

Unsaturated Binuclear Cyclopentadienylrhenium Carbonyl Derivatives: Metal-Metal Multiple Bonds, Rhenocene Structures, and Agostic Hydrogen Atoms

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Supporting Information

Tables S1-S9: Theoretical harmonic vibrational frequencies for $\text{Cp}_2\text{Re}_2(\text{CO})_5$ (8 structures), $\text{Cp}_2\text{Re}_2(\text{CO})_4$ (12 structures), $\text{Cp}_2\text{Re}_2(\text{CO})_3$ (8 structures) and $\text{Cp}_2\text{Re}_2(\text{CO})_2$ (9 structures) using the BP86 method.

Tables S10-S46: Theoretical Cartesian coordinates for $\text{Cp}_2\text{Re}_2(\text{CO})_5$ (8 structures), $\text{Cp}_2\text{Re}_2(\text{CO})_4$ (12 structures), $\text{Cp}_2\text{Re}_2(\text{CO})_3$ (8 structures) and $\text{Cp}_2\text{Re}_2(\text{CO})_2$ (9 structures) using the MPW1PW91 method..

Complete Gaussian 03 reference (Reference 34)

Table S1. Theoretical harmonic vibrational frequencies (in cm^{-1}) for $\text{Cp}_2\text{Re}_2(\text{CO})_5$ using the BP86/SDD method (infrared intensities in parentheses are in km/mol).

5S-1 (C_2)	5S-2 (C_s)	5S-3 (C_1)	5S-4 (C_s)
36.6 (b, 1.3)	108.8i (a", 5.7)	25.2 (a, 0.4)	27.0i (a", 0.1)
37.1 (a, 0.0)	37.3i (a", 0.1)	29.8 (a, 1.1)	22.7i (a", 0.0)
38.5 (b, 0.0)	23.5i (a", 0.0)	39.0 (a, 0.1)	32.3 (a', 0.1)
46.0 (a, 1.4)	31.4 (a', 1.2)	47.3 (a, 0.1)	51.7 (a", 0.7)
72.1 (b, 0.4)	44.2 (a", 1.6)	66.4 (a, 0.5)	53.6 (a', 0.6)
77.9 (a, 0.2)	78.5 (a", 0.5)	79.4 (a, 0.8)	80.9 (a", 0.7)
93.8 (a, 0.1)	82.5 (a', 0.6)	84.9 (a, 0.0)	89.9 (a', 0.2)
95.2 (a, 0.6)	93.4 (a', 0.8)	91.9 (a, 0.1)	93.4 (a", 0.1)
97.0 (b, 0.7)	98.3 (a", 0.5)	94.8 (a, 0.3)	94.9 (a', 0.7)
99.2 (a, 0.4)	100.2 (a', 0.1)	98.8 (a, 0.3)	97.3 (a', 0.3)
102.6 (b, 0.1)	103.2 (a", 0.8)	103.5 (a, 0.2)	101.5 (a", 0.2)
106.7 (a, 0.1)	106.0 (a', 0.3)	108.8 (a, 0.6)	115.3 (a", 2.6)
108.0 (b, 0.9)	113.3 (a', 2.3)	117.6 (a, 0.4)	119.1 (a', 0.1)
116.6 (b, 3.6)	144.6 (a', 3.9)	125.0 (a, 1.5)	132.8 (a', 0.8)
149.8 (a, 0.2)	146.8 (a", 0.6)	144.0 (a, 0.3)	161.8 (a', 0.1)
240.7 (b, 1.4)	189.4 (a', 4.0)	255.6 (a, 0.3)	248.5 (a", 3.2)
291.9 (a, 2.8)	278.0 (a', 20.4)	282.7 (a, 6.4)	290.2 (a', 1.7)
292.0 (b, 4.9)	290.6 (a', 5.5)	289.9 (a, 3.8)	291.3 (a", 0.4)
310.9 (b, 2.5)	319.2 (a", 8.5)	306.3 (a, 5.7)	299.1 (a", 6.2)
311.6 (a, 9.5)	328.7 (a', 1.0)	323.2 (a, 3.3)	299.5 (a', 13.7)
352.8 (b, 1.1)	333.4 (a', 11.3)	342.4 (a, 4.2)	351.1 (a", 0.2)
356.7 (a, 0.7)	334.5 (a", 12.0)	356.8 (a, 0.7)	354.5 (a', 0.6)
411.6 (a, 0.3)	349.1 (a", 0.2)	406.0 (a, 9.9)	396.0 (a', 6.7)
414.8 (b, 11.2)	405.0 (a', 109.5)	422.2 (a, 2.1)	434.9 (a", 3.2)
482.0 (a, 0.0)	470.6 (a", 0.9)	459.7 (a, 1.4)	459.6 (a', 0.2)
485.3 (b, 7.3)	479.0 (a", 24.5)	472.7 (a, 82.1)	475.1 (a", 56.9)
492.7 (a, 34.0)	493.5 (a', 66.3)	488.4 (a, 24.0)	486.4 (a', 33.2)
493.3 (b, 105.9)	505.4 (a", 1.2)	497.4 (a, 45.0)	503.5(a", 127.7)
502.4 (b, 63.7)	505.7 (a", 2.7)	501.9 (a, 17.7)	503.5 (a', 10.3)
519.8 (a, 0.0)	512.4 (a', 47.6)	511.6 (a, 10.7)	519.2 (a", 4.3)
521.4 (b, 9.1)	520.6 (a', 3.9)	517.2 (a, 15.2)	519.8 (a', 2.9)
528.7 (a, 8.4)	539.5 (a", 4.8)	533.3 (a, 13.1)	541.6 (a', 9.1)
553.5 (a, 3.1)	555.4 (a', 37.1)	549.7 (a, 42.7)	557.8 (a", 25.2)
571.5 (b, 33.1)	570.3 (a', 0.3)	567.5 (a, 25.9)	569.3 (a', 2.4)
574.4 (a, 0.7)	573.0 (a", 1.4)	572.5 (a, 5.8)	569.8 (a", 0.6)
574.5 (b, 1.5)	574.0 (a', 21.2)	574.2 (a, 2.2)	573.1 (a", 8.0)
576.5 (a, 0.0)	578.4 (a", 0.0)	575.8 (a, 4.3)	575.4 (a', 2.5)
577.6 (b, 42.4)	585.2 (a', 22.2)	579.7 (a, 5.0)	588.4 (a', 11.9)
593.5 (b, 45.6)	587.7 (a", 4.0)	587.1 (a, 18.1)	590.5 (a", 20.5)
598.7 (a, 2.4)	593.3 (a', 72.4)	598.3 (a, 24.8)	594.6 (a', 24.7)

633.1 (b, 311.4)	627.0 (a', 219.9)	635.8 (a, 310.8)	648.7(a", 386.8)
794.1 (a, 0.7)	790.0 (a', 72.6)	774.0 (a, 46.6)	744.0 (a", 24.9)
796.5 (b, 90.1)	793.3 (a", 8.9)	782.9 (a, 33.8)	781.7 (a', 35.2)
803.2 (b, 8.6)	794.7 (a", 2.9)	787.7 (a, 45.1)	798.7 (a", 33.3)
804.0 (a, 0.0)	799.0 (a', 78.5)	791.0 (a, 11.8)	801.4 (a', 19.2)
813.0 (a, 0.3)	809.2 (a", 0.0)	804.8 (a, 2.8)	803.0 (a", 1.1)
813.3 (b, 34.2)	812.2 (a", 0.0)	810.6 (a, 0.7)	805.2 (a', 20.2)
815.3 (b, 8.3)	813.8 (a', 2.6)	812.1 (a, 13.9)	811.1 (a", 0.3)
815.3 (a, 1.0)	814.4 (a', 3.2)	812.8 (a, 8.7)	813.1 (a', 2.2)
821.5 (b, 28.2)	825.2 (a', 2.3)	817.2 (a, 2.1)	815.0 (a", 23.0)
822.1 (a, 8.8)	830.1 (a', 10.6)	823.3 (a, 12.4)	819.7 (a', 19.1)
878.0 (b, 1.6)	872.8 (a', 1.2)	863.9 (a, 2.1)	863.2 (a", 0.0)
878.2 (a, 1.1)	874.6 (a", 0.0)	872.0 (a, 1.8)	868.4 (a', 1.8)
884.1 (a, 0.3)	876.1 (a", 1.9)	876.8 (a, 2.0)	874.3 (a", 0.4)
884.3 (b, 1.0)	887.2 (a', 4.9)	878.1 (a, 0.8)	878.2 (a', 1.2)
983.6 (b, 11.9)	986.7 (a", 9.7)	980.1 (a, 6.0)	978.0 (a", 9.7)
983.6 (a, 1.2)	989.3 (a", 7.4)	980.4 (a, 8.6)	982.2 (a', 3.3)
993.1 (b, 1.6)	992.5 (a', 3.2)	992.5 (a, 6.5)	989.8 (a", 0.3)
993.3 (a, 9.6)	992.9 (a', 10.5)	994.2 (a, 7.5)	995.2 (a', 15.3)
1040.3 (a, 1.1)	1041.8 (a', 1.2)	1034.8 (a, 0.3)	1033.4 (a", 0.1)
1040.9 (b, 0.2)	1042.7 (a', 1.3)	1040.8 (a, 1.3)	1041.2 (a", 0.2)
1043.1 (b, 0.6)	1043.9 (a", 0.6)	1041.4 (a, 0.8)	1042.9 (a', 0.2)
1043.4 (a, 0.3)	1048.2 (a", 0.0)	1042.0 (a, 0.8)	1044.8 (a', 1.8)
1096.6 (a, 0.0)	1097.4 (a', 1.8)	1095.6 (a, 3.0)	1096.3 (a", 1.3)
1096.6 (b, 3.8)	1097.7 (a', 2.4)	1096.9 (a, 4.4)	1098.0 (a', 7.6)
1224.8 (b, 0.0)	1225.0 (a", 0.0)	1221.6 (a, 0.0)	1220.5 (a", 0.0)
1224.8 (a, 0.0)	1227.3 (a", 0.0)	1223.1 (a, 0.0)	1224.8 (a', 0.0)
1350.6 (b, 1.1)	1348.9 (a', 2.8)	1349.7 (a, 1.7)	1352.5 (a", 0.0)
1350.7 (a, 1.6)	1352.9 (a", 2.8)	1353.0 (a, 2.7)	1353.4 (a', 4.0)
1357.6 (a, 0.3)	1357.5 (a', 0.9)	1356.5 (a, 0.7)	1356.7 (a", 0.1)
1359.2 (b, 0.4)	1360.4 (a", 0.7)	1359.0 (a, 0.7)	1358.6 (a', 1.4)
1397.7 (b, 7.4)	1401.5 (a', 3.0)	1395.8 (a, 4.7)	1397.2 (a", 7.4)
1397.8 (a, 1.0)	1402.1 (a", 2.2)	1396.5 (a, 2.1)	1398.8 (a', 1.7)
1409.9 (b, 0.5)	1403.8 (a', 3.7)	1407.1 (a, 2.3)	1406.5 (a", 0.6)
1410.1 (a, 4.0)	1404.4 (a", 3.1)	1410.8 (a, 2.6)	1409.9 (a', 3.9)
1743.3(a,362.7)	1825.9(a",620.7)	1727.4(a, 391.4)	1721.4(a',373.1)
1903.4(b, 101.1)	1832.7 (a', 6.0)	1904.1(a, 453.5)	1911.4 (a", 2.2)
1921.5(a,1286.8)	1915.3(a",964.3)	1934.6(a, 632.6)	1944.9(a',1418.1)
1949.9(b,1657.3)	1938.6(a',1633.3)	1950.2(a, 849.6)	1955.0(a", 539.3)
1975.6 (a, 40.0)	1969.6(a', 176.7)	1995.4(a,1143.3)	1998.5(a',1203.6)
3176.8 (b, 0.2)	3175.4 (a", 0.2)	3173.4 (a, 0.0)	3174.5 (a", 0.2)
3176.8 (a, 0.1)	3175.7 (a', 0.3)	3176.1 (a, 0.1)	3174.6 (a', 0.2)
3179.0 (a, 0.1)	3176.6 (a', 0.1)	3178.4 (a, 0.3)	3178.8 (a", 0.1)
3179.0 (b, 0.0)	3177.3 (a", 0.0)	3179.2 (a, 0.2)	3179.3 (a', 0.2)

3189.6 (b, 0.0)	3186.2 (a', 0.9)	3187.8 (a, 0.3)	3188.0 (a'', 0.3)
3189.7 (a, 0.3)	3188.1 (a', 0.3)	3189.1 (a, 0.0)	3188.4 (a', 0.1)
3191.0 (b, 1.0)	3189.1 (a'', 0.3)	3189.9 (a, 0.6)	3193.3 (a'', 0.5)
3191.0 (a, 0.0)	3193.1 (a'', 0.6)	3191.4 (a, 0.8)	3193.5 (a', 0.1)
3199.9 (b, 0.0)	3198.0 (a', 0.0)	3199.7 (a, 0.7)	3203.6 (a'', 1.4)
3200.0 (a, 0.0)	3199.5 (a', 0.0)	3201.1 (a, 1.3)	3204.4 (a', 2.6)

Table S2. Theoretical harmonic vibrational frequencies (in cm^{-1}) for $\text{Cp}_2\text{Re}_2(\text{CO})_5$ using the BP86/SDD method (infrared intensities in parentheses are in km/mol).

5S-5 (C_{2v})	5S-6 (C_1)	5S-7 (C_{2v})	5S-8 (C_{2v})
10.5i (b ₁ , 0.3)	28.2 (a, 0.0)	51.0 (b ₁ , 2.1)	13.1i (b ₂ , 1.2)
33.8 (a ₂ , 0.0)	44.9 (a, 0.8)	53.0 (b ₂ , 0.0)	45.1 (b ₂ , 0.0)
53.0 (b ₁ , 0.1)	52.1 (a, 1.3)	61.5 (a ₂ , 0.0)	48.2 (a ₂ , 0.0)
58.6 (a ₁ , 2.5)	54.7 (a, 1.3)	69.3 (a ₁ , 0.0)	58.7 (a ₁ , 0.1)
63.1 (b ₂ , 0.1)	73.6 (a, 0.1)	75.8 (b ₂ , 2.3)	59.5 (b ₁ , 0.6)
71.1 (b ₁ , 0.0)	74.1 (a, 0.6)	79.9 (a ₁ , 0.1)	63.1 (b ₂ , 0.8)
74.6 (a ₂ , 0.0)	85.7 (a, 0.0)	81.7 (b ₁ , 1.4)	78.5 (a ₂ , 0.0)
84.9 (b ₂ , 0.3)	88.8 (a, 0.3)	86.0 (a ₂ , 0.0)	85.2 (a ₁ , 0.5)
89.0 (b ₁ , 0.1)	95.0 (a, 0.2)	87.0 (b ₂ , 1.3)	85.5 (b ₁ , 0.5)
89.3 (a ₂ , 0.0)	98.0 (a, 0.2)	90.4 (b ₁ , 0.1)	93.3 (b ₂ , 0.2)
93.6 (a ₁ , 0.4)	112.4 (a, 1.1)	98.9 (a ₁ , 0.0)	102.0 (b ₁ , 0.2)
93.9 (b ₂ , 0.1)	120.3 (a, 1.2)	120.9 (b ₁ , 2.0)	120.5 (a ₂ , 0.0)
104.3 (a ₁ , 2.4)	133.0 (a, 0.8)	133.5 (b ₂ , 1.7)	137.7 (a ₁ , 0.5)
126.9 (b ₂ , 0.3)	147.4 (a, 0.8)	163.0 (b ₁ , 1.2)	139.9 (b ₂ , 2.4)
134.4 (b ₁ , 3.8)	170.9 (a, 4.6)	169.3 (a ₂ , 0.0)	177.7 (b ₁ , 0.2)
185.1 (a ₁ , 23.0)	188.8 (a, 13.2)	234.4 (a ₁ , 0.3)	200.1 (a ₁ , 36.6)
319.8 (b ₂ , 11.9)	195.4 (a, 12.1)	272.1 (b ₂ , 0.4)	252.9 (b ₂ , 15.7)
330.3 (a ₁ , 1.2)	244.1 (a, 0.3)	290.4 (a ₁ , 32.1)	273.0 (b ₁ , 6.6)
338.5 (a ₂ , 0.0)	294.1 (a, 3.0)	306.6 (b ₁ , 3.5)	274.1 (a ₁ , 2.2)
351.7 (b ₂ , 4.5)	312.0 (a, 6.5)	351.6 (a ₂ , 0.0)	284.4 (a ₂ , 0.0)
353.2 (b ₁ , 8.5)	345.2 (a, 1.0)	354.0 (b ₂ , 31.5)	355.1 (b ₁ , 6.5)
367.4 (a ₂ , 0.0)	362.2 (a, 33.0)	390.6 (a ₁ , 0.0)	400.4 (b ₂ , 27.3)
371.0 (b ₁ , 1.4)	382.1 (a, 49.2)	410.6 (b ₁ , 40.8)	401.9 (a ₁ , 0.7)
398.3 (a ₁ , 12.3)	405.1 (a, 4.4)	414.0 (a ₂ , 0.0)	402.5 (a ₂ , 0.0)
405.8 (b ₂ , 2.6)	411.0 (a, 12.6)	419.8 (b ₁ , 1.6)	411.6 (b ₂ , 0.5)
413.5 (b ₂ , 27.3)	432.9 (a, 11.8)	450.7 (b ₂ , 4.7)	437.0 (b ₂ , 4.4)
417.2 (b ₁ , 8.7)	437.2 (a, 4.1)	464.3 (a ₁ , 0.2)	458.7 (a ₁ , 1.0)
438.5(a ₁ ,113.2)	473.6 (a, 13.6)	475.4 (a ₁ , 0.7)	466.7 (b ₂ , 32.1)
459.0 (a ₁ , 9.2)	480.7 (a, 6.7)	482.4 (b ₂ , 0.4)	470.0 (a ₂ , 0.0)
461.4 (a ₁ , 11.9)	509.6 (a, 15.3)	498.5 (b ₁ , 3.4)	485.6 (a ₁ , 6.2)
476.4 (b ₁ , 9.9)	511.4 (a, 23.5)	504.1 (b ₂ , 7.6)	502.1 (b ₁ , 4.8)
486.8 (a ₁ , 17.3)	547.6 (a, 6.0)	535.9 (a ₂ , 0.0)	509.4 (a ₁ , 2.6)
488.8 (a ₂ , 0.0)	552.5 (a, 21.0)	539.1 (a ₁ , 39.6)	514.5 (b ₁ , 55.1)
529.3 (a ₂ , 0.0)	565.5 (a, 7.4)	550.9 (a ₁ , 4.8)	542.8 (b ₂ , 13.7)
529.9 (b ₂ , 1.1)	569.2 (a, 7.6)	552.8 (a ₂ , 0.0)	562.3 (a ₁ , 25.0)
541.8 (b ₁ , 0.1)	575.2 (a, 19.1)	553.0 (b ₁ , 16.7)	578.2 (a ₁ , 42.5)
552.8 (a ₁ , 0.0)	581.0 (a, 10.5)	567.5 (b ₁ , 27.6)	584.7 (b ₁ , 28.7)
557.8 (b ₂ , 2.8)	593.0 (a, 24.4)	573.0 (b ₂ , 17.4)	588.6 (b ₂ , 0.5)
573.5 (b ₂ , 46.9)	598.6 (a, 40.3)	590.3 (a ₁ , 124.0)	594.3 (b ₁ , 3.9)
587.9 (b ₁ , 55.7)	608.5 (a, 208.3)	600.7 (b ₂ , 24.4)	596.8 (a ₂ , 0.0)

603.6(a ₁ , 109.2)	630.8 (a, 123.3)	620.4 (a ₁ , 11.0)	607.2 (a ₁ , 1.3)
748.8 (a ₂ , 0.0)	750.3 (a, 88.0)	763.5 (b ₂ , 0.1)	750.0 (a ₂ , 0.0)
760.4 (b ₁ , 3.2)	760.2 (a, 8.5)	778.2 (a ₂ , 0.0)	752.9 (b ₁ , 2.1)
772.1 (b ₂ , 16.9)	784.5 (a, 7.0)	783.4 (b ₁ , 0.9)	759.3 (a ₁ , 0.2)
773.3 (b ₂ , 30.2)	786.9 (a, 68.4)	790.6 (a ₁ , 3.4)	760.9 (b ₂ , 3.2)
775.1 (a ₂ , 0.0)	787.8 (a, 0.0)	801.8 (b ₂ , 46.6)	792.5 (b ₁ , 0.2)
779.1 (a ₁ , 0.0)	793.2 (a, 8.0)	805.9 (a ₂ , 0.0)	800.4 (a ₂ , 0.0)
799.3 (b ₁ , 3.5)	806.2 (a, 47.6)	813.1 (a ₁ , 23.8)	804.6 (b ₂ , 0.4)
811.4 (a ₁ , 1.6)	810.9 (a, 0.3)	814.6 (b ₁ , 5.1)	804.8 (a ₁ , 4.9)
815.3 (a ₁ , 28.5)	816.2 (a, 6.7)	832.8 (b ₂ , 4.1)	812.4 (b ₁ , 32.9)
817.9 (b ₂ , 6.1)	820.0 (a, 5.3)	858.8 (a ₁ , 71.5)	822.9 (a ₁ , 0.5)
833.9 (a ₂ , 0.0)	849.5 (a, 7.6)	873.9 (b ₂ , 21.5)	863.3 (b ₁ , 2.7)
841.5 (b ₁ , 0.4)	870.5 (a, 1.2)	881.6 (b ₁ , 0.1)	864.0 (b ₂ , 10.4)
844.6 (b ₂ , 9.4)	883.4 (a, 4.7)	883.8 (a ₁ , 0.9)	865.0 (a ₁ , 2.2)
862.7 (a ₁ , 11.6)	892.4 (a, 16.8)	885.4 (a ₂ , 0.0)	873.1 (a ₂ , 0.0)
950.6 (b ₂ , 1.0)	982.6 (a, 21.1)	954.7 (a ₂ , 0.0)	923.3 (a ₂ , 0.0)
957.1 (a ₁ , 6.7)	985.0 (a, 8.4)	957.0 (b ₂ , 1.5)	928.3 (b ₂ , 7.0)
989.1 (a ₂ , 0.0)	990.9 (a, 7.8)	964.5 (a ₁ , 0.4)	975.8 (b ₁ , 0.3)
1002.1(b ₁ ,17.3)	1005.7 (a, 3.7)	966.0 (b ₁ , 13.5)	980.2 (a ₁ , 3.4)
1023.0 (a ₂ , 0.0)	1041.6 (a, 0.5)	1035.8 (b ₂ , 0.7)	1003.7 (a ₁ , 0.7)
1036.4 (b ₁ , 0.0)	1042.0 (a, 1.2)	1037.9 (a ₁ , 2.9)	1004.9 (b ₁ , 0.4)
1036.5 (b ₂ , 0.0)	1050.3 (a, 0.3)	1041.1 (a ₂ , 0.0)	1027.9 (a ₂ , 0.0)
1042.1 (a ₁ , 0.0)	1057.9 (a, 8.2)	1043.0 (b ₁ , 19.8)	1031.7 (b ₂ , 2.6)
1091.1 (a ₁ , 4.8)	1096.4 (a, 2.9)	1064.1 (a ₁ , 0.0)	1064.0 (b ₁ , 7.9)
1091.6(b ₂ , 31.3)	1096.9 (a, 2.1)	1065.1 (b ₂ , 12.9)	1067.5 (a ₁ , 0.0)
1216.5 (a ₂ , 0.0)	1223.2 (a, 0.0)	1114.9 (b ₁ , 7.5)	1209.2 (a ₂ , 0.0)
1217.6 (b ₁ , 0.0)	1224.7 (a, 0.1)	1121.2 (a ₂ , 0.0)	1209.4 (b ₂ , 0.7)
1347.0 (a ₂ , 0.0)	1338.9 (a, 20.8)	1221.4 (b ₁ , 0.2)	1282.6 (a ₂ , 0.0)
1349.4 (b ₂ , 0.1)	1345.2 (a, 12.3)	1223.4 (a ₂ , 0.0)	1291.1 (b ₂ , 13.1)
1356.6 (a ₁ , 1.4)	1351.9 (a, 2.3)	1343.5 (b ₂ , 0.0)	1314.1 (a ₁ , 13.7)
1360.9 (b ₁ , 1.6)	1355.4 (a, 1.9)	1345.3 (a ₁ , 0.1)	1314.8 (b ₁ , 20.1)
1378.1 (b ₂ , 1.2)	1393.8 (a, 25.7)	1370.8 (b ₂ , 2.0)	1344.8 (a ₂ , 0.0)
1384.9(a ₁ , 12.0)	1401.0 (a, 2.6)	1377.4 (a ₁ , 0.2)	1346.8 (b ₂ , 1.1)
1402.6 (a ₂ , 0.0)	1403.0 (a, 3.8)	1410.0 (b ₁ , 2.2)	1393.2 (b ₁ , 1.8)
1406.4 (b ₁ , 2.5)	1446.7 (a, 25.3)	1411.6 (a ₂ , 0.0)	1394.8 (a ₁ , 3.9)
1943.1(b ₁ ,1255.2)	1713.4 (a, 354.1)	1921.7(a ₁ ,1258.7)	1904.7 (a ₁ , 878.7)
1950.1 (a ₁ , 783.0)	1739.9 (a, 419.6)	1933.9 (b ₂ , 963.4)	1930.7 (b ₂ , 133.5)
1956.5(b ₂ ,1307.5)	1910.1 (a, 977.5)	1941.5(b ₁ ,1549.1)	1940.2(b ₂ ,2009.5)
1966.8 (a ₁ , 3.6)	1946.0 (a, 1232.9)	1958.5 (a ₁ , 478.7)	1980.9(a ₁ ,1604.2)
2044.8 (a ₁ , 577.1)	2010.1 (a, 218.0)	2040.8 (a ₁ , 381.2)	2006.8 (a ₁ , 50.4)
3173.6 (b ₂ , 0.3)	3133.6 (a, 0.9)	2936.5 (a ₁ , 0.0)	3143.0 (a ₂ , 0.0)
3178.6 (a ₁ , 0.0)	3137.7 (a, 1.3)	2942.6 (b ₂ , 10.1)	3143.8 (b ₂ , 0.8)
3181.7 (a ₂ , 0.0)	3149.9 (a, 2.0)	3155.7 (b ₁ , 0.0)	3145.4 (b ₁ , 0.6)
3183.0 (b ₁ , 1.9)	3154.2 (a, 3.5)	3156.0 (a ₂ , 0.0)	3145.6 (a ₁ , 0.1)

3189.4 (b ₂ , 0.1)	3171.6 (a, 5.1)	3161.2 (b ₂ , 0.0)	3155.2 (a ₂ , 0.0)
3194.6 (a ₁ , 11.0)	3173.8 (a, 0.2)	3162.6 (a ₁ , 0.1)	3155.6 (b ₂ , 3.5)
3202.6 (b ₁ , 1.3)	3179.7 (a, 0.2)	3169.9 (a ₂ , 0.0)	3157.4 (b ₁ , 0.2)
3203.2 (a ₂ , 0.0)	3188.0 (a, 0.1)	3170.8 (b ₁ , 2.5)	3157.6 (a ₁ , 0.6)
3211.9 (b ₂ , 0.0)	3192.2 (a, 0.2)	3176.6 (b ₂ , 1.8)	3166.5 (b ₁ , 6.2)
3212.5 (a ₁ , 0.2)	3199.9 (a, 0.1)	3177.1 (a ₁ , 2.4)	3166.8 (a ₁ , 0.6)

Table S3. Theoretical harmonic vibrational frequencies (in cm^{-1}) for $\text{Cp}_2\text{Re}_2(\text{CO})_4$ using the BP86/SDD method (infrared intensities in parentheses are in km/mol).

4S-1 (C_i)	4S-2(C_{2h})	4S-3 (C_2)	4S-4 (C_s)
8.9 (a_u , 2.9)	13.2i (b_g , 0.0)	32.6 (a, 1.8)	2.5i (a'' , 0.1)
18.1 (a_u , 0.5)	13.1 (a_u , 0.7)	33.6 (b, 0.1)	17.7 (a' , 0.4)
30.0 (a_g , 0.0)	29.7 (b_g , 0.0)	44.4 (a, 0.0)	26.9 (a'' , 0.0)
58.2 (a_u , 1.6)	37.6 (a_u , 0.2)	51.8 (b, 1.0)	54.3 (a' , 3.3)
67.7 (a_u , 2.0)	83.3 (a_u , 0.7)	63.7 (a, 0.7)	64.1 (a'' , 1.0)
72.3 (a_g , 0.0)	86.2 (b_u , 0.9)	68.8 (b, 0.2)	73.5 (a' , 0.2)
78.3 (a_g , 0.0)	89.2 (a_g , 0.0)	82.8 (b, 1.0)	90.0 (a' , 0.0)
92.0 (a_g , 0.0)	94.9 (a_u , 0.7)	82.8 (a, 0.1)	98.0 (a' , 0.0)
96.2 (a_u , 1.0)	99.0 (b_u , 1.3)	95.7 (a, 0.0)	102.9 (a'' , 0.6)
104.5 (a_u , 1.3)	103.0 (b_g , 0.0)	104.6 (b, 0.7)	113.5 (a' , 0.4)
108.9 (a_g , 0.0)	105.8 (a_g , 0.0)	109.8 (a, 0.2)	122.4 (a'' , 0.0)
135.4 (a_g , 0.0)	112.5 (b_u , 5.9)	140.0 (a, 0.0)	166.6 (a' , 0.5)
139.5 (a_u , 0.5)	125.9 (a_g , 0.0)	145.9 (b, 1.2)	185.1 (a'' , 6.7)
157.7 (a_g , 0.0)	181.7 (a_g , 0.0)	160.1 (a, 0.2)	224.4 (a'' , 0.5)
274.4 (a_u , 7.8)	283.2 (b_u , 3.1)	275.5 (b, 1.9)	265.5 (a'' , 0.1)
278.5 (a_g , 0.0)	287.8 (a_g , 0.0)	282.5 (a, 5.9)	301.4 (a' , 4.9)
321.2 (a_g , 0.0)	293.8 (a_u , 10.7)	320.5 (a, 0.8)	307.3 (a'' , 0.3)
329.0 (a_u , 3.2)	298.6 (b_g , 0.0)	330.2 (b, 3.9)	310.4 (a' , 8.3)
339.1 (a_u , 5.1)	303.1 (a_g , 0.0)	345.4 (b, 0.6)	323.1 (a'' , 15.7)
347.4 (a_g , 0.0)	304.0 (b_u , 0.9)	354.8 (a, 0.6)	358.6 (a'' , 0.5)
394.3 (a_u , 16.8)	416.3 (b_g , 0.0)	385.7 (b, 11.1)	359.6 (a' , 7.0)
402.2 (a_g , 0.0)	463.4 (a_u , 6.5)	407.0 (a, 1.3)	417.0 (a' , 3.3)
480.9 (a_g , 0.0)	488.8 (a_u , 22.4)	481.4 (b, 7.3)	427.5 (a'' , 3.6)
486.3 (a_u , 22.6)	489.0 (b_g , 0.0)	483.1 (a, 6.3)	436.0 (a' , 4.7)
510.4 (a_g , 0.0)	511.2 (b_u , 158.5)	498.9 (b, 10.9)	454.9 (a' , 3.2)
511.4 (a_u , 0.9)	519.7 (b_g , 0.0)	512.7 (b, 19.8)	476.9 (a' , 5.0)
530.6 (a_u , 29.8)	522.6 (a_g , 0.0)	513.5 (a, 3.0)	482.6 (a' , 3.7)
530.6 (a_g , 0.0)	525.1 (a_u , 12.1)	519.5 (a, 1.0)	482.9 (a'' , 68.6)
534.9 (a_g , 0.0)	538.1 (b_u , 1.4)	540.2 (b, 72.5)	522.8 (a' , 7.5)
545.0 (a_u , 74.0)	547.0 (a_g , 0.0)	547.7 (a, 1.9)	523.3 (a'' , 0.4)
567.7 (a_g , 0.0)	557.4 (b_u , 2.4)	558.7 (b, 10.6)	553.9 (a'' , 79.6)
570.9 (a_g , 0.0)	561.5 (a_g , 0.0)	568.0 (a, 0.5)	559.4 (a' , 0.6)
571.1 (a_u , 0.3)	573.4 (b_g , 0.0)	572.3 (a, 0.5)	566.5 (a' , 2.8)
573.3 (a_u , 20.2)	575.1 (a_u , 0.1)	573.3 (b, 7.5)	569.4 (a'' , 4.1)
590.1 (a_u , 17.7)	598.3 (b_u , 23.2)	577.1 (b, 2.7)	577.0 (a'' , 33.7)
592.1 (a_g , 0.0)	603.6 (a_g , 0.0)	585.5 (a, 10.6)	583.8 (a' , 9.5)
785.6 (a_g , 0.0)	789.5 (b_u , 45.1)	738.7 (b, 26.1)	770.0 (a'' , 22.5)
787.2 (a_u , 70.5)	791.7 (a_g , 0.0)	757.3 (a, 29.8)	780.9 (a' , 30.5)
792.1 (a_g , 0.0)	801.2 (b_u , 146.2)	795.5 (a, 12.4)	797.4 (a'' , 45.7)
792.5 (a_u , 63.0)	802.7 (a_g , 0.0)	796.1 (b, 33.0)	799.0 (a' , 13.8)

803.0 (a _g , 0.0)	809.6 (a _g , 0.0)	801.8 (b, 2.0)	803.4 (a', 0.0)
803.4 (a _u , 7.6)	809.7 (b _u , 22.0)	804.0 (a, 0.0)	803.7 (a'', 3.8)
807.8 (a _g , 0.0)	811.7 (b _g , 0.0)	805.7 (b, 10.3)	810.5 (a'', 8.6)
811.7 (a _u , 9.6)	815.1 (a _u , 3.1)	809.2 (a, 9.4)	813.0 (a', 7.9)
817.9 (a _g , 0.0)	822.6 (b _g , 0.0)	824.7 (b, 14.7)	820.4 (a'', 0.5)
818.1 (a _u , 7.7)	824.1 (a _u , 6.8)	825.2 (a, 1.9)	820.5 (a', 1.3)
875.7 (a _u , 7.2)	867.4 (b _u , 1.9)	871.1 (a, 0.1)	865.9 (a'', 0.0)
876.4 (a _g , 0.0)	868.9 (a _g , 0.0)	872.1 (b, 3.2)	866.5 (a', 0.7)
885.2 (a _u , 5.3)	881.2 (b _g , 0.0)	878.7 (b, 6.4)	879.4 (a'', 1.9)
885.4 (a _g , 0.0)	881.8 (a _u , 1.5)	879.6 (a, 3.9)	882.9 (a', 4.1)
976.0 (a _g , 0.0)	987.9 (b _g , 0.0)	974.6 (b, 15.7)	979.5 (a'', 0.1)
976.3 (a _u , 16.6)	988.4 (a _u , 15.3)	977.0 (a, 2.3)	981.4 (a', 17.8)
995.9 (a _g , 0.0)	997.6 (b _u , 14.4)	994.5 (b, 9.4)	987.6 (a'', 5.3)
996.2 (a _u , 13.0)	998.0 (a _g , 0.0)	994.6 (a, 6.5)	989.2 (a', 8.8)
1039.1 (a _u , 0.6)	1043.5 (b _g , 0.0)	1037.6 (b, 0.9)	1035.0 (a'', 0.6)
1039.3 (a _g , 0.0)	1044.3 (a _u , 0.1)	1038.7 (a, 0.6)	1037.1 (a', 2.6)
1040.7 (a _u , 1.6)	1045.5 (b _u , 1.4)	1040.3 (b, 2.3)	1039.9 (a'', 0.5)
1041.7 (a _g , 0.0)	1048.2 (a _g , 0.0)	1041.3 (a, 0.2)	1040.6 (a', 0.3)
1094.8 (a _g , 0.0)	1101.5 (a _g , 0.0)	1092.5 (b, 6.7)	1093.4 (a'', 10.5)
1094.9 (a _u , 5.5)	1101.5 (b _u , 1.1)	1093.0 (a, 5.1)	1094.0 (a', 4.4)
1224.7 (a _g , 0.0)	1229.2 (b _g , 0.0)	1223.5 (b, 0.0)	1221.6 (a'', 0.0)
1224.7 (a _u , 0.0)	1229.2 (a _u , 0.0)	1224.4 (a, 0.0)	1222.3 (a', 0.0)
1345.4 (a _u , 11.1)	1349.6 (b _u , 15.9)	1345.0 (b, 9.3)	1349.1 (a', 0.6)
1347.2 (a _g , 0.0)	1355.7 (a _g , 0.0)	1348.2 (a, 6.1)	1349.9 (a'', 9.7)
1353.0 (a _u , 1.3)	1358.6 (a _u , 0.2)	1353.4 (a, 0.6)	1356.1 (a', 1.7)
1354.4 (a _g , 0.0)	1358.7 (b _g , 0.0)	1353.9 (b, 1.4)	1356.5 (a'', 0.0)
1392.1 (a _g , 0.0)	1398.2 (b _g , 0.0)	1390.7 (b, 4.6)	1392.6 (a'', 0.1)
1392.5 (a _u , 7.9)	1399.1 (a _u , 13.1)	1391.0 (a, 0.8)	1392.9 (a', 2.7)
1414.5 (a _u , 6.3)	1416.7 (b _u , 6.8)	1411.3 (b, 5.9)	1401.2 (a'', 2.9)
1414.9 (a _g , 0.0)	1417.0 (a _g , 0.0)	1411.9 (a, 0.5)	1401.9 (a', 4.6)
1832.7 (a _g , 0.0)	1873.9 (b _g , 0.0)	1816.6 (a, 82.1)	1732.2 (a', 473.3)
1844.5(a _u ,1036.7)	1895.9(a _u ,1517.0)	1829.6 (b, 925.7)	1755.5 (a', 618.0)
1907.9(a _u ,1735.7)	1935.1(b _u ,1626.9)	1908.3 (b, 351.3)	1900.6 (a'', 451.8)
1927.0 (a _g , 0.0)	1962.4 (a _g , 0.0)	1948.9 (a, 1399.5)	1950.0(a', 1333.2)
3174.4 (a _g , 0.0)	3174.6 (b _u , 0.5)	3172.2 (b, 0.1)	3175.4 (a'', 0.1)
3174.6 (a _u , 0.9)	3174.6 (a _g , 0.0)	3172.2 (a, 0.1)	3175.6 (a', 0.1)
3175.8 (a _g , 0.0)	3177.5 (b _g , 0.0)	3174.0 (b, 0.4)	3175.8 (a'', 0.9)
3175.9 (a _u , 0.2)	3177.6 (a _u , 1.2)	3174.0 (a, 0.1)	3175.9 (a', 0.1)
3186.2 (a _g , 0.0)	3189.7 (b _g , 0.0)	3184.5 (b, 2.0)	3186.1 (a'', 0.3)
3186.2 (a _u , 1.0)	3189.9 (a _u , 0.1)	3184.6 (a, 0.0)	3186.2 (a', 0.1)
3190.2 (a _u , 0.5)	3192.3 (b _u , 0.4)	3191.6 (b, 0.4)	3190.5 (a'', 0.1)
3190.3 (a _g , 0.0)	3192.4 (a _g , 0.0)	3191.6 (a, 0.0)	3190.8 (a', 0.2)
3197.5 (a _u , 0.2)	3201.7 (b _u , 1.2)	3198.2 (b, 0.2)	3197.8 (a'', 0.0)
3197.5 (a _g , 0.0)	3201.9 (a _g , 0.0)	3198.3 (a, 1.2)	3198.1 (a', 0.6)

Table S4. Theoretical harmonic vibrational frequencies (in cm^{-1}) for $\text{Cