Cp_2Mo_2(CO)_5$ by BP86/SDD method (infrared intensities in parentheses are in km/mol).

5S-1(C_1)	**5S-2(C_2)**	**5S-3(C_{2v})**
18.2(a, 0.7)	4.8(b, 0.9)	14.6i (a", 0.0)
36.5(a, 1.7)	17.1(b, 0.4)	6.2i (a", 0.1)
43.6(a, 0.3)	17.6(a, 0.0)	46.4(a', 0.2)
66.8(a, 0.0)	41.0(a, 0.7)	59.0(a', 0.0)
74.3(a, 0.2)	55.5(b, 0.6)	64.4(a", 0.1)
76.5(a, 0.4)	73.3(a, 2.1)	67.7(a", 1.0)
81.2(a, 1.3)	79.8(b, 0.2)	69.6(a", 0.0)
92.3(a, 1.4)	88.7(a, 0.0)	78.3(a', 0.2)
99.4(a, 0.6)	92.6(b, 0.7)	84.6(a', 0.2)
101.0(a, 0.1)	104.2(a, 0.4)	88.1(a", 0.1)
111.2(a, 0.9)	108.4(a, 0.0)	88.6(a', 0.1)
121.7(a, 0.3)	111.8(b, 1.6)	94.4(a", 0.0)
124.6(a, 1.7)	124.7(a, 0.0)	101.9(a", 2.2)
133.6(a, 0.2)	130.2(b, 1.0)	127.4(a', 4.6)
169.5(a, 0.4)	153.6(a, 0.8)	130.1(a', 0.1)
252.0(a, 0.5)	261.5(b, 10.1)	182.0(a', 11.4)
270.6(a, 4.6)	304.4(b, 8.2)	277.2(a', 0.2)
300.3(a, 1.3)	312.4(a, 4.4)	286.2(a", 9.3)
303.4(a, 6.7)	322.5(b, 3.5)	296.8(a', 0.0)
313.3(a, 5.3)	329.2(a, 3.6)	336.0(a", 0.0)
336.5(a, 5.9)	335.9(b, 5.8)	340.9(a", 0.0)
341.6(a, 1.5)	347.6(a, 1.2)	359.4(a", 0.0)
389.1(a, 3.0)	389.3(a, 0.1)	361.5(a', 3.7)
414.4(a, 3.9)	396.3(b, 2.2)	369.7(a', 3.0)
418.0(a, 19.8)	410.1(a, 0.1)	400.2(a', 3.7)
443.5(a, 4.8)	417.0(b, 37.6)	407.9(a', 10.2)
456.4(a, 5.1)	446.3(b, 52.6)	416.1(a", 3.1)
461.5(a, 32.9)	451.5(a, 1.8)	417.9(a', 0.6)
470.9(a, 3.2)	461.2(b, 82.4)	418.2(a', 19.6)
489.5(a, 35.0)	475.7(a, 16.5)	435.6(a', 0.4)
496.1(a, 63.2)	483.0(b, 1.3)	446.5(a", 16.6)
507.9(a, 3.6)	498.8(a, 2.9)	467.1(a", 0.0)
533.9(a, 38.2)	524.7(a, 0.4)	479.9(a', 49.5)
540.9(a, 12.4)	528.1(b, 10.1)	516.6(a', 1.5)
562.9(a, 6.4)	564.1(b, 10.4)	551.1(a', 13.6)
573.5(a, 3.5)	569.7(b, 11.5)	553.8(a", 0.0)
575.5(a, 0.8)	575.3(a, 0.1)	559.0(a', 0.1)
581.2(a, 3.3)	580.6(b, 0.1)	571.0(a", 5.7)
581.5(a, 1.8)	580.8(a, 0.2)	571.8(a', 40.1)
592.4(a, 15.9)	584.6(a, 20.2)	576.9(a", 48.4)
601.3(a, 47.9)	625.8(b, 175.1)	604.4(a', 56.2)
784.3(a, 65.1)	785.8(b, 93.5)	765.1(a', 33.8)
795.0(a, 19.1)	786.3(a, 18.4)	766.4(a", 0.0)
795.6(a, 106.0)	793.4(b, 0.0)	792.3(a', 5.1)
806.6(a, 16.4)	794.2(a, 15.9)	800.7(a", 1.0)
810.6(a, 1.9)	808.6(b, 7.0)	802.5(a", 0.0)
811.7(a, 0.4)	809.1(a, 4.5)	804.0(a", 3.0)
813.3(a, 1.8)	810.9(b, 14.4)	809.4(a', 65.9)
814.2(a, 4.9)	814.0(a, 0.4)	814.1(a', 3.1)
816.0(a, 1.2)	816.9(a, 4.2)	819.7(a', 0.1)
816.2(a, 0.7)	817.1(b, 9.7)	830.0(a', 10.9)
870.4(a, 2.9)	864.1(a, 0.0)	856.0(a', 23.1)
871.5(a, 0.8)	864.4(b, 4.0)	882.2(a", 0.0)

878.8(a, 0.7)	886.3(a, 0.1)	882.4(a", 3.7)
889.6(a, 2.2)	886.9(b, 5.1)	885.1(a', 17.3)
991.7(a, 6.8)	990.3(b, 11.9)	983.2(a', 2.2)
993.2(a, 5.3)	990.4(a, 4.1)	984.9(a', 10.6)
993.4(a, 5.2)	992.8(b, 9.3)	988.1(a", 0.0)
995.4(a, 5.8)	993.0(a, 4.1)	997.3(a", 13.1)
1040.6(a, 1.9)	1039.1(b, 3.3)	1033.0(a", 0.0)
1043.3(a, 1.4)	1040.2(a, 0.1)	1041.1(a", 0.0)
1044.0(a, 0.3)	1045.2(b, 0.4)	1056.0(a', 6.9)
1045.4(a, 0.9)	1045.4(a, 1.0)	1056.4(a', 0.2)
1103.5(a, 0.9)	1103.3(b, 2.5)	1101.0(a', 5.4)
1105.3(a, 0.2)	1103.3(a, 0.2)	1101.6(a', 3.8)
1226.2(a, 0.0)	1225.1(a, 0.0)	1226.7(a", 0.0)
1228.0(a, 0.1)	1225.2(b, 0.0)	1228.7(a", 0.0)
1355.7(a, 14.2)	1353.3(b, 14.2)	1347.4(a", 0.0)
1359.6(a, 0.6)	1354.0(a, 2.1)	1360.0(a", 0.1)
1361.9(a, 2.5)	1366.7(a, 0.0)	1360.7(a', 1.8)
1363.1(a, 0.7)	1366.8(b, 2.4)	1361.0(a', 1.5)
1406.5(a, 4.3)	1407.2(b, 9.3)	1403.0(a", 8.0)
1409.9(a, 3.7)	1407.3(a, 0.4)	1405.1(a", 0.0)
1410.6(a, 3.6)	1408.1(b, 0.9)	1412.6(a', 3.7)
1411.8(a, 2.6)	1408.3(a, 4.8)	1414.1(a', 1.9)
1720.9(a, 370.9)	1689.4(a, 579.9)	1901.7(a', 1582.5)
1857.4(a, 454.5)	1894.5(a, 157.9)	1915.6(a", 1516.8)
1908.7(a, 1006.0)	1910.2(b, 907.0)	1923.3(a', 193.5)
1932.1(a, 963.7)	1915.4(b, 862.6)	1933.9(a', 354.2)
1981.5(a, 833.7)	1976.5(a, 908.7)	2000.6(a', 1128.6)
3172.2(a, 0.4)	3170.6(b, 0.1)	3175.1(a', 0.3)
3173.0(a, 0.2)	3170.7(a, 0.0)	3178.6(a', 0.0)
3173.9(a, 0.2)	3172.2(b, 0.1)	3180.3(a", 0.0)
3178.6(a, 0.0)	3172.2(a, 0.2)	3181.1(a", 1.1)
3184.4(a, 0.1)	3182.5(b, 1.5)	3191.2(a', 0.0)
3186.6(a, 0.4)	3182.6(a, 0.0)	3196.9(a", 0.0)
3188.6(a, 0.3)	3187.0(b, 0.0)	3197.6(a", 0.0)
3191.1(a, 0.2)	3187.0(a, 0.1)	3199.1(a', 7.2)
3195.2(a, 0.2)	3194.7(b, 0.3)	3208.5(a', 0.0)
3204.2(a, 0.1)	3194.7(a, 0.1)	3208.9(a', 0.2)

Table S3. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the triplet structures of $Cp_2Mo_2(CO)_5$ by BP86/SDD method (infrared intensities in parentheses are in km/mol).

5T-1(C_S)	**5T-2(C_S)**	**5T-3(C_{2v})**
18i(a",0.2)	16i(a",0.0)	15.7(b_1,0.1)
28.0(a',1.0)	29.8(a",0.0)	24.6(a_2,0.0)
34.5(a",0.1)	35.3(a',1.7)	39.6(a_1,0.2)
47.4(a",0.7)	45.5(a",0.0)	49.8(b_2,0.2)
48.4(a",0.4)	61.1(a",0.1)	62.2(b_1,0.0)
73.3(a',0.0)	73.8(a",0.2)	67.4(b_2,0.1)
76.8(a",0.0)	75.0(a',0.3)	74.5(a_2,0.0)
81.8(a',0.5)	83.3(a',0.6)	77.6(a_1,0.0)
83.3(a',0.4)	85.9(a",0.0)	79.2(b_1,0.7)
85.5(a",0.0)	90.2(a',0.2)	82.8(b_1,0.0)
96.1(a',0.1)	95.7(a',0.4)	85.7(b_1,0.3)
99.0(a",0.1)	105.2(a",0.3)	85.9(a_2,0.0)
103.0(a',2.4)	110.3(a',1.0)	87.5(b_2,0.5)
122.2(a",0.0)	151.7(a",0.0)	91.0(a_1,0.0)
148.3(a',0.6)	156.8(a',0.4)	107.3(b_2,0.0)
160.8(a',0.1)	171.0(a',0.4)	151.5(a_1,6.2)
295.0(a",0.1)	296.6(a",0.0)	280.1(a_1,4.5)
299.6(a",7.4)	302.3(a',5.1)	317.9(b_2,0.0)
306.1(a',6.2)	304.6(a",8.2)	326.6(b_1,6.3)
314.5(a',0.0)	328.2(a',2.4)	332.6(a_2,0.0)
333.1(a',0.7)	336.8(a',0.3)	343.7(a_2,0.0)
338.9(a',1.9)	344.8(a',0.8)	354.4(a_1,67.9)
362.2(a",4.1)	371.9(a",8.0)	366.8(b_2,0.4)
396.4(a',36.0)	380.4(a',27.6)	368.2(b_1,0.2)
428.1(a",0.1)	404.5(a",3.3)	388.1(b_2,0.0)
441.4(a',22.5)	428.8(a",3.0)	403.0(b_1,20.1)
445.1(a",16.4)	436.0(a',8.8)	412.9(b_2,24.7)
448.6(a",3.1)	438.6(a",6.5)	415.8(a_1,0.1)
468.4(a',32.5)	450.1(a',40.4)	419.6(a_1,0.1)
471.9(a",0.1)	463.6(a",0.0)	468.1(a_1,1.4)
475.3(a',47.7)	471.3(a',44.5)	473.7(a_2,0.0)
485.7(a',11.5)	479.5(a',9.8)	502.5(b_1,0.4)
489.0(a",10.7)	479.8(a",7.1)	508.4(a_1,26.9)
514.5(a',73.6)	514.9(a',29.4)	537.2(b_2,0.8)
551.7(a',30.1)	544.9(a',36.4)	552.7(a_2,0.0)
553.8(a",15.1)	548.5(a",6.2)	569.6(b_1,0.7)
573.8(a",0.0)	572.0(a',4.3)	570.1(b_2,11.9)
574.0(a',0.2)	575.0(a",0.0)	573.3(a_1,2.0)
577.5(a',5.3)	575.8(a',0.9)	579.4(b_2,34.6)
580.9(a",0.2)	579.7(a",0.0)	587.9(b_1,51.2)
582.4(a',7.2)	581.2(a',1.4)	617.2(a_1,97.6)
783.7(a',86.6)	772.6(a',29.4)	771.4(a_2,0.0)
785.5(a',78.0)	786.2(a',80.4)	777.4(b_1,1.3)
790.1(a',4.1)	790.2(a',38.6)	779.3(b_2,122.5)
791.7(a',10.5)	798.1(a',14.0)	784.9(a_1,3.4)
798.9(a",2.5)	803.8(a",2.3)	790.0(b_2,3.8)
805.0(a",3.7)	807.9(a",3.6)	790.2(a_1,3.8)
809.8(a',2.5)	808.7(a',2.3)	801.0(a_2,0.0)
813.3(a",0.8)	812.3(a",1.9)	809.4(b_2,4.5)
813.3(a',6.2)	813.6(a",0.0)	810.5(b_1,1.2)
814.4(a",0.3)	815.2(a',11.5)	820.0(a_1,2.0)
866.2(a",0.6)	869.4(a',2.5)	851.6(b_2,0.0)
867.3(a',1.7)	870.4(a",1.4)	858.5(a_2,0.0)

874.6(a",0.0)	873.2(a',2.7)	862.1(b_1,1.2)
874.9(a',0.1)	874.7(a",0.1)	877.7(a_1,3.7)
985.8(a',6.0)	988.0(a',9.9)	982.8(b_2,1.4)
987.6(a',6.4)	989.4(a',5.2)	982.8(a_1,36.8)
992.9(a",5.9)	993.9(a",2.2)	987.6(a_2,0.0)
995.9(a",7.6)	994.2(a",12.0)	988.5(b_1,25.6)
1040.5(a',0.1)	1042.1(a",0.0)	1035.2(a_2,0.0)
1041.1(a",0.3)	1042.9(a",0.5)	1043.1(b_1,0.0)
1042.1(a",0.7)	1043.0(a',0.0)	1047.4(b_2,7.5)
1042.5(a',0.8)	1044.2(a',0.3)	1049.0(a_1,0.5)
1098.6(a',1.5)	1100.1(a',3.1)	1094.9(a_1,13.7)
1099.3(a',1.3)	1100.2(a',1.3)	1095.1(b_2,14.0)
1225.1(a",0.0)	1225.9(a",0.0)	1223.6(b_1,0.0)
1226.0(a",0.0)	1226.7(a",0.0)	1223.6(a_2,0.0)
1354.9(a',0.6)	1356.1(a",0.2)	1346.7(a_2,0.0)
1355.3(a",0.2)	1358.4(a',1.4)	1358.2(b_1,0.6)
1355.4(a',1.7)	1359.1(a',2.2)	1359.0(b_2,1.8)
1357.0(a",0.1)	1360.5(a",0.0)	1367.2(a_1,13.4)
1402.9(a',2.6)	1404.4(a',2.0)	1396.6(b_2,0.2)
1403.6(a',3.3)	1404.6(a',4.4)	1396.8(a_1,0.1)
1406.5(a",2.8)	1407.7(a",2.8)	1397.1(b_1,2.8)
1410.8(a",2.0)	1409.2(a",2.9)	1403.0(a_2,0.0)
1827.4(a",578.4)	1790.7(a",702.0)	1908.5(b_2,1608.6)
1841.9(a',50.3)	1804.4(a',284.5)	1916.1(b_1,1658.3)
1900.6(a",1040.7)	1912.8(a',517.5)	1919.4(a_1,562.6)
1923.1(a',2130.1)	1914.3(a",864.1)	1936.8(a_1,85.7)
1954.5(a',11.4)	1970.9(a',1199.9)	2013.6(a_1,749.4)
3172.3(a",0.1)	3168.6(a',1.4)	3169.0(a_1,5.9)
3172.5(a',0.1)	3172.8(a",0.0)	3169.0(b_2,0.0)
3173.1(a",0.2)	3174.5(a",0.1)	3173.3(b_1,0.2)
3174.3(a',0.1)	3174.9(a',0.1)	3173.4(a_2,0.0)
3184.1(a",0.1)	3183.3(a',0.1)	3186.9(b_2,0.0)
3185.1(a',0.4)	3184.2(a",0.1)	3187.2(a_1,0.0)
3187.0(a",0.0)	3186.6(a',0.3)	3202.3(b_1,0.6)
3187.6(a',0.2)	3187.3(a",0.1)	3202.9(a_2,0.0)
3195.6(a',0.0)	3193.9(a',0.1)	3212.5(b_2,0.7)
3195.7(a',0.0)	3196.5(a',0.1)	3212.6(a_1,1.0)

Table S4. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the $Cp_2Mo_2(CO)_4$ structures by BP86/SDD method (infrared intensities in parentheses are in km/mol).

4S-1(C_2)	**4T-1(C_S)**	**4T-2(C_i)**
19.3(a, 1.4)	11.2(a", 0.6)	16.2(a_u, 1.1)
29.3(b, 0.0)	16.9(a", 0.1)	24.9(a_u, 0.2)
30.6(a, 0.0)	38.3(a', 0.8)	25.5(a_g, 0.0)
37.2(b, 0.3)	44.9(a", 0.6)	51.7(a_u, 1.2)
61.3(b, 1.9)	64.7(a", 0.4)	67.3(a_g, 0.0)
76.1(a, 0.0)	74.2(a", 0.0)	75.2(a_u, 2.2)
88.9(a, 0.2)	78.3(a', 0.0)	75.9(a_g, 0.0)
90.8(b, 1.8)	82.7(a', 0.5)	80.0(a_u, 0.7)
100.5(a, 0.2)	97.8(a', 0.8)	93.3(a_g, 0.0)
109.4(a, 0.1)	102.5(a', 0.1)	95.3(a_u, 0.5)
111.8(b, 0.0)	112.6(a", 0.0)	112.7(a_g, 0.0)
114.8(a, 0.0)	150.9(a", 0.4)	133.7(a_g, 0.0)
122.5(b, 0.6)	156.0(a', 0.2)	135.3(a_u, 1.5)
209.5(a, 0.0)	170.5(a', 1.2)	196.3(a_g, 0.0)
308.4(b, 7.8)	291.2(a', 5.2)	286.6(a_u, 8.6)
316.7(b, 4.1)	301.8(a", 4.0)	291.3(a_g, 0.0)
316.8(a, 0.4)	315.6(a', 0.1)	314.1(a_u, 1.1)
325.1(a, 1.6)	317.1(a", 2.9)	314.7(a_g, 0.0)
326.2(b, 0.4)	322.1(a', 2.7)	331.0(a_u, 5.0)
355.0(a, 0.0)	331.9(a", 2.4)	331.3(a_g, 0.0)
407.1(b, 3.2)	340.1(a', 0.3)	403.1(a_u, 9.1)
438.8(a, 13.5)	414.3(a", 1.3)	408.9(a_g, 0.0)
453.1(b, 8.7)	421.6(a', 8.2)	437.1(a_u, 3.7)
474.6(a, 15.9)	441.8(a", 1.1)	446.8(a_g, 0.0)
483.7(b, 87.1)	449.9(a', 22.0)	465.2(a_u, 48.0)
489.8(a, 0.5)	468.6(a', 30.4)	470.1(a_g, 0.0)
516.1(b, 0.5)	476.1(a", 6.7)	485.2(a_g, 0.0)
516.7(a, 7.2)	477.1(a', 16.0)	487.2(a_u, 4.7)
524.4(a, 3.1)	489.1(a', 14.5)	495.3(a_g, 0.0)
527.9(b, 75.7)	529.3(a', 90.8)	506.0(a_u, 48.0)
569.6(a, 0.1)	557.8(a", 18.7)	555.3(a_u, 33.8)
571.9(b, 0.7)	561.3(a', 20.3)	561.6(a_g, 0.0)
580.2(b, 0.1)	563.4(a", 0.7)	574.7(a_u, 2.0)
581.0(a, 0.0)	565.1(a', 1.9)	575.3(a_g, 0.0)
582.3(b, 10.6)	580.1(a", 0.3)	576.4(a_g, 0.0)
596.7(a, 0.6)	584.8(a', 0.3)	578.0(a_u, 4.9)
776.4(a, 0.5)	766.1(a', 23.9)	772.6(a_u, 106.2)
776.9(b, 107.4)	776.9(a', 48.5)	772.9(a_g, 0.0)
786.5(a, 4.6)	781.4(a', 88.6)	784.1(a_u, 12.8)
787.7(b, 4.9)	783.8(a", 2.1)	785.1(a_g, 0.0)
804.7(b, 49.1)	800.8(a', 12.0)	805.4(a_g, 0.0)
807.7(a, 0.2)	802.2(a", 0.7)	805.9(a_u, 52.7)
812.1(b, 15.0)	808.2(a", 0.6)	809.4(a_g, 0.0)
812.6(a, 0.1)	811.2(a', 2.2)	810.6(a_u, 7.6)
813.4(b, 0.0)	812.6(a", 0.0)	812.5(a_u, 14.4)
814.1(a, 0.1)	816.6(a', 5.1)	813.2(a_g, 0.0)
858.0(b, 1.8)	861.0(a", 1.9)	861.4(a_u, 3.6)
858.7(a, 0.1)	865.0(a", 0.6)	862.1(a_g, 0.0)
877.8(b, 0.0)	871.5(a', 3.5)	872.9(a_u, 0.4)
877.9(a, 0.8)	877.4(a', 4.3)	873.0(a_g, 0.0)
987.8(a, 18.6)	983.8(a", 10.1)	984.1(a_u, 20.5)
988.1(b, 0.3)	989.3(a", 9.7)	984.5(a_g, 0.0)
992.5(b, 20.8)	990.3(a', 8.2)	996.5(a_g, 0.0)
993.0(a, 0.3)	994.2(a', 3.7)	996.6(a_u, 13.5)

1036.8(a, 0.7)	1040.4(a", 0.3)	1038.9(a_u, 1.9)
1038.8(b, 0.0)	1040.9(a', 0.1)	1039.1(a_g, 0.0)
1043.4(b, 1.6)	1042.8(a', 2.9)	1042.3(a_u, 1.6)
1043.7(a, 0.1)	1043.3(a", 0.6)	1042.7(a_g, 0.0)
1099.7(b, 5.0)	1093.4(a', 7.7)	1100.1(a_g, 0.0)
1099.7(a, 0.1)	1102.4(a', 0.6)	1100.2(a_u, 4.0)
1224.3(a, 0.0)	1225.0(a", 0.0)	1224.9(a_g, 0.0)
1224.3(b, 0.0)	1225.5(a", 0.0)	1225.0(a_u, 0.0)
1350.2(a, 0.0)	1349.0(a', 3.3)	1352.9(a_u, 1.7)
1351.8(b, 0.4)	1352.8(a", 0.1)	1353.8(a_g, 0.0)
1363.3(b, 0.7)	1353.9(a', 3.7)	1359.8(a_u, 3.3)
1363.6(a, 0.2)	1360.9(a", 1.2)	1360.5(a_g, 0.0)
1403.1(b, 0.2)	1396.2(a", 3.1)	1402.4(a_u, 6.9)
1403.2(a, 4.0)	1403.4(a', 2.8)	1402.5(a_g, 0.0)
1410.5(b, 8.6)	1406.7(a", 2.5)	1412.4(a_g, 0.0)
1410.8(a, 0.2)	1409.3(a', 2.9)	1412.5(a_u, 6.6)
1858.2(b, 208.2)	1810.1(a", 998.9)	1795.3(a_u, 1002.6)
1870.4(a, 1265.9)	1824.9(a', 90.8)	1795.7(a_g, 0.0)
1900.1(b, 1142.7)	1873.6(a',1221.1)	1887.5(a_u, 2168.1)
1937.6(a, 289.9)	1939.5(a', 802.5)	1912.9(a_g, 0.0)
3168.4(b, 0.1)	3168.1(a', 0.2)	3169.9(a_u, 1.0)
3168.6(a, 0.0)	3170.0(a', 0.1)	3169.9(a_g, 0.0)
3171.3(a, 0.1)	3170.9(a", 0.2)	3172.4(a_g, 0.0)
3171.3(b, 0.0)	3175.2(a", 0.1)	3172.5(a_u, 0.2)
3181.9(b, 2.4)	3183.0(a", 0.0)	3184.0(a_u, 1.3)
3182.0(a, 0.0)	3184.8(a', 0.4)	3184.1(a_g, 0.0)
3183.7(a, 0.0)	3185.2(a', 0.8)	3184.2(a_u, 0.8)
3183.8(b, 0.1)	3186.6(a", 0.1)	3184.3(a_g, 0.0)
3193.0(b, 0.1)	3194.4(a', 0.1)	3194.2(a_u, 0.1)
3193.1(a, 0.0)	3196.5(a', 0.1)	3194.2(a_g, 0.0)

Table S5. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structures of $Cp_2Mo_2(CO)_3$ by BP86/SDD method (infrared intensities in parentheses are in km/mol).

3T-1(C_1)	**3T-2(C_2)**	**3T-3(C_s)**	**3S-2(C_s)**
11.4 (a, 0.0)	18.3i (b, 2.8)	22.4 (a", 0.0)	14.2i (a", 0.0)
17.6 (a, 0.0)	17.3 (a, 0.0)	49.1 (a', 0.7)	31.9 (a", 0.1)
32.7 (a, 0.8)	25.6 (b, 0.5)	66.6 (a", 0.4)	58.9 (a", 0.4)
62.5 (a, 1.5)	54.2 (a, 0.4)	68.4 (a', 0.0)	62.0 (a', 2.8)
64.9 (a, 0.8)	71.5 (b, 2.1)	68.6 (a", 0.2)	87.8 (a', 0.1)
73.4 (a, 0.9)	78.3 (a, 0.0)	77.7 (a', 1.7)	96.1 (a", 0.9)
99.8 (a, 0.0)	95.5 (b, 1.2)	83.0 (a', 0.1)	106.1 (a', 1.2)
110.2 (a, 0.2)	100.3 (a, 0.0)	86.0 (a", 0.6)	118.7 (a", 3.6)
125.3 (a, 0.1)	120.2 (b, 1.2)	93.4 (a', 1.4)	148.1 (a", 4.7)
129.4 (a, 3.3)	146.1 (b, 0.6)	103.1 (a", 0.3)	159.2 (a', 3.5)
190.9 (a, 1.1)	153.0 (a, 0.5)	131.8 (a', 1.5)	211.5 (a', 1.1)
208.0 (a, 0.5)	196.8 (a, 0.0)	178.1 (a', 0.7)	214.9 (a', 2.0)
315.5 (a, 5.3)	251.2 (b, 1.1)	297.3 (a', 2.9)	306.0 (a", 3.4)
318.9 (a, 2.3)	318.1 (a, 7.0)	304.2 (a', 9.1)	308.9 (a', 3.7)
320.5 (a, 4.0)	319.5 (b, 0.3)	330.4 (a", 0.0)	328.2 (a', 2.6)
326.1 (a, 3.7)	329.0 (a, 1.8)	350.7 (a", 0.0)	335.1 (a", 9.6)
336.3 (a, 0.2)	339.8 (b, 2.5)	372.0 (a", 4.1)	343.4 (a', 4.1)
355.2 (a, 0.5)	344.9 (b, 4.4)	389.1 (a', 16.2)	373.7 (a", 0.4)
399.1 (a, 2.0)	353.6 (a, 1.2)	404.1 (a", 0.0)	390.3 (a', 1.4)
402.9 (a, 0.7)	397.9 (b, 0.3)	409.7 (a', 0.6)	418.6 (a", 0.0)
424.4 (a, 6.5)	421.4 (a, 0.4)	420.6 (a", 0.1)	435.5 (a', 9.9)
456.4 (a, 2.8)	442.5 (b, 13.8)	465.3 (a', 0.4)	458.6 (a', 0.6)
468.5 (a, 2.8)	453.6 (a, 2.7)	485.3 (a", 3.7)	471.9 (a", 5.1)
476.2 (a, 18.9)	478.0 (a, 23.4)	488.3 (a', 9.5)	521.3 (a", 1.1)
502.7 (a, 11.4)	479.2 (b, 13.8)	552.8 (a", 0.1)	533.0 (a', 20.2)
523.5 (a, 30.7)	482.5 (a, 1.4)	565.2 (a', 1.0)	546.9 (a', 26.0)
557.3 (a, 5.3)	537.0 (b, 1.2)	569.8 (a', 2.2)	562.6 (a', 7.4)
561.8 (a, 0.3)	570.0 (a, 0.0)	570.2 (a", 0.6)	573.8 (a", 0.2)
569.5 (a, 4.4)	571.9 (b, 0.2)	581.8 (a", 6.5)	574.2 (a", 0.1)
579.5 (a, 0.2)	573.3 (a, 0.0)	586.1 (a', 8.6)	579.4 (a', 1.1)
582.4 (a, 0.3)	574.9 (b, 0.3)	588.6 (a', 7.3)	625.0 (a', 36.2)
776.8 (a, 87.4)	775.4 (b, 135.5)	736.8 (a", 25.4)	775.7 (a', 48.2)
778.3 (a, 33.3)	776.3 (a, 3.0)	748.3 (a', 1.7)	777.9 (a', 81.8)
781.3 (a, 29.9)	782.0 (a, 0.2)	756.9 (a", 25.5)	778.2 (a", 0.1)
782.7 (a, 0.2)	782.2 (b, 2.6)	766.4 (a', 2.4)	789.8 (a", 3.2)
793.6 (a, 1.8)	792.1 (b, 1.8)	774.8 (a", 62.5)	791.6 (a', 2.6)
798.5 (a, 3.9)	793.5 (a, 3.7)	775.3 (a', 0.3)	812.0 (a", 0.1)
809.4 (a, 0.2)	810.8 (a, 0.2)	781.1 (a", 0.2)	812.9 (a', 3.8)
810.5 (a, 1.3)	812.1 (b, 1.2)	787.4 (a', 1.1)	813.4 (a", 0.1)
815.1 (a, 0.2)	812.3 (a, 0.1)	802.6 (a", 0.0)	816.7 (a', 0.5)
816.0 (a, 1.8)	814.3 (b, 0.2)	813.3 (a', 1.1)	821.6 (a', 10.6)
855.1 (a, 1.8)	856.5 (b, 1.0)	832.0 (a", 0.2)	855.8 (a", 0.6)
861.3 (a, 0.2)	856.7 (a, 2.4)	837.9 (a', 2.4)	864.2 (a', 0.2)
862.2 (a, 2.0)	863.6 (a, 0.1)	848.1 (a", 0.0)	866.8 (a", 5.0)
869.4 (a, 2.7)	864.0 (b, 0.7)	849.9 (a', 0.3)	867.6 (a', 5.0)
987.3 (a, 12.9)	988.2 (b, 12.2)	964.8 (a", 0.5)	981.2 (a', 8.7)
989.3 (a, 8.4)	988.7 (a, 6.6)	970.3 (a', 28.9)	985.3 (a", 9.8)
989.6 (a, 12.0)	989.9 (b, 10.1)	972.3 (a", 0.1)	987.5 (a', 10.2)
993.3 (a, 10.3)	990.4 (a, 12.6)	972.6 (a', 16.3)	993.6 (a", 8.5)
1039.8 (a, 0.2)	1039.4 (a, 1.6)	1025.9 (a", 4.7)	1036.1 (a', 0.1)
1040.3 (a, 0.2)	1039.9 (b, 0.3)	1029.3 (a', 4.6)	1037.6 (a", 3.0)
1041.3 (a, 0.7)	1040.2 (a, 0.9)	1033.6 (a", 0.0)	1041.1 (a', 0.3)
1042.4 (a, 0.8)	1041.0 (b, 0.2)	1036.8 (a', 1.3)	1041.1 (a", 0.0)

1096.3 (a, 9.3)	1097.5 (b, 14.5)	1079.0 (a", 21.0)	1091.3 (a', 12.2)
1101.9 (a, 3.7)	1097.6 (a, 0.0)	1079.6 (a', 2.9)	1100.8 (a', 4.2)
1224.0 (a, 0.0)	1223.7 (b, 0.0)	1210.6 (a", 0.0)	1220.4 (a", 0.1)
1224.3 (a, 0.0)	1223.7 (a, 0.0)	1210.9 (a', 0.5)	1223.6 (a", 0.0)
1350.6 (a, 0.0)	1354.5 (b, 1.2)	1319.7 (a", 2.1)	1347.9 (a', 3.0)
1357.1 (a, 0.9)	1354.8 (a, 0.0)	1328.6 (a', 5.2)	1353.0 (a", 2.2)
1358.8 (a, 1.5)	1358.7 (b, 0.9)	1342.2 (a", 0.0)	1356.3 (a', 0.0)
1362.8 (a, 0.4)	1359.3 (a, 0.9)	1352.7 (a', 5.5)	1359.8 (a", 0.0)
1400.1 (a, 1.5)	1402.0 (b, 3.2)	1382.8 (a", 0.3)	1394.0 (a', 3.5)
1402.2 (a, 3.7)	1402.3 (a, 0.6)	1383.1 (a', 1.0)	1402.0 (a', 2.9)
1405.3 (a, 1.7)	1404.0 (b, 1.5)	1390.6 (a", 0.0)	1402.0 (a", 0.0)
1409.5 (a, 2.6)	1404.4 (a, 4.1)	1394.3 (a', 0.8)	1409.2 (a", 3.2)
1753.2 (a, 790.4)	1748.1 (a, 899.3)	1865.4 (a", 945.5)	1709.5 (a', 613.3)
1808.9 (a, 912.8)	1789.8 (b, 986.5)	1865.8 (a', 1096.5)	1744.4 (a", 1087.5)
1848.6 (a, 310.9)	1811.8 (a, 108.9)	1941.1 (a', 1195.8)	1761.4 (a', 40.3)
3163.9 (a, 0.0)	3165.3 (a, 0.0)	3105.6 (a", 3.4)	3155.8 (a', 0.3)
3166.7 (a, 0.3)	3165.4 (b, 0.1)	3105.9 (a', 5.9)	3162.8 (a', 0.5)
3168.5 (a, 0.4)	3170.3 (a, 0.1)	3162.6 (a", 0.1)	3171.8 (a", 0.1)
3170.2 (a, 0.0)	3170.3 (b, 0.5)	3163.8 (a', 0.8)	3176.4 (a", 0.0)
3176.5 (a, 0.0)	3179.5 (a, 0.0)	3171.4 (a', 0.7)	3180.9 (a', 0.2)
3180.4 (a, 0.3)	3179.5 (b, 0.2)	3171.5 (a", 0.2)	3183.4 (a', 0.4)
3181.5 (a, 0.5)	3183.0 (b, 0.1)	3180.1 (a", 0.3)	3185.7 (a", 0.1)
3183.4 (a, 0.3)	3183.0 (a, 0.2)	3180.3 (a', 0.5)	3187.9 (a", 0.3)
3188.9 (a, 0.1)	3191.8 (b, 0.1)	3187.3 (a', 0.7)	3193.2 (a', 0.0)
3192.7 (a, 0.1)	3191.9 (a, 0.0)	3187.7 (a", 0.9)	3194.3 (a', 0.1)

Table S6. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the triplet structures of $Cp_2Mo_2(CO)_2$ by BP86/SDD method (infrared intensities in parentheses are in km/mol).

2T-1(C_s)	**2T-2(C_i)**	**2T-3(C_s)**	**2T-4(C_s)**
18.7i (a", 0.0)	13.1 (a_u, 1.4)	16.1 (a", 0.2)	-39.7 (a", 0.3)
16.7 (a", 0.3)	26.9 (a_u, 0.1)	25.5 (a", 0.6)	34.3 (a", 0.2)
38.8 (a", 0.1)	35.1 (a_g, 0.0)	28.5 (a', 0.7)	49.1 (a", 0.2)
42.5 (a', 1.1)	47.6 (a_u, 2.8)	33.7 (a", 0.0)	71.6 (a', 0.6)
79.5 (a', 0.7)	76.2 (a_u, 2.3)	68.4 (a', 1.4)	77.3 (a', 2.0)
88.9 (a", 0.3)	104.6 (a_g, 0.0)	82.0 (a', 0.3)	85.7 (a", 0.8)
98.1 (a", 0.4)	117.0 (a_g, 0.0)	85.8 (a", 0.4)	126.6 (a", 0.0)
105.1 (a', 0.7)	145.1 (a_u, 2.5)	101.8 (a", 0.0)	131.9 (a', 0.3)
125.9 (a', 2.3)	154.0 (a_g, 0.0)	112.7 (a', 0.8)	178.6 (a', 5.0)
212.7 (a', 1.3)	209.4 (a_g, 0.0)	187.2 (a', 1.8)	210.1 (a', 0.0)
290.1 (a", 4.9)	295.7 (a_u, 1.2)	281.3 (a', 6.3)	297.4 (a', 5.0)
291.0 (a', 2.5)	307.7 (a_u, 5.3)	300.8 (a', 3.9)	317.0 (a", 4.5)
304.6 (a', 3.7)	309.0 (a_g, 0.0)	302.7 (a", 5.5)	328.2 (a', 4.9)
314.8 (a", 1.1)	318.7 (a_g, 0.0)	314.9 (a', 1.2)	334.3 (a", 7.2)
318.7 (a', 0.1)	347.3 (a_u, 3.0)	317.0 (a", 0.4)	374.6 (a', 11.9)
362.6 (a', 0.9)	352.9 (a_g, 0.0)	337.6 (a', 7.4)	388.4 (a", 0.8)
419.5 (a", 2.3)	414.7 (a_g, 0.0)	418.8 (a", 0.4)	400.2 (a', 5.3)
470.8 (a", 9.1)	432.4 (a_u, 9.7)	466.6 (a", 14.2)	429.5 (a", 1.5)
485.5 (a', 19.2)	497.1 (a_g, 0.0)	478.0 (a', 17.1)	457.1 (a', 2.0)
489.9 (a', 6.4)	500.2 (a_u, 18.5)	501.9 (a', 8.7)	483.2 (a', 0.5)
511.7 (a", 7.4)	501.1 (a_g, 0.0)	521.4 (a", 3.6)	501.3 (a", 14.9)
549.8 (a', 0.6)	510.3 (a_u, 4.7)	550.8 (a", 0.8)	545.0 (a", 0.9)
552.0 (a", 1.1)	564.0 (a_g, 0.0)	553.9 (a', 0.4)	552.1 (a', 2.1)
572.0 (a", 0.1)	564.2 (a_u, 2.7)	570.5 (a", 0.1)	572.8 (a", 0.3)
572.1 (a', 1.3)	565.7 (a_g, 0.0)	577.2 (a', 1.8)	580.5 (a', 5.7)
582.6 (a', 3.9)	566.1 (a_u, 1.4)	582.2 (a', 2.7)	598.1 (a', 5.0)
750.2 (a', 47.4)	757.6 (a_u, 72.0)	754.6 (a', 63.4)	714.2 (a", 0.3)
757.5 (a', 24.3)	758.3 (a_g, 0.0)	762.6 (a", 1.5)	722.7 (a', 14.9)
765.1 (a", 0.7)	774.9 (a_u, 13.0)	764.1 (a', 60.7)	741.9 (a", 1.1)
766.9 (a", 0.3)	776.4 (a_g, 0.0)	771.6 (a", 0.1)	761.7 (a", 0.6)
769.3 (a', 44.5)	781.1 (a_g, 0.0)	775.4 (a', 17.9)	763.9 (a', 68.2)
779.6 (a', 22.7)	781.3 (a_u, 40.8)	777.9 (a', 20.6)	771.5 (a', 0.2)
797.7 (a', 11.1)	803.1 (a_u, 5.9)	801.3 (a', 1.9)	795.3 (a', 1.2)
802.7 (a", 0.7)	805.4 (a_g, 0.0)	803.6 (a", 0.4)	797.8 (a", 0.5)
811.1 (a", 0.1)	808.6 (a_g, 0.0)	810.4 (a', 0.7)	805.2 (a', 3.6)
811.8 (a', 0.4)	808.8 (a_u, 1.3)	811.8 (a", 0.1)	819.5 (a", 0.8)
833.1 (a', 0.4)	842.4 (a_g, 0.0)	842.1 (a', 0.0)	827.1 (a', 11.5)
838.4 (a", 0.1)	842.9 (a_u, 0.7)	846.5 (a", 0.2)	832.6 (a", 0.8)
843.1 (a', 0.1)	852.5 (a_g, 0.0)	847.8 (a', 0.5)	839.4 (a', 0.7)
859.9 (a", 0.8)	852.8 (a_u, 0.7)	855.5 (a", 0.3)	866.8 (a", 2.4)
975.2 (a", 11.3)	981.3 (a_g, 0.0)	983.8 (a", 8.0)	955.1 (a", 19.2)
982.5 (a", 15.5)	981.4 (a_u, 25.7)	984.4 (a', 14.9)	956.6 (a', 8.0)
983.5 (a', 10.1)	986.4 (a_u, 22.5)	984.5 (a", 17.0)	969.6 (a', 4.5)
990.5 (a', 14.1)	987.3 (a_g, 0.0)	989.8 (a', 10.7)	1012.2 (a", 13.9)
1034.2 (a", 0.1)	1033.8 (a_u, 1.1)	1034.0 (a', 0.4)	1017.0 (a', 12.1)
1036.5 (a", 0.8)	1035.1 (a_g, 0.0)	1034.8 (a", 1.2)	1032.0 (a', 0.6)
1037.3 (a', 1.3)	1037.8 (a_u, 1.4)	1036.2 (a", 0.0)	1034.2 (a", 1.2)
1041.6 (a', 1.6)	1038.0 (a_g, 0.0)	1038.8 (a', 1.4)	1065.5 (a', 21.2)
1089.9 (a', 15.8)	1092.1 (a_u, 21.4)	1088.5 (a', 6.0)	1075.9 (a', 22.7)
1097.0 (a', 6.3)	1092.3 (a_g, 0.0)	1097.2 (a', 6.8)	1140.2 (a', 15.6)
1219.6 (a", 0.0)	1220.8 (a_g, 0.0)	1220.5 (a", 0.0)	1183.0 (a", 0.1)
1220.3 (a", 0.0)	1220.8 (a_u, 0.0)	1221.2 (a", 0.0)	1209.5 (a", 0.4)
1342.0 (a", 0.0)	1350.5 (a_u, 0.4)	1344.1 (a", 0.2)	1301.2 (a', 8.8)

1354.0 (a", 0.0)	1351.4 (a_g, 0.0)	1344.8 (a', 0.4)	1313.3 (a", 0.0)
1355.9 (a', 1.4)	1351.7 (a_g, 0.0)	1352.6 (a", 0.1)	1329.8 (a", 3.6)
1357.6 (a', 0.2)	1352.6 (a_u, 4.4)	1355.7 (a', 1.3)	1345.5 (a', 2.0)
1396.1 (a', 2.0)	1394.7 (a_g, 0.0)	1394.8 (a', 1.4)	1373.3 (a', 1.1)
1398.0 (a", 1.1)	1395.1 (a_u, 2.7)	1398.1 (a", 0.9)	1381.2 (a', 1.3)
1399.1 (a", 0.7)	1403.6 (a_u, 4.3)	1399.5 (a", 1.3)	1384.3 (a", 0.0)
1409.8 (a', 3.3)	1404.4 (a_g, 0.0)	1407.8 (a', 5.3)	1388.3 (a", 3.1)
1792.9(a", 905.0)	1758.2 (a_u, 1234.9)	1813.0 (a", 925.3)	1821.7 (a", 1323.7)
1834.3(a', 585.6)	1766.0 (a_g, 0.0)	1851.2 (a', 455.1)	1875.6 (a', 1042.6)
3159.2 (a', 0.8)	3159.4 (a_u, 0.0)	3157.8 (a", 0.2)	2422.0 (a', 10.4)
3161.8 (a", 0.0)	3159.5 (a_g, 0.0)	3160.3 (a', 0.4)	3097.2 (a", 0.4)
3166.4 (a', 0.2)	3169.5 (a_u, 0.3)	3165.3 (a', 0.2)	3108.2 (a', 0.3)
3168.9 (a", 0.2)	3169.5 (a_g, 0.0)	3169.1 (a", 0.1)	3164.0 (a', 0.1)
3175.0 (a", 0.1)	3179.5 (a_u, 0.7)	3175.7 (a', 0.0)	3165.2 (a", 1.0)
3177.7 (a', 2.2)	3179.6 (a_g, 0.0)	3175.8 (a", 0.2)	3171.2 (a", 0.1)
3180.5 (a", 0.9)	3182.1 (a_u, 1.0)	3178.3 (a', 1.6)	3171.9 (a', 0.3)
3182.1 (a', 0.3)	3182.2 (a_g, 0.0)	3181.0 (a", 0.9)	3179.5 (a", 0.1)
3191.9 (a', 0.3)	3192.4 (a_u, 0.2)	3187.3 (a', 0.3)	3182.5 (a', 0.1)
3196.6 (a', 0.1)	3192.5 (a_g, 0.0)	3191.9 (a', 0.4)	3186.0 (a', 0.1)

Table S7. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Cp_2Mo_2(CO)_2$ by BP86/SDD method (infrared intensities in parentheses are in km/mol).

2S-1(C_2)	**2S-2(C_s)**
30.4 (b, 0.9)	41.2i (a, 1.9)
51.3 (a, 0.1)	28.7 (a, 0.8)
51.4 (b, 1.0)	46.3 (a, 0.2)
56.6 (a, 1.0)	63.4 (a, 1.4)
65.7 (b, 0.9)	107.2 (a, 0.1)
85.9 (a, 0.9)	122.2 (a, 5.0)
86.5 (a, 0.2)	139.2 (a, 1.9)
117.9 (b, 3.5)	173.2 (a, 2.1)
162.8 (a, 0.3)	196.7 (a, 1.4)
205.3 (a, 0.9)	207.4 (a, 0.6)
254.1 (b, 2.4)	293.4 (a, 7.6)
281.0 (a, 0.0)	312.1 (a, 0.0)
300.9 (b, 0.0)	327.1 (a, 0.9)
302.9 (a, 1.9)	339.0 (a, 0.0)
322.0 (a, 8.0)	357.6 (a, 14.4)
326.4 (b, 0.2)	374.2 (a, 7.7)
427.9 (b, 8.1)	388.3 (a, 3.2)
443.7 (a, 4.3)	403.1 (a, 8.8)
490.9 (b, 27.0)	425.3 (a, 0.2)
502.2 (a, 0.6)	461.0 (a, 1.8)
511.3 (b, 2.7)	468.0 (a, 2.6)
523.0 (a, 0.7)	514.0 (a, 3.5)
562.2 (a, 5.2)	557.9 (a, 1.3)
563.5 (b, 14.6)	558.0 (a, 0.4)
579.8 (a, 5.4)	587.0 (a, 1.5)
580.9 (b, 0.7)	596.2 (a, 3.9)
739.2 (b, 6.5)	737.3 (a, 10.1)
745.6 (a, 10.3)	762.2 (a, 29.4)
757.2 (b, 69.9)	771.7 (a, 1.9)
759.2 (a, 43.8)	779.8 (a, 3.9)
779.1 (b, 2.1)	784.0 (a, 56.0)
788.8 (a, 4.5)	792.8 (a, 0.0)
806.0 (a, 0.1)	793.5 (a, 0.1)
806.1 (b, 2.8)	800.9 (a, 1.1)
811.6 (a, 3.1)	806.3 (a, 0.2)
812.7 (b, 1.0)	821.1 (a, 5.4)
835.1 (b, 0.4)	844.4 (a, 0.1)
839.4 (a, 0.0)	847.7 (a, 0.7)
868.2 (a, 1.6)	884.1 (a, 3.6)
868.4 (b, 1.6)	901.0 (a, 15.6)
979.7 (b, 22.4)	956.9 (a, 3.7)
982.7 (a, 0.4)	957.5 (a, 2.2)
987.0 (a, 21.3)	1012.4 (a, 1.0)
987.3 (b, 2.9)	1016.4 (a, 11.7)
1035.6 (a, 0.4)	1033.1 (a, 2.2)
1036.6 (b, 0.5)	1037.2 (a, 2.6)
1039.1 (a, 1.4)	1044.6 (a, 50.6)
1040.1 (b, 0.5)	1061.4 (a, 0.5)
1091.7 (a, 4.0)	1080.1 (a, 8.8)
1091.8 (b, 12.4)	1083.3 (a, 17.7)
1220.7 (b, 0.0)	1188.0 (a, 0.2)
1222.3 (a, 0.0)	1191.2 (a, 0.9)

1339.9 (b, 3.4)	1286.1 (a, 2.0)
1341.1 (a, 0.1)	1296.5 (a, 2.4)
1346.9 (b, 4.3)	1338.8 (a, 0.2)
1347.0 (a, 0.4)	1347.7 (a, 3.6)
1396.6 (b, 5.7)	1372.4 (a, 0.7)
1396.8 (a, 0.0)	1374.3 (a, 17.7)
1412.2 (b, 2.7)	1398.2 (a, 0.3)
1412.9 (a, 0.1)	1401.1 (a, 6.5)
1774.5 (b, 1156.1)	1859.9 (a, 840.9)
1780.5 (a, 246.9)	1898.9 (a, 1495.0)
3150.2 (a, 0.6)	2487.1 (a, 33.9)
3150.3 (b, 1.3)	2501.8 (a, 5.9)
3174.9 (a, 0.1)	3156.4 (a, 0.0)
3175.5 (b, 0.3)	3156.7 (a, 1.1)
3181.1 (a, 1.1)	3166.5 (a, 4.7)
3181.3 (b, 0.3)	3166.8 (a, 0.2)
3186.9 (a, 0.5)	3174.3 (a, 3.3)
3187.8 (b, 0.3)	3175.3 (a, 1.5)
3195.1 (a, 0.7)	3186.0 (a, 0.1)
3197.3 (b, 0.1)	3186.3 (a, 0.4)

Table S8. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the triplet structures of $Cp_2Mo_2(CO)$ by BP86/SDD method (infrared intensities in parentheses are in km/mol).

1T-1(C_1)	**1T-2(C_1)**	**1T-3(C_1)**
17.3 (a, 0.1)	25.2 (a, 0.1)	44.6 (a, 0.9)
28.6 (a, 0.2)	40.2 (a, 0.3)	56.3 (a, 0.7)
42.8 (a, 0.1)	47.6 (a, 1.0)	79.4 (a, 0.5)
57.9 (a, 1.3)	61.6 (a, 1.5)	91.5 (a, 0.3)
69.9 (a, 1.7)	81.0 (a, 1.9)	111.3 (a, 1.7)
118.2 (a, 1.3)	94.0 (a, 0.2)	122.0 (a, 1.2)
209.5 (a, 1.4)	156.2 (a, 2.6)	136.6 (a, 1.2)
215.8 (a, 3.2)	215.9 (a, 1.4)	193.5 (a, 0.4)
289.5 (a, 4.3)	256.5 (a, 1.1)	269.6 (a, 3.0)
297.5 (a, 2.3)	263.3 (a, 2.7)	294.8 (a, 0.3)
310.2 (a, 1.0)	290.4 (a, 2.8)	303.6 (a, 0.6)
312.7 (a, 1.7)	314.0 (a, 1.6)	321.7 (a, 13.8)
330.6 (a, 0.2)	325.0 (a, 4.9)	328.8 (a, 5.2)
349.7 (a, 0.3)	331.5 (a, 1.4)	352.1 (a, 11.8)
403.7 (a, 1.1)	451.6 (a, 2.1)	377.6 (a, 3.1)
479.2 (a, 14.2)	502.1 (a, 8.8)	461.7 (a, 10.5)
550.7 (a, 0.1)	552.4 (a, 3.3)	495.4 (a, 13.4)
554.4 (a, 0.3)	558.6 (a, 6.6)	542.6 (a, 2.0)
557.8 (a, 1.0)	561.7 (a, 0.4)	555.5 (a, 1.7)
564.6 (a, 0.3)	575.0 (a, 2.8)	564.1 (a, 1.0)
717.6 (a, 7.2)	688.4 (a, 9.8)	567.6 (a, 0.1)
730.6 (a, 12.0)	732.1 (a, 2.8)	681.7 (a, 17.9)
747.2 (a, 44.0)	743.5 (a, 53.8)	711.6 (a, 1.6)
753.0 (a, 3.6)	745.0 (a, 35.4)	734.8 (a, 19.5)
757.1 (a, 38.1)	758.7 (a, 14.0)	751.4 (a, 26.0)
761.2 (a, 30.0)	762.0 (a, 24.8)	762.9 (a, 5.0)
774.8 (a, 0.2)	773.3 (a, 5.2)	772.7 (a, 7.7)
790.5 (a, 0.2)	791.7 (a, 2.6)	779.8 (a, 31.0)
800.7 (a, 0.3)	796.0 (a, 1.5)	796.8 (a, 15.9)
802.8 (a, 1.5)	806.2 (a, 4.4)	801.5 (a, 4.1)
808.9 (a, 1.1)	808.9 (a, 1.3)	808.9 (a, 8.8)
825.5 (a, 0.1)	826.0 (a, 0.5)	818.6 (a, 2.6)
828.2 (a, 0.1)	834.6 (a, 2.4)	827.1 (a, 8.0)
836.5 (a, 2.3)	838.4 (a, 0.3)	834.7 (a, 5.4)
843.4 (a, 1.0)	848.6 (a, 1.0)	851.4 (a, 1.1)
973.1 (a, 15.6)	971.3 (a, 12.9)	957.0 (a, 11.1)
978.9 (a, 13.9)	972.9 (a, 10.4)	964.6 (a, 14.0)
983.0 (a, 16.9)	981.0 (a, 21.1)	981.1 (a, 11.2)
987.5 (a, 8.0)	987.5 (a, 10.3)	990.4 (a, 15.9)
1030.9 (a, 0.2)	1029.4 (a, 0.6)	1011.8 (a, 2.7)
1034.0 (a, 0.0)	1034.4 (a, 1.1)	1031.5 (a, 1.3)
1036.9 (a, 1.5)	1035.3 (a, 1.8)	1037.6 (a, 0.0)
1038.5 (a, 0.6)	1037.2 (a, 2.4)	1043.6 (a, 6.7)
1088.8 (a, 32.0)	1085.5 (a, 12.5)	1068.0 (a, 25.9)
1089.3 (a, 5.3)	1089.9 (a, 17.6)	1098.5 (a, 8.6)
1217.1 (a, 0.0)	1217.9 (a, 0.0)	1206.4 (a, 0.2)
1218.6 (a, 0.0)	1218.8 (a, 0.0)	1220.7 (a, 0.0)
1343.3 (a, 0.1)	1331.4 (a, 1.0)	1318.7 (a, 2.4)
1348.9 (a, 0.2)	1339.6 (a, 2.3)	1335.5 (a, 0.2)
1353.3 (a, 2.8)	1344.2 (a, 0.5)	1351.8 (a, 0.4)
1355.6 (a, 4.9)	1351.0 (a, 11.1)	1364.7 (a, 1.2)
1383.9 (a, 2.3)	1389.3 (a, 2.5)	1376.3 (a, 1.4)

1392.6 (a, 0.9)	1389.7 (a, 2.8)	1387.2 (a, 1.4)
1399.4 (a, 4.6)	1405.0 (a, 1.0)	1397.8 (a, 1.0)
1401.6 (a, 3.6)	1409.5 (a, 1.0)	1406.1 (a, 2.1)
1435.0 (a, 257.5)	1531.1 (a, 362.1)	1807.6 (a, 1483.6)
3154.9 (a, 0.2)	3151.6 (a, 0.1)	3117.9 (a, 3.3)
3156.4 (a, 0.1)	3159.6 (a, 0.3)	3139.9 (a, 1.1)
3157.6 (a, 0.7)	3164.2 (a, 0.3)	3159.2 (a, 0.5)
3165.5 (a, 0.9)	3166.2 (a, 0.6)	3161.6 (a, 2.8)
3173.9 (a, 1.6)	3173.2 (a, 1.5)	3171.0 (a, 2.5)
3177.1 (a, 0.1)	3175.5 (a, 1.6)	3175.6 (a, 0.8)
3179.7 (a, 1.1)	3180.3 (a, 0.0)	3179.2 (a, 1.1)
3186.5 (a, 0.2)	3181.5 (a, 0.9)	3182.3 (a, 0.3)
3191.8 (a, 0.1)	3191.9 (a, 0.8)	3188.2 (a, 0.4)
3192.4 (a, 0.7)	3192.3 (a, 0.2)	3200.2 (a, 0.2)

Table S9. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structures of $Cp_2Mo_2(CO)$ by BP86/SDD method (infrared intensities in parentheses are in km/mol).

1S-1(C_1)	**1S-2(C_1)**	**1S-3(C_s)**
23.3 (a, 0.1)	56.0 (a, 1.2)	10.8 (a", 0.8)
43.6 (a, 0.5)	61.1 (a, 0.8)	77.8 (a', 1.1)
51.5 (a, 0.3)	69.6 (a, 0.6)	117.8 (a", 4.0)
64.3 (a, 0.5)	72.9 (a, 0.1)	129.7 (a', 3.6)
115.0 (a, 1.1)	85.1 (a, 0.4)	154.7 (a', 2.9)
115.9 (a, 0.1)	119.1 (a, 0.6)	166.9 (a', 1.5)
201.6 (a, 2.4)	169.7 (a, 2.2)	168.7 (a", 22.2)
225.6 (a, 0.6)	233.9 (a, 1.1)	260.3 (a', 1.0)
275.0 (a, 1.7)	252.1 (a, 0.2)	286.1 (a', 3.5)
296.8 (a, 2.8)	267.9 (a, 5.2)	326.5 (a", 2.5)
298.0 (a, 1.0)	298.6 (a, 0.2)	339.2 (a", 0.3)
307.7 (a, 4.1)	326.7 (a, 2.1)	357.8 (a', 6.9)
333.1 (a, 1.0)	358.3 (a, 4.3)	382.6 (a", 11.7)
348.7 (a, 1.0)	384.1 (a, 0.6)	395.2 (a', 0.4)
444.9 (a, 4.4)	413.6 (a, 5.6)	429.0 (a', 4.2)
482.5 (a, 11.8)	494.6 (a, 1.4)	450.3 (a", 0.0)
556.8 (a, 0.6)	519.1 (a, 1.6)	523.3 (a', 2.4)
560.0 (a, 1.0)	544.6 (a, 0.6)	545.9 (a', 1.1)
561.9 (a, 0.2)	560.8 (a, 2.2)	549.8 (a", 0.1)
568.8 (a, 1.7)	569.7 (a, 3.9)	578.8 (a", 34.3)
720.7 (a, 11.8)	586.1 (a, 4.2)	605.4 (a', 5.4)
744.9 (a, 62.9)	721.3 (a, 31.0)	711.0 (a", 26.9)
746.8 (a, 11.0)	742.0 (a, 41.4)	748.6 (a", 37.4)
751.5 (a, 48.0)	746.9 (a, 5.3)	758.4 (a', 1.7)
760.8 (a, 4.3)	757.9 (a, 40.9)	764.5 (a', 3.5)
778.2 (a, 23.4)	764.8 (a, 5.2)	775.7 (a", 53.7)
789.8 (a, 10.2)	777.7 (a, 9.3)	789.3 (a", 8.4)
794.1 (a, 6.5)	784.0 (a, 12.0)	791.9 (a', 0.6)
803.0 (a, 0.7)	787.6 (a, 2.7)	796.1 (a", 0.1)
808.2 (a, 0.5)	804.9 (a, 1.3)	801.0 (a', 0.9)
809.7 (a, 0.2)	807.2 (a, 1.5)	812.3 (a', 2.9)
825.2 (a, 0.3)	826.7 (a, 0.9)	838.4 (a", 2.5)
842.3 (a, 1.7)	835.2 (a, 0.8)	841.2 (a', 0.7)
844.1 (a, 0.5)	843.6 (a, 2.2)	850.7 (a", 1.4)
846.5 (a, 1.4)	853.8 (a, 1.9)	897.8 (a', 11.0)
971.7 (a, 13.3)	944.2 (a, 3.8)	953.4 (a", 27.3)
977.5 (a, 13.9)	960.5 (a, 15.0)	953.4 (a', 2.1)
983.7 (a, 16.1)	963.6 (a, 9.9)	1006.8 (a", 8.6)
996.7 (a, 6.1)	969.3 (a, 13.5)	1013.3 (a', 19.0)
1029.4 (a, 0.8)	1018.0 (a, 4.9)	1032.6 (a", 6.8)
1033.6 (a, 0.2)	1019.4 (a, 3.7)	1038.3 (a", 30.7)
1037.2 (a, 1.6)	1034.9 (a, 0.3)	1039.0 (a', 2.0)
1040.0 (a, 1.9)	1037.4 (a, 2.0)	1067.1 (a', 2.0)
1089.4 (a, 10.4)	1075.3 (a, 14.2)	1074.8 (a", 29.8)
1095.7 (a, 10.6)	1079.3 (a, 13.3)	1095.9 (a', 34.6)
1217.4 (a, 0.0)	1199.9 (a, 0.1)	1179.4 (a", 1.5)
1220.1 (a, 0.0)	1212.9 (a, 0.0)	1187.0 (a', 0.8)
1339.3 (a, 0.1)	1302.6 (a, 2.7)	1272.2 (a", 2.9)
1348.2 (a, 3.6)	1309.1 (a, 0.6)	1285.8 (a', 1.4)
1353.9 (a, 2.3)	1330.4 (a, 3.6)	1340.8 (a", 1.5)
1356.0 (a, 5.7)	1342.2 (a, 8.4)	1346.1 (a', 0.9)
1386.7 (a, 3.2)	1376.2 (a, 1.9)	1377.4 (a", 2.3)
1391.8 (a, 0.7)	1382.3 (a, 5.2)	1380.7 (a', 10.9)

1405.7 (a, 3.1)	1399.3 (a, 1.1)	1389.8 (a", 2.1)
1421.7 (a, 1.3)	1426.0 (a, 0.9)	1393.5 (a', 7.3)
1465.9 (a, 307.2)	1795.5 (a, 847.1)	1847.0 (a', 927.4)
3154.2 (a, 0.1)	2916.4 (a, 7.0)	2274.1 (a", 307.7)
3156.0 (a, 0.2)	3144.4 (a, 0.8)	2333.5 (a', 8.0)
3159.9 (a, 0.2)	3153.1 (a, 2.6)	3153.7 (a", 0.1)
3161.9 (a, 0.4)	3155.8 (a, 0.2)	3153.8 (a', 1.4)
3172.2 (a, 1.1)	3161.4 (a, 4.4)	3164.9 (a', 6.7)
3173.0 (a, 1.8)	3170.6 (a, 0.7)	3165.2 (a", 0.1)
3177.4 (a, 0.9)	3171.5 (a, 3.4)	3172.2 (a', 4.1)
3181.7 (a, 0.1)	3178.6 (a, 1.8)	3173.9 (a", 2.2)
3189.5 (a, 0.3)	3181.8 (a, 0.7)	3188.0 (a', 0.2)
3190.5 (a, 0.1)	3187.3 (a, 0.2)	3188.1 (a", 1.1)

Table S10. Theoretical Cartesian coordinates (in Å) for the structure **6S-1** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	0.112782	1.616526	0.000000
2	6	0	-2.493747	-1.330713	0.000000
3	6	0	-2.127480	-2.078149	1.155907
4	6	0	-1.539635	-3.297429	0.717849
5	6	0	-1.539635	-3.297429	-0.717849
6	6	0	-2.127480	-2.078149	-1.155907
7	1	0	-2.976271	-0.362096	0.000000
8	1	0	-2.283740	-1.773327	2.182889
9	1	0	-1.188303	-4.099433	1.355230
10	1	0	-1.188303	-4.099433	-1.355230
11	1	0	-2.283740	-1.773327	-2.182889
12	6	0	1.539635	3.297429	-0.717849
13	6	0	2.127480	2.078149	-1.155907
14	6	0	2.493747	1.330713	0.000000
15	6	0	2.127480	2.078149	1.155907
16	6	0	1.539635	3.297429	0.717849
17	1	0	1.188303	4.099433	-1.355230
18	1	0	2.283740	1.773327	-2.182889
19	1	0	2.976271	0.362096	0.000000
20	1	0	2.283740	1.773327	2.182889
21	1	0	1.188303	4.099433	1.355230
22	6	0	-0.930850	1.045117	-1.580040
23	8	0	-1.539635	0.835422	-2.547771
24	6	0	-0.930850	1.045117	1.580040
25	8	0	-1.539635	0.835422	2.547771
26	6	0	0.930850	-1.045117	-1.580040
27	8	0	1.539635	-0.835422	-2.547771
28	6	0	0.930850	-1.045117	1.580040
29	8	0	1.539635	-0.835422	2.547771
30	6	0	-1.341191	2.934672	0.000000
31	8	0	-2.186480	3.728121	0.000000
32	42	0	-0.112782	-1.616526	0.000000
33	6	0	1.341191	-2.934672	0.000000
34	8	0	2.186480	-3.728121	0.000000

Table S11. Theoretical Cartesian coordinates (in Å) for the structure **6S-2** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.034548	2.140598	-2.309958
2	6	0	1.224281	1.542939	-2.019088
3	6	0	1.902335	2.361252	-1.072611
4	6	0	1.066155	3.476552	-0.780231
5	6	0	-0.136620	3.338815	-1.547702
6	1	0	-0.770472	1.773922	-3.014835
7	1	0	1.606850	0.625261	-2.445315
8	1	0	2.884508	2.168532	-0.660265
9	1	0	1.310931	4.301035	-0.122082
10	1	0	-0.961575	4.040070	-1.571988
11	6	0	-1.902335	-2.361252	-1.072611
12	6	0	-1.066155	-3.476552	-0.780231
13	6	0	0.136620	-3.338815	-1.547702
14	6	0	0.034548	-2.140598	-2.309958
15	6	0	-1.224281	-1.542939	-2.019088
16	1	0	-2.884508	-2.168532	-0.660265
17	1	0	-1.310931	-4.301035	-0.122082
18	1	0	0.961575	-4.040070	-1.571988
19	1	0	0.770472	-1.773922	-3.014835
20	1	0	-1.606850	-0.625261	-2.445315
21	42	0	-0.072216	1.617251	0.001925
22	42	0	0.072216	-1.617251	0.001925
23	6	0	1.066155	-2.760395	1.246693
24	8	0	1.650402	-3.462331	1.960137
25	6	0	1.867361	-0.792616	-0.039467
26	8	0	2.983799	-0.471053	-0.115270
27	6	0	-0.822475	-1.165407	1.721350
28	8	0	-1.383717	-1.016168	2.722597
29	6	0	-1.867361	0.792616	-0.039467
30	8	0	-2.983799	0.471053	-0.115270
31	6	0	0.822475	1.165407	1.721350
32	8	0	1.383717	1.016168	2.722597
33	6	0	-1.066155	2.760395	1.246693
34	8	0	-1.650402	3.462331	1.960137

Table S12. Theoretical Cartesian coordinates (in Å) for the structure **5S-1** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.203536	1.273498	-0.912752
2	6	0	-2.976798	1.612248	0.448494
3	6	0	-3.248210	0.456167	1.237252
4	6	0	-3.660469	-0.594504	0.364169
5	6	0	-3.617473	-0.086718	-0.973151
6	1	0	-3.042299	1.932056	-1.757707
7	1	0	-2.630963	2.571915	0.812168
8	1	0	-3.183130	0.393451	2.316665
9	1	0	-3.970060	-1.588173	0.663055
10	1	0	-3.887769	-0.631005	-1.869726
11	6	0	3.054179	-0.931919	-1.235942
12	6	0	1.981274	-1.868466	-1.208582
13	6	0	1.762928	-2.248376	0.142007
14	6	0	2.682683	-1.538991	0.958826
15	6	0	3.498770	-0.732702	0.110142
16	1	0	3.490763	-0.490203	-2.123110
17	1	0	1.440565	-2.239331	-2.069819
18	1	0	1.019436	-2.951095	0.492928
19	1	0	2.765874	-1.620554	2.035781
20	1	0	4.329437	-0.111837	0.421665
21	6	0	-0.128291	1.501593	-0.680369
22	8	0	-0.399262	2.583208	-1.104648
23	6	0	1.437559	1.160287	1.659433
24	8	0	1.518716	1.715591	2.669924
25	6	0	-1.129207	-1.841635	-0.986744
26	8	0	-1.055990	-2.896167	-1.475631
27	6	0	-0.706721	-0.995540	1.459415
28	8	0	-0.468350	-1.558575	2.456997
29	6	0	2.212320	1.777088	-0.783416
30	8	0	2.719018	2.723891	-1.216895
31	42	0	1.379592	0.176148	-0.057540
32	42	0	-1.441472	-0.115695	-0.112759

Table S13. Theoretical Cartesian coordinates (in Å) for the structure **5S-2** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.165896	-2.804230	1.541008
2	6	0	0.214043	-2.919284	1.873354
3	6	0	0.882200	-3.501781	0.762275
4	6	0	-0.077942	-3.761251	-0.257533
5	6	0	-1.354169	-3.323602	0.225555
6	1	0	-1.931481	-2.378940	2.179124
7	1	0	0.671175	-2.578005	2.793509
8	1	0	1.942282	-3.716581	0.701766
9	1	0	0.119081	-4.225435	-1.215953
10	1	0	-2.295910	-3.405078	-0.303330
11	6	0	-0.214043	2.919284	1.873354
12	6	0	-0.882200	3.501781	0.762275
13	6	0	0.077942	3.761251	-0.257533
14	6	0	1.354169	3.323602	0.225555
15	6	0	1.165896	2.804230	1.541008
16	1	0	-0.671175	2.578005	2.793509
17	1	0	-1.942282	3.716581	0.701766
18	1	0	-0.119081	4.225435	-1.215953
19	1	0	2.295910	3.405078	-0.303330
20	1	0	1.931481	2.378940	2.179124
21	6	0	-1.835147	1.080680	-0.576734
22	8	0	-2.946546	1.001964	-0.911063
23	6	0	0.571309	1.241149	-1.867437
24	8	0	0.941343	1.268881	-2.963858
25	6	0	-0.571309	-1.241149	-1.867437
26	8	0	-0.941343	-1.268881	-2.963858
27	6	0	1.835147	-1.080680	-0.576734
28	8	0	2.946546	-1.001964	-0.911063
29	6	0	-0.000000	0.000000	1.535533
30	8	0	-0.000000	0.000000	2.737713
31	42	0	0.000000	1.456552	0.025806
32	42	0	-0.000000	-1.456552	0.025806

Table S14. Theoretical Cartesian coordinates (in Å) for the structure **5S-3** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.164502	-2.275581	0.707821
2	6	0	-1.164502	-2.275581	-0.707821
3	6	0	-2.402535	-1.740111	-1.164318
4	6	0	-3.184808	-1.452092	0.000000
5	6	0	-2.402535	-1.740111	1.164318
6	1	0	-0.362619	-2.621768	1.344993
7	1	0	-0.362619	-2.621768	-1.344993
8	1	0	-2.725695	-1.668734	-2.194916
9	1	0	-4.209664	-1.107007	0.000000
10	1	0	-2.725695	-1.668734	2.194916
11	6	0	-1.164502	2.275582	0.707821
12	6	0	-2.402535	1.740111	1.164318
13	6	0	-3.184808	1.452093	0.000000
14	6	0	-2.402535	1.740111	-1.164318
15	6	0	-1.164502	2.275582	-0.707821
16	1	0	-0.362619	2.621768	1.344993
17	1	0	-2.725695	1.668738	2.194916
18	1	0	-4.209664	1.107008	0.000000
19	1	0	-2.725695	1.668738	-2.194916
20	1	0	-0.362619	2.621768	-1.344993
21	42	0	-1.472556	-0.000000	0.000000
22	6	0	1.724623	-2.013409	0.000000
23	6	0	1.724622	2.013416	0.000000
24	8	0	1.988349	-3.142023	0.000000
25	8	0	1.988348	3.142029	0.000000
26	6	0	1.271711	-0.000004	-2.032736
27	6	0	1.271711	-0.000004	2.032736
28	8	0	1.126872	-0.000010	-3.181347
29	8	0	1.126872	-0.000010	3.181347
30	42	0	1.490400	0.000002	0.000000
31	6	0	3.484837	0.000005	0.000000
32	8	0	4.642649	-0.000002	0.000000

Table S15. Theoretical Cartesian coordinates (in Å) for the structure **5T-1** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.716767	2.657044	0.713661
2	6	0	-1.716767	2.657044	-0.713661
3	6	0	-0.535238	3.311603	-1.155912
4	6	0	0.204028	3.721486	0.000000
5	6	0	-0.535238	3.311603	1.155912
6	1	0	-2.474509	2.218844	1.351791
7	1	0	-2.474509	2.218844	-1.351791
8	1	0	-0.254573	3.484530	-2.187605
9	1	0	1.130852	4.281690	0.000000
10	1	0	-0.254573	3.484530	2.187605
11	6	0	0.395184	-3.570964	0.717449
12	6	0	1.408127	-2.672041	1.152730
13	6	0	2.039159	-2.118837	0.000000
14	6	0	1.408127	-2.672041	-1.152730
15	6	0	0.395184	-3.570964	-0.717449
16	1	0	-0.241116	-4.171070	1.355982
17	1	0	1.663956	-2.451864	2.182197
18	1	0	2.864491	-1.418568	0.000000
19	1	0	1.663956	-2.451864	-2.182197
20	1	0	-0.241116	-4.171070	-1.355982
21	6	0	-0.752133	-0.419568	1.621925
22	8	0	-1.093828	-0.054997	2.680657
23	6	0	-0.752133	-0.419568	-1.621925
24	8	0	-1.093828	-0.054997	-2.680657
25	6	0	1.616545	1.122260	1.338423
26	8	0	2.459498	1.021869	2.129443
27	6	0	1.616545	1.122260	-1.338423
28	8	0	2.459498	1.021869	-2.129443
29	6	0	-2.154425	-1.945068	0.000000
30	8	0	-3.267644	-2.271805	0.000000
31	42	0	-0.250378	-1.443582	0.000000
32	42	0	0.188149	1.410130	0.000000

Table S16. Theoretical Cartesian coordinates (in Å) for the structure **5T-2** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.820908	3.006218	0.000000
2	6	0	1.019004	3.262981	1.151782
3	6	0	-0.265748	3.691043	0.717313
4	6	0	-0.265748	3.691043	-0.717313
5	6	0	1.019004	3.262981	-1.151782
6	1	0	2.854384	2.681529	0.000000
7	1	0	1.335994	3.158255	2.182412
8	1	0	-1.088156	3.987056	1.356556
9	1	0	-1.088156	3.987056	-1.356556
10	1	0	1.335994	3.158255	-2.182412
11	6	0	2.222159	-1.950931	-0.712618
12	6	0	1.317251	-2.953731	-1.155845
13	6	0	0.754758	-3.585000	0.000000
14	6	0	1.317251	-2.953731	1.155845
15	6	0	2.222159	-1.950931	0.712618
16	1	0	2.795496	-1.290561	-1.351371
17	1	0	1.109059	-3.207711	-2.187942
18	1	0	0.065469	-4.420181	0.000000
19	1	0	1.109059	-3.207711	2.187942
20	1	0	2.795496	-1.290561	1.351371
21	6	0	-1.455591	-1.722867	-1.307584
22	8	0	-2.278799	-1.985038	-2.078231
23	6	0	-1.455591	-1.722867	1.307584
24	8	0	-2.278799	-1.985038	2.078231
25	6	0	0.290292	0.427030	-1.657759
26	8	0	0.556984	0.175294	-2.775453
27	6	0	-1.962077	1.233540	0.000000
28	8	0	-3.121128	1.195373	0.000000
29	6	0	0.290292	0.427030	1.657759
30	8	0	0.556984	0.175294	2.775453
31	42	0	0.000786	-1.419178	0.000000
32	42	0	0.001202	1.487432	0.000000

Table S17. Theoretical Cartesian coordinates (in Å) for the structure **5T-3** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.713140	2.204732	1.180384
2	6	0	0.713140	2.204732	1.180384
3	6	0	1.154407	1.846969	2.484013
4	6	0	-0.000000	1.615964	3.299072
5	6	0	-1.154407	1.846969	2.484013
6	1	0	-1.350525	2.466638	0.347935
7	1	0	1.350525	2.466638	0.347935
8	1	0	2.186520	1.767832	2.804802
9	1	0	-0.000000	1.376947	4.355025
10	1	0	-2.186520	1.767832	2.804802
11	6	0	-0.713140	-2.204732	1.180384
12	6	0	-1.154407	-1.846969	2.484013
13	6	0	-0.000000	-1.615964	3.299072
14	6	0	1.154407	-1.846969	2.484013
15	6	0	0.713140	-2.204732	1.180384
16	1	0	-1.350525	-2.466638	0.347935
17	1	0	-2.186520	-1.767832	2.804802
18	1	0	-0.000000	-1.376947	4.355025
19	1	0	2.186520	-1.767832	2.804802
20	1	0	1.350525	-2.466638	0.347935
21	42	0	-0.000000	0.000000	1.725889
22	6	0	0.000000	2.019259	-1.831999
23	6	0	-0.000000	-2.019259	-1.831999
24	8	0	0.000000	3.149877	-2.081061
25	8	0	-0.000000	-3.149877	-2.081061
26	6	0	2.033046	-0.000000	-1.459318
27	6	0	-2.033046	0.000000	-1.459318
28	8	0	3.183250	-0.000000	-1.341576
29	8	0	-3.183250	0.000000	-1.341576
30	42	0	0.000000	-0.000000	-1.613768
31	6	0	0.000000	-0.000000	-3.572496
32	8	0	0.000000	-0.000000	-4.733941

Table S18. Theoretical Cartesian coordinates (in Å) for the structure **4S-1** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.836371	-2.674027	-0.242537
2	6	0	-0.982141	-2.905360	-1.364045
3	6	0	0.240888	-3.453607	-0.875745
4	6	0	0.146577	-3.560408	0.535413
5	6	0	-1.140237	-3.079629	0.935991
6	6	0	0.982141	2.905360	-1.364045
7	6	0	1.836371	2.674027	-0.242537
8	6	0	1.140237	3.079629	0.935991
9	6	0	-0.146577	3.560408	0.535413
10	6	0	-0.240888	3.453607	-0.875745
11	1	0	-2.840161	-2.267458	-0.284453
12	1	0	-1.222098	-2.704998	-2.401316
13	1	0	1.098220	-3.730377	-1.477144
14	1	0	0.917929	-3.938304	1.195305
15	1	0	-1.522392	-3.050113	1.949095
16	1	0	1.222098	2.704998	-2.401316
17	1	0	2.840161	2.267458	-0.284453
18	1	0	1.522392	3.050113	1.949095
19	1	0	-0.917929	3.938304	1.195305
20	1	0	-1.098220	3.730377	-1.477144
21	42	0	0.025227	1.253648	-0.007306
22	42	0	-0.025227	-1.253648	-0.007306
23	6	0	1.140237	-0.896194	1.525048
24	6	0	-1.140237	0.896194	1.525048
25	6	0	-1.468315	0.681874	-1.123506
26	6	0	1.468315	-0.681874	-1.123506
27	8	0	2.390616	-0.511339	-1.824983
28	8	0	-2.390616	0.511339	-1.824983
29	8	0	-1.846524	0.807640	2.447689
30	8	0	1.846524	-0.807640	2.447689

Table S19. Theoretical Cartesian coordinates (in Å) for the structure **4T-1** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.486020	3.521761	0.718162
2	6	0	0.486020	3.521761	-0.718162
3	6	0	-0.814002	3.115397	-1.148040
4	6	0	-1.630044	2.900747	0.000000
5	6	0	-0.814002	3.115397	1.148040
6	6	0	0.948867	-3.073058	1.154858
7	6	0	1.930649	-2.133305	0.710918
8	6	0	1.930649	-2.133305	-0.710918
9	6	0	0.948867	-3.073058	-1.154858
10	6	0	0.353055	-3.652928	0.000000
11	1	0	1.309411	3.808371	1.359825
12	1	0	1.309411	3.808371	-1.359825
13	1	0	-1.124402	2.981268	-2.178026
14	1	0	-2.665423	2.581740	0.000000
15	1	0	-1.124402	2.981268	2.178026
16	1	0	0.719060	-3.320845	2.183713
17	1	0	2.573175	-1.536600	1.346032
18	1	0	2.573175	-1.536600	-1.346032
19	1	0	0.719060	-3.320845	-2.183713
20	1	0	-0.426861	-4.405001	0.000000
21	6	0	-0.738802	-0.310642	-1.595332
22	6	0	-2.104786	-1.844542	0.000000
23	6	0	-0.738802	-0.310642	1.595332
24	6	0	2.115960	1.122586	0.000000
25	8	0	3.282377	1.117281	0.000000
26	8	0	-1.082273	0.080193	2.647727
27	8	0	-3.224011	-2.151849	0.000000
28	8	0	-1.082273	0.080193	-2.647727
29	42	0	-0.198339	-1.356941	0.000000
30	42	0	0.170466	1.365400	0.000000

Table S20. Theoretical Cartesian coordinates (in Å) for the structure **4T-2** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.206945	-3.104408	1.105047
2	6	0	-0.059791	-3.632427	0.735393
3	6	0	-0.246445	-3.413050	-0.658927
4	6	0	0.932080	-2.766315	-1.160264
5	6	0	1.823053	-2.572399	-0.071828
6	6	0	0.246445	3.413050	0.658927
7	6	0	-0.932080	2.766315	1.160264
8	6	0	-1.823053	2.572399	0.071828
9	6	0	-1.206945	3.104408	-1.105047
10	6	0	0.059791	3.632427	-0.735393
11	1	0	1.633448	-3.105848	2.101120
12	1	0	-0.769348	-4.105469	1.403667
13	1	0	-1.103477	-3.719441	-1.245459
14	1	0	1.109191	-2.480931	-2.190018
15	1	0	2.796755	-2.099773	-0.119728
16	1	0	1.103477	3.719441	1.245459
17	1	0	-1.109191	2.480931	2.190018
18	1	0	-2.796755	2.099773	0.119728
19	1	0	-1.633448	3.105848	-2.101120
20	1	0	0.769348	4.105469	-1.403667
21	6	0	-1.251791	-0.561112	-1.081737
22	6	0	1.727477	1.109627	-1.467100
23	6	0	1.251791	0.561112	1.081737
24	6	0	-1.727477	-1.109627	1.467100
25	8	0	-2.691761	-1.060869	2.114501
26	8	0	1.977879	0.349148	1.986614
27	8	0	2.691761	1.060869	-2.114501
28	8	0	-1.977879	-0.349148	-1.986614
29	42	0	0.126899	1.302757	-0.323908
30	42	0	-0.126899	-1.302757	0.323908

Table S21. Theoretical Cartesian coordinates (in Å) for the structure **3T-1** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	1.321862	0.001917	0.000586
2	42	0	-1.228251	-0.071512	-0.001352
3	6	0	-3.234676	0.085590	-1.197263
4	6	0	-3.016924	1.342386	-0.569802
5	1	0	-3.266208	-0.096523	-2.264580
6	1	0	-2.832676	2.285582	-1.069695
7	6	0	3.209292	1.328994	-0.029258
8	6	0	3.281790	0.461780	-1.161843
9	1	0	3.131503	2.408903	-0.053356
10	1	0	3.245701	0.770018	-2.200334
11	6	0	-0.442734	-1.188467	-1.409110
12	8	0	-0.173050	-1.889978	-2.312027
13	6	0	0.103503	1.661560	-0.013282
14	8	0	-0.014583	2.842008	-0.018425
15	6	0	-3.311934	-0.233920	1.084328
16	6	0	-3.066299	1.145858	0.843150
17	1	0	-3.402012	-0.702468	2.057057
18	1	0	-2.929848	1.913419	1.595365
19	6	0	3.283522	0.514140	1.141351
20	6	0	3.392276	-0.847332	0.731521
21	1	0	3.248406	0.869492	2.164728
22	1	0	3.447317	-1.708189	1.387772
23	6	0	-0.437301	-1.157332	1.429820
24	8	0	-0.166870	-1.839942	2.347063
25	6	0	3.391088	-0.879925	-0.690811
26	1	0	3.446708	-1.769629	-1.307275
27	6	0	-3.412728	-0.898888	-0.173050
28	1	0	-3.617774	-1.951012	-0.324912

Table S22. Theoretical Cartesian coordinates (in Å) for the structure **3T-2** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.131162	1.312609
2	6	0	-1.127916	3.272184	0.446703
3	6	0	-0.645921	3.369291	-0.894773
4	6	0	0.772888	3.289799	-0.855176
5	6	0	1.177665	3.149509	0.505040
6	1	0	-0.030836	3.039438	2.391558
7	1	0	-2.166887	3.304682	0.751813
8	1	0	-1.253618	3.480353	-1.784248
9	1	0	1.433074	3.304785	-1.714896
10	1	0	2.197402	3.064345	0.861040
11	6	0	-1.177665	-3.149509	0.505040
12	6	0	-0.000000	-3.131162	1.312609
13	6	0	1.127916	-3.272184	0.446703
14	6	0	0.645921	-3.369291	-0.894773
15	6	0	-0.772888	-3.289799	-0.855176
16	1	0	-2.197402	-3.064345	0.861040
17	1	0	0.030836	-3.039438	2.391558
18	1	0	2.166887	-3.304682	0.751813
19	1	0	1.253618	-3.480353	-1.784248
20	1	0	-1.433074	-3.304785	-1.714896
21	6	0	0.000000	-0.000000	1.669463
22	8	0	0.000000	-0.000000	2.854315
23	6	0	1.542027	-0.330558	-0.987746
24	6	0	-1.542027	0.330558	-0.987746
25	8	0	2.506269	-0.027334	-1.588660
26	8	0	-2.506269	0.027334	-1.588660
27	42	0	-0.081577	1.257840	-0.032895
28	42	0	0.081577	-1.257840	-0.032895

Table S23. Theoretical Cartesian coordinates (in Å) for the structure **3T-3** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.612496	-0.644232	2.166062
2	6	0	0.815071	-0.683974	2.054173
3	6	0	1.188790	-2.049796	1.806735
4	6	0	-0.003321	-2.844530	1.769311
5	6	0	-1.109461	-1.964282	1.981976
6	1	0	-1.202382	0.235390	2.393389
7	1	0	1.491161	0.132262	2.285480
8	1	0	2.203164	-2.419210	1.714338
9	1	0	-0.054623	-3.919826	1.655321
10	1	0	-2.154763	-2.250309	1.998221
11	6	0	-0.612496	-0.644232	-2.166062
12	6	0	-1.109461	-1.964282	-1.981976
13	6	0	-0.003321	-2.844530	-1.769311
14	6	0	1.188790	-2.049796	-1.806735
15	6	0	0.815071	-0.683974	-2.054173
16	1	0	-1.202382	0.235390	-2.393389
17	1	0	-2.154763	-2.250309	-1.998221
18	1	0	-0.054623	-3.919826	-1.655321
19	1	0	2.203164	-2.419210	-1.714338
20	1	0	1.491161	0.132262	-2.285480
21	42	0	-0.020203	-1.432596	0.000000
22	42	0	0.274323	1.361653	-0.000000
23	6	0	0.513792	2.728199	1.344751
24	6	0	-1.570218	1.860852	-0.000000
25	6	0	0.513792	2.728199	-1.344751
26	8	0	-2.699275	2.166088	-0.000000
27	8	0	0.641803	3.527033	2.188542
28	8	0	0.641803	3.527033	-2.188542

Table S24. Theoretical Cartesian coordinates (in Å) for the structure **3S-1** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-1.185056	-0.058732	-0.010323
2	42	0	1.289045	0.087237	-0.314721
3	6	0	3.383865	1.098648	-0.143054
4	6	0	3.646138	-0.175058	-0.719702
5	6	0	3.219763	-1.194018	0.168540
6	1	0	3.622211	2.063484	-0.571764
7	1	0	4.045097	-0.340714	-1.716050
8	1	0	3.287460	-2.262082	0.002211
9	6	0	-2.897888	1.514060	0.072883
10	6	0	-3.431515	-0.668881	-0.457108
11	6	0	-3.184217	0.627176	-1.008289
12	1	0	-2.656727	2.567159	-0.011055
13	1	0	-3.674637	-1.564082	-1.016127
14	1	0	-3.226368	0.890178	-2.058238
15	6	0	-0.546148	-1.240536	-1.415668
16	8	0	-0.288079	-1.955409	-2.315353
17	6	0	0.402323	1.797506	-0.201037
18	8	0	0.175522	2.949879	-0.055245
19	6	0	2.792501	0.867438	1.149400
20	6	0	2.685421	-0.550237	1.334023
21	1	0	2.526710	1.630609	1.869667
22	1	0	2.295969	-1.054760	2.209580
23	6	0	-2.973983	0.768528	1.285793
24	6	0	-3.301886	-0.579644	0.953206
25	1	0	-2.810582	1.155508	2.284592
26	1	0	-3.419745	-1.397212	1.653953
27	6	0	-0.332964	-1.289624	1.243439
28	8	0	-0.028116	-2.086650	2.049412

Table S25. Theoretical Cartesian coordinates (in Å) for the structure **3S-2** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	0.093697	1.249534	0.000000
2	42	0	0.258947	-1.278107	0.000000
3	6	0	-0.110710	-3.246076	1.160299
4	6	0	0.633675	-3.598970	0.000000
5	6	0	-0.110710	-3.246076	-1.160299
6	1	0	0.191424	-3.385267	2.190599
7	1	0	1.641965	-4.000435	0.000000
8	1	0	0.191424	-3.385267	-2.190599
9	6	0	-0.631810	3.161551	1.156430
10	6	0	0.703502	3.383500	-0.716702
11	6	0	0.703502	3.383500	0.716702
12	1	0	-0.963272	3.095756	2.185493
13	1	0	1.565384	3.533584	-1.355023
14	1	0	1.565384	3.533584	1.355023
15	6	0	1.820323	0.365551	0.000000
16	8	0	2.714456	-0.423954	0.000000
17	6	0	-0.492238	-0.032022	1.550056
18	8	0	-1.026520	-0.127557	2.608863
19	6	0	-1.346462	-2.672200	0.717065
20	6	0	-1.346462	-2.672200	-0.717065
21	1	0	-2.138347	-2.313673	1.362405
22	1	0	-2.138347	-2.313673	-1.362405
23	6	0	-1.454287	3.033382	0.000000
24	6	0	-0.631810	3.161551	-1.156430
25	1	0	-2.520390	2.835451	0.000000
26	1	0	-0.963272	3.095756	-2.185493
27	6	0	-0.492238	-0.032022	-1.550056
28	8	0	-1.026520	-0.127557	-2.608863

Table S26. Theoretical Cartesian coordinates (in Å) for the structure **2T-1** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.002384	-3.299485	0.708958
2	6	0	1.216533	-2.699987	1.156076
3	6	0	1.966247	-2.329694	0.000000
4	6	0	1.216533	-2.699987	-1.156076
5	6	0	-0.002384	-3.299485	-0.708958
6	1	0	-0.792165	-3.681635	1.343908
7	1	0	1.522948	-2.574516	2.187465
8	1	0	2.948978	-1.871419	0.000000
9	1	0	1.522948	-2.574516	-2.187465
10	1	0	-0.792165	-3.681635	-1.343908
11	6	0	0.310172	3.543051	0.711608
12	6	0	0.310172	3.543051	-0.711608
13	6	0	1.213149	2.536046	-1.151352
14	6	0	1.786694	1.898544	0.000000
15	6	0	1.213149	2.536046	1.151352
16	1	0	-0.287211	4.183620	1.349630
17	1	0	-0.287211	4.183620	-1.349630
18	1	0	1.430222	2.284832	-2.183043
19	1	0	2.589384	1.173926	0.000000
20	1	0	1.430222	2.284832	2.183043
21	6	0	-1.258589	-0.562472	1.380430
22	8	0	-2.043743	-0.434906	2.253074
23	6	0	-1.258589	-0.562472	-1.380430
24	8	0	-2.043743	-0.434906	-2.253074
25	42	0	-0.425383	1.397767	0.000000
26	42	0	0.024186	-1.026042	0.000000

able S27. Theoretical Cartesian coordinates (in Å) for the structure **2T-2** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	1.229631	0.163170	0.304207
2	6	0	3.468704	0.380707	1.078107
3	6	0	3.249404	1.358620	0.060705
4	6	0	3.289134	-0.907125	0.511643
5	1	0	3.706601	0.586666	2.115809
6	1	0	3.308828	2.433927	0.180953
7	1	0	3.393311	-1.853659	1.027186
8	6	0	-0.404245	1.544110	-0.697950
9	8	0	-0.209085	2.687497	-0.955526
10	6	0	2.934759	0.668716	-1.145307
11	6	0	2.946239	-0.736802	-0.872836
12	1	0	2.712563	1.131366	-2.099564
13	1	0	2.790801	-1.532429	-1.590166
14	42	0	-1.229631	-0.163170	-0.304207
15	6	0	-2.934759	-0.668716	1.145307
16	6	0	-3.249404	-1.358620	-0.060705
17	6	0	-2.946239	0.736802	0.872836
18	1	0	-2.712563	-1.131366	2.099564
19	1	0	-3.308828	-2.433927	-0.180953
20	1	0	-2.790801	1.532429	1.590166
21	6	0	0.404245	-1.544110	0.697950
22	8	0	0.209085	-2.687497	0.955526
23	6	0	-3.468704	-0.380707	-1.078107
24	6	0	-3.289134	0.907125	-0.511643
25	1	0	-3.706601	-0.586666	-2.115809
26	1	0	-3.393311	1.853659	-1.027186

Table S28. Theoretical Cartesian coordinates (in Å) for the structure **2T-3** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.597335	-3.378192	0.709039
2	6	0	0.746425	-3.174380	1.155420
3	6	0	1.572866	-3.049448	0.000000
4	6	0	0.746425	-3.174380	-1.155420
5	6	0	-0.597335	-3.378192	-0.709039
6	1	0	-1.465040	-3.506063	1.344440
7	1	0	1.076640	-3.144611	2.186573
8	1	0	2.646271	-2.897784	0.000000
9	1	0	1.076640	-3.144611	-2.186573
10	1	0	-1.465040	-3.506063	-1.344440
11	6	0	-0.317965	3.188608	1.155811
12	6	0	-1.131349	2.967662	0.000000
13	6	0	-0.317965	3.188608	-1.155811
14	6	0	0.990354	3.528012	-0.713495
15	6	0	0.990354	3.528012	0.713495
16	1	0	-0.644419	3.094459	2.185111
17	1	0	-2.181719	2.701217	0.000000
18	1	0	-0.644419	3.094459	-2.185111
19	1	0	1.839834	3.747374	-1.350352
20	1	0	1.839834	3.747374	1.350352
21	6	0	-0.954877	-0.376958	1.394277
22	8	0	-1.649206	-0.022027	2.279670
23	6	0	-0.954877	-0.376958	-1.394277
24	8	0	-1.649206	-0.022027	-2.279670
25	42	0	0.446379	1.292068	0.000000
26	42	0	0.107440	-1.215584	0.000000

Table S29. Theoretical Cartesian coordinates (in Å) for the structure **2T-4** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.737706	0.317648	0.000000
2	6	0	-1.987885	-0.494628	1.159370
3	6	0	-2.273536	-1.813635	0.719317
4	6	0	-2.273536	-1.813635	-0.719317
5	6	0	-1.987885	-0.494628	-1.159370
6	1	0	-1.612144	1.452002	0.000000
7	1	0	-1.898551	-0.155961	2.184609
8	1	0	-2.492439	-2.665982	1.350886
9	1	0	-2.492439	-2.665982	-1.350886
10	1	0	-1.898551	-0.155961	-2.184609
11	6	0	1.969539	-0.756630	-0.726273
12	6	0	1.643611	-2.096155	-1.152737
13	6	0	1.480685	-2.912032	0.000000
14	6	0	1.643611	-2.096155	1.152737
15	6	0	1.969539	-0.756630	0.726273
16	1	0	2.356364	0.024149	-1.378338
17	1	0	1.571842	-2.426745	-2.182012
18	1	0	1.233023	-3.966742	0.000000
19	1	0	1.571842	-2.426745	2.182012
20	1	0	2.356364	0.024149	1.378338
21	42	0	-0.134008	-1.232812	0.000000
22	42	0	0.387654	1.359324	0.000000
23	6	0	0.114603	2.631437	1.431876
24	6	0	0.114603	2.631437	-1.431876
25	8	0	-0.087643	3.348248	2.337094
26	8	0	-0.087643	3.348248	-2.337094

Table S30. Theoretical Cartesian coordinates (in Å) for the structure **2S-1** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	0.054341	1.205349	-0.413180
2	6	0	-0.300586	1.807892	1.727778
3	6	0	-1.148409	2.702226	0.991241
4	6	0	1.061359	2.102957	1.388345
5	1	0	-0.633451	1.070700	2.446932
6	1	0	-2.229463	2.747071	1.035571
7	1	0	1.945038	1.645082	1.814869
8	6	0	-1.730173	-0.464012	-1.012623
9	8	0	-2.858323	-0.207580	-1.267324
10	6	0	-0.300586	3.547052	0.225644
11	6	0	1.050747	3.196815	0.455809
12	1	0	-0.640914	4.301913	-0.476689
13	1	0	1.922181	3.663385	0.014293
14	42	0	-0.054341	-1.205349	-0.413180
15	6	0	0.300586	-1.807892	1.727778
16	6	0	1.148409	-2.702226	0.991241
17	6	0	-1.061359	-2.102957	1.388345
18	1	0	0.633451	-1.070700	2.446932
19	1	0	2.229463	-2.747071	1.035571
20	1	0	-1.945038	-1.645082	1.814869
21	6	0	1.730173	0.464012	-1.012623
22	8	0	2.858323	0.207580	-1.267324
23	6	0	0.300586	-3.547052	0.225644
24	6	0	-1.050747	-3.196815	0.455809
25	1	0	0.640914	-4.301913	-0.476689
26	1	0	-1.922181	-3.663385	0.014293

Table S31. Theoretical Cartesian coordinates (in Å) for the structure **2S-2** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.061382	1.875343	-0.223120
2	6	0	1.051454	1.854360	-1.286522
3	6	0	2.330999	1.921629	-0.661122
4	6	0	2.149226	2.067186	0.748493
5	6	0	0.768473	2.072117	1.026003
6	1	0	-1.055944	2.058529	-0.368818
7	1	0	0.849677	1.855795	-2.350479
8	1	0	3.288108	1.898092	-1.169702
9	1	0	2.942667	2.141877	1.482953
10	1	0	0.306063	2.162500	2.001108
11	6	0	0.768618	-2.072199	1.025773
12	6	0	2.149377	-2.067121	0.748299
13	6	0	2.331173	-1.921400	-0.661295
14	6	0	1.051636	-1.854167	-1.286719
15	6	0	0.061536	-1.875347	-0.223344
16	1	0	0.306194	-2.162728	2.000858
17	1	0	2.942804	-2.141828	1.482773
18	1	0	3.288292	-1.897732	-1.169849
19	1	0	0.849885	-1.855505	-2.350681
20	1	0	-1.055765	-2.058626	-0.369086
21	42	0	1.185435	0.000032	-0.004387
22	42	0	-1.340748	-0.000047	-0.296756
23	6	0	-3.305592	0.000066	-0.774956
24	6	0	-1.776612	-0.000210	1.571466
25	8	0	-4.441437	0.000163	-1.029048
26	8	0	-2.057171	-0.000322	2.709198

Table S32. Theoretical Cartesian coordinates (in Å) for the structure **1T-1** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	1.369084	0.474747	-0.009691
2	42	0	-1.100678	-0.001994	-0.022725
3	6	0	-2.938197	-0.894661	1.140388
4	6	0	-2.869644	-1.619362	-0.084917
5	6	0	-3.069885	-0.703858	-1.156735
6	6	0	-3.274610	0.592373	-0.599752
7	6	0	-3.191190	0.477696	0.827661
8	1	0	-2.839608	-1.313352	2.135177
9	1	0	-2.680494	-2.682605	-0.185721
10	1	0	-3.070444	-0.949736	-2.212321
11	1	0	-3.476132	1.499164	-1.155282
12	1	0	-3.335974	1.278349	1.541345
13	6	0	1.890596	-1.649315	0.718664
14	6	0	2.928666	-0.763955	1.154583
15	6	0	3.608867	-0.248095	0.015323
16	6	0	2.948113	-0.772260	-1.132972
17	6	0	1.903778	-1.655896	-0.709129
18	1	0	1.256660	-2.250735	1.357348
19	1	0	3.157218	-0.527872	2.188279
20	1	0	4.444573	0.439621	0.020436
21	1	0	3.196451	-0.545234	-2.164129
22	1	0	1.282115	-2.263481	-1.354024
23	6	0	-0.292448	1.714244	-0.005093
24	8	0	0.616037	2.574851	0.022780

Table S33. Theoretical Cartesian coordinates (in Å) for the structure **1T-2** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-1.182488	0.142536	-0.472901
2	42	0	1.218637	0.401018	0.121333
3	6	0	1.954466	-1.636640	-0.693568
4	6	0	2.128227	-1.634835	0.725318
5	6	0	3.135806	-0.677770	1.061910
6	6	0	3.572149	-0.068189	-0.141780
7	6	0	2.838438	-0.640334	-1.219069
8	1	0	1.339138	-2.317058	-1.265646
9	1	0	1.602626	-2.273990	1.425163
10	1	0	3.490337	-0.450102	2.060061
11	1	0	4.306608	0.724295	-0.225289
12	1	0	2.946379	-0.380346	-2.265884
13	6	0	-3.422456	-0.935400	-0.548248
14	6	0	-3.515472	0.303638	0.123413
15	6	0	-2.605809	0.261898	1.238822
16	6	0	-1.977433	-1.033689	1.253944
17	6	0	-2.487308	-1.766245	0.124305
18	1	0	-3.947064	-1.195462	-1.462162
19	1	0	-4.149455	1.136762	-0.153357
20	1	0	-2.496500	1.028405	1.995280
21	1	0	-1.344668	-1.425578	2.039180
22	1	0	-2.238339	-2.786319	-0.143741
23	6	0	-0.384568	1.833039	-0.153578
24	8	0	0.444557	2.634661	0.266678

Table S34. Theoretical Cartesian coordinates (in Å) for the structure **1T-3** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.387790	2.175534	0.664583
2	6	0	-0.508418	2.061252	-0.755113
3	6	0	0.805929	2.103944	-1.308703
4	6	0	1.733788	2.263287	-0.236007
5	6	0	0.995373	2.295809	0.981392
6	1	0	-1.212648	2.186048	1.363893
7	1	0	-1.436331	2.011609	-1.307325
8	1	0	1.056035	2.049518	-2.361658
9	1	0	2.811480	2.322464	-0.330671
10	1	0	1.414706	2.397767	1.975486
11	6	0	0.686639	-2.023400	0.762971
12	6	0	1.761270	-1.293448	1.387019
13	6	0	2.688527	-0.920465	0.374059
14	6	0	2.171128	-1.332383	-0.882401
15	6	0	0.950681	-2.056389	-0.657263
16	1	0	-0.039036	-2.626652	1.302846
17	1	0	1.870761	-1.128325	2.451737
18	1	0	3.606625	-0.366307	0.528874
19	1	0	2.643730	-1.183385	-1.845997
20	1	0	0.429453	-2.649068	-1.402685
21	42	0	0.702137	0.202859	0.011233
22	42	0	-1.463020	-0.997715	-0.215735
23	6	0	-2.766733	0.257772	0.278237
24	8	0	-3.496255	1.147652	0.570244

Table S35. Theoretical Cartesian coordinates (in Å) for the structure **1S-1** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-1.036685	0.122346	-0.351434
2	6	0	-3.344882	-0.729707	-0.746646
3	6	0	-3.413516	0.431699	0.055191
4	6	0	-2.558377	-1.709537	-0.077613
5	1	0	-3.783857	-0.841347	-1.732808
6	1	0	-3.935856	1.348501	-0.188851
7	1	0	-2.367268	-2.717777	-0.426421
8	6	0	-0.314264	1.859268	-0.085799
9	8	0	0.530699	2.694759	0.244795
10	6	0	-2.654257	0.186110	1.251071
11	6	0	-2.139573	-1.149157	1.176699
12	1	0	-2.555941	0.860690	2.091675
13	1	0	-1.593497	-1.663745	1.957618
14	42	0	1.277084	0.501806	0.010650
15	6	0	2.281998	-1.175113	-1.168177
16	6	0	1.447126	-1.733002	-0.142796
17	6	0	3.386902	-0.533414	-0.515207
18	1	0	2.174878	-1.326325	-2.234372
19	1	0	0.608927	-2.402897	-0.298309
20	1	0	4.175787	0.017937	-1.015540
21	6	0	1.997742	-1.345214	1.125178
22	6	0	3.220396	-0.639568	0.873691
23	1	0	1.619970	-1.627354	2.100095
24	1	0	3.858739	-0.194309	1.627889

Table S36. Theoretical Cartesian coordinates (in Å) for the structure **1S-2** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	1.112865	0.321157	0.539929
2	42	0	-0.933917	-0.126554	-0.456193
3	6	0	-2.223706	-1.405478	0.865878
4	6	0	-3.059684	-1.310929	-0.298812
5	6	0	-3.378277	0.035237	-0.522307
6	6	0	-2.743869	0.841198	0.478176
7	6	0	-2.073759	-0.065558	1.386718
8	1	0	-1.916224	-2.322899	1.351540
9	1	0	-3.344746	-2.139964	-0.937775
10	1	0	-3.934899	0.415909	-1.372478
11	1	0	-2.874268	1.907935	0.612464
12	1	0	-1.658168	0.203833	2.350965
13	6	0	2.909576	-1.358344	0.564595
14	6	0	3.299312	-0.213335	-0.193850
15	6	0	2.358669	-0.046042	-1.255881
16	6	0	1.377514	-1.114031	-1.133184
17	6	0	1.772966	-1.947521	-0.026268
18	1	0	3.410440	-1.718041	1.457179
19	1	0	4.164557	0.410553	-0.005928
20	1	0	2.425575	0.668881	-2.066290
21	1	0	0.635430	-1.390459	-1.900736
22	1	0	1.257259	-2.838225	0.308712
23	6	0	0.504950	2.103004	0.033862
24	8	0	0.232130	3.189994	-0.338514

Table S37. Theoretical Cartesian coordinates (in Å) for the structure **1S-3** using the MPW1PW91/SDD method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.030192	-0.144062	2.058679
2	6	0	0.365955	0.202700	1.888324
3	6	0	1.132783	-1.028389	1.875881
4	6	0	0.188381	-2.098379	1.909208
5	6	0	-1.124820	-1.553784	2.031356
6	1	0	-1.848060	0.559354	2.145907
7	1	0	0.808046	1.255474	2.042358
8	1	0	2.211735	-1.117179	1.892011
9	1	0	0.429690	-3.154687	1.872012
10	1	0	-2.043336	-2.126807	2.083937
11	6	0	-1.030192	-0.144062	-2.058679
12	6	0	-1.124820	-1.553784	-2.031356
13	6	0	0.188381	-2.098379	-1.909208
14	6	0	1.132783	-1.028389	-1.875881
15	6	0	0.365955	0.202700	-1.888324
16	1	0	-1.848060	0.559354	-2.145907
17	1	0	-2.043336	-2.126807	-2.083937
18	1	0	0.429690	-3.154687	-1.872012
19	1	0	2.211735	-1.117179	-1.892011
20	1	0	0.808046	1.255474	-2.042358
21	42	0	-0.128278	-0.799662	0.000000
22	42	0	0.788122	1.453144	0.000000
23	6	0	-0.925995	2.335600	0.000000
24	8	0	-1.957363	2.896351	0.000000

Table S38. Dissociation Gibbs free energies (ΔG in kcal/mol) for the successive removal of carbonyl groups from $Cp_2Mo_2(CO)_n$

	MPW1PW91/DZP	BP86/DZP
$Cp_2Mo_2(CO)_6$ (**6S-1**) → $Cp_2Mo_2(CO)_5$(**5S-1**) + CO	27.4	26.2
$Cp_2Mo_2(CO)_5$(**5S-1**) → $Cp_2Mo_2(CO)_4$(**4S-1**) + CO	2.4	5.9
$Cp_2Mo_2(CO)_4$(**4S-1**) → $Cp_2Mo_2(CO)_3$(**3T-1**) + CO	38.0	44.2
$Cp_2Mo_2(CO)_3$(**3T-1**) → $Cp_2Mo_2(CO)_2$(**2T-1**) + CO	51.3	53.8
$Cp_2Mo_2(CO)_2$(**2T-1**) → $Cp_2Mo_2(CO)$(**1T-1**) + CO	52.4	53.0

Table S39. Disproportionation dissociation Gibbs free energies (ΔG in kcal/mol) of the $Cp_2Mo_2(CO)_n$ (n = 5, 4, 3, 2) species

	MPW1PW91/DZP	BP86/DZP
$2Cp_2Mo_2(CO)_5$ → $Cp_2Mo_2(CO)_6$ + $Cp_2Mo_2(CO)_4$	-25.1	-20.4
$2Cp_2Mo_2(CO)_4$ → $Cp_2Mo_2(CO)_5$ + $Cp_2Mo_2(CO)_3$	35.6	38.3
$2Cp_2Mo_2(CO)_3$ → $Cp_2Mo_2(CO)_4$ + $Cp_2Mo_2(CO)_2$	13.3	9.6
$2Cp_2Mo_2(CO)_2$ → $Cp_2Mo_2(CO)_3$ + $Cp_2Mo_2(CO)$	1.1	-0.8

Table S40. Dissociation Gibbs free energies (ΔG in kcal/mol) of the binuclear $Cp_2Mo_2(CO)_n$ into mononuclear fragments (kcal/mol)

	MPW1PW91/DZP	BP86/DZP
$Cp_2Mo_2(CO)_2$ → $2MoCp(CO)$	64.9	71.1
$Cp_2Mo_2(CO)_4$ → $2MoCp(CO)_2$	66.2	72.2
$Cp_2Mo_2(CO)_6$ → $2MoCp(CO)_3$	9.3	10.9
$Cp_2Mo_2(CO)_3$ → $MoCp(CO)_2$ + $MoCp(CO)$	72.2	76.4
$Cp_2Mo_2(CO)_4$ → $MoCp(CO)_3$ + $MoCp(CO)$	66.9	73.9
$Cp_2Mo_2(CO)_5$ → $MoCp(CO)_4$ + $MoCp(CO)$	70.7	75.6
$Cp_2Mo_2(CO)_5$ → $MoCp(CO)_3$ + $MoCp(CO)_2$	25.2	31.4
$Cp_2Mo_2(CO)_6$ → $MoCp(CO)_2$ + $MoCp(CO)_4$	54.2	53.5

Table S41. Dissociation enthalpies (ΔH in kcal/mol) for the successive removal of carbonyl groups from $Cp_2Mo_2(CO)_n$

	MPW1PW91/DZP	BP86/DZP
$Cp_2Mo_2(CO)_6$ (**6S-1**) → $Cp_2Mo_2(CO)_5$(**5S-1**) + CO	40.1	38.5
$Cp_2Mo_2(CO)_5$(**5S-1**) → $Cp_2Mo_2(CO)_4$(**4S-1**) + CO	14.3	17.8
$Cp_2Mo_2(CO)_4$(**4S-1**) → $Cp_2Mo_2(CO)_3$(**3T-1**) + CO	50.3	56.5
$Cp_2Mo_2(CO)_3$(**3T-1**) → $Cp_2Mo_2(CO)_2$(**2T-1**) + CO	63.1	65.0
$Cp_2Mo_2(CO)_2$(**2T-1**) → $Cp_2Mo_2(CO)$(**1T-1**) + CO	62.3	63.5

Table S42. Disproportionation dissociation enthalpies (ΔH in kcal/mol) of the $Cp_2Mo_2(CO)_n$ (*n* = 5, 4, 3, 2) species

	MPW1PW91/DZP	BP86/DZP
$2Cp_2Mo_2(CO)_5$ → $Cp_2Mo_2(CO)_6$ + $Cp_2Mo_2(CO)_4$	-25.8	-20.8
$2Cp_2Mo_2(CO)_4$ → $Cp_2Mo_2(CO)_5$ + $Cp_2Mo_2(CO)_3$	36.0	38.7
$2Cp_2Mo_2(CO)_3$ → $Cp_2Mo_2(CO)_4$ + $Cp_2Mo_2(CO)_2$	12.9	8.5
$2Cp_2Mo_2(CO)_2$ → $Cp_2Mo_2(CO)_3$ + $Cp_2Mo_2(CO)$	-0.9	-1.5

Table S43. Dissociation dissociation enthalpies (ΔH in kcal/mol) of the binuclear $Cp_2Mo_2(CO)_n$ into mononuclear fragments (kcal/mol)

	MPW1PW91/DZP	BP86/DZP
$Cp_2Mo_2(CO)_2$ → $2MoCp(CO)$	75.6	82.0
$Cp_2Mo_2(CO)_4$ → $2MoCp(CO)_2$	79.8	85.7
$Cp_2Mo_2(CO)_6$ → $2MoCp(CO)_3$	27.4	28.5
$Cp_2Mo_2(CO)_3$ → $MoCp(CO)_2$ + $MoCp(CO)$	84.1	88.1
$Cp_2Mo_2(CO)_4$ → $MoCp(CO)_3$ + $MoCp(CO)$	81.0	87.9
$Cp_2Mo_2(CO)_5$ → $MoCp(CO)_4$ + $MoCp(CO)$	86.3	90.9
$Cp_2Mo_2(CO)_5$ → $MoCp(CO)_3$ + $MoCp(CO)_2$	40.7	46.7
$Cp_2Mo_2(CO)_6$ → $MoCp(CO)_2$ + $MoCp(CO)_4$	71.7	70.5

Table S44. Infrared active ν(CO) vibrational frequencies (cm^{-1}) predicted for the two lowest energy isomers of $Cp_2Mo_2(CO)_6$ (infrared intensities in parentheses are in km/mol).

	MPW1PW91	BP86
6S-1 (***C_{2h}***)	1993 (0), 2018 (375), 2027 (2199), 2034 (0), 2070 (2868), 2108 (0)	1881 (0), 1902(397), 1912(1831), 1915(0), 1955(2266), 1986 (0)
Expt.		1916, 1960
6S-2 (***C_2***)	2001(452), 2008(874), 2042(1139) 2047 (0), 2072(1687), 2124(1223)	1887 (381), 1892 (711), 1925 (1038), 1928(4), 1957(1348), 2001 (978)

Table S45. Infrared active ν(CO) vibrational frequencies (cm^{-1}) predicted for the six lowest energy structures of $Cp_2Mo_2(CO)_5$ (infrared intensities in parentheses are in km/mol).

	MPW1PW91	BP86
5S-1 (C_1)	1817 (537), 1971 (554), 2027 (1322), 2055 (1118), 2108 (976)	1721 (371), 1857 (455), 1909 (1006), 1932 (964), 1982 (834),
Expt		1665, 1872, 1944, 1982
5S-2 (C_2)	1782 (738), 2010 (142), 2027 (1724), 2037 (385), 2105 (1154)	1689 (580), 1895 (158), 1910 (907), 1915 (863), 1977 (909)
5S-3 (C_s)	2017 (1943), 2038 (1874), 2043 (535), 2057 (244), 2129 (1173)	1902 (1583), 1916 (1517), 1923 (194), 1934 (354), 2001 (1129)
5T-1 (C_s)	1950 (686), 1973(124), 2023(1380), 2041 (2675), 2082 (20)	1827 (578), 1842 (50), 1901 (1041), 1923 (2130), 1955 (11)
5T-2 (C_s)	1913 (917), 1929 (373), 2026 (694), 2040 (1097), 2099 (1473)	1791 (702), 1804 (285), 1913 (518), 1914 (864), 1971 (1200)
5T-3 (C_{2v})	2027 (1966), 2030 (823), 2042(2015), 2065 (79), 2144 (721)	1909 (1609), 1916 (1658), 1919 (563), 1937 (86), 2014 (749)

Table S46. Infrared active ν(CO) vibrational frequencies (cm^{-1}) predicted for the six lowest energy isomers of $Cp_2Mo_2(CO)_4$ (infrared intensities in parentheses are in km/mol).

	MPW1PW91	BP86
4S-1 (C_2)	1970 (298),1983 (1536),2010(1424), 2057 (341)	1858 (208),1870(1266),1900(1143), 1938(290)
4T-1 (C_S)	1938(1312),1961(172),1998(1525), 2065(918)	1810(999),1825 (91),1874(1221), 1940(803)
4T-2 (C_i)	1910(1394),1914(0),2012(2690), 2043(0)	1795 (1003),1796 (0),1888 (2168), 1913(0)

Table S47. Infrared active ν(CO) vibrational frequencies (cm^{-1}) predicted for the six lowest energy isomers of $Cp_2Mo_2(CO)_3$ (infrared intensities in parentheses are in km/mol).

	MPW1PW91	BP86
3T-1(C_1)	1876 (1088), 1934 (1185), 1981(401)	1753 (790), 1809(913), 1849(311)
3T-2(C_2)	1873(1242), 1932(1281), 1958 (210)	1748 (899), 1790 (987), 1812 (109)
3T-3 (C_s)	1970(1304), 1971(1121), 2051 (1728)	1865(946), 1866(1097), 1941(1196)
3S-1 (C_1)	1913 (1030), 1932(1024), 1985(552)	(converges to **3S-2**)
3S-2 (C_s)	1827(824), 1858 (1432), 1876(36)	1710 (613), 1744 (1088), 1761(40)

Table S48. Infrared active ν(CO) vibrational frequencies (cm^{-1}) predicted for the six lowest energy isomers of $Cp_2Mo_2(CO)_2$ (infrared intensities in parentheses are in km/mol).

	MPW1PW91	BP86
2T-1 (C_1)	1906 (1149), 1955 (836)	1793 (906), 1834 (586)
2T-2 (C_i)	1864 (1671), 1878 (0)	1758 (1235), 1766 (0)
2T-3 (C_s)	1909 (1141), 1956 (30)	1813 (925), 1851 (455)
2T-4 (C_s)	1940 (1594), 2000 (1556)	1822 (1324), 1876 (1043)
2S-1 (C_2)	1904 (1630), 1913 (372)	1775 (1156), 1781 (247)
2S-2 (C_s)	1972 (932), 2022 (2063)	1860 (841), 1899 (1495)

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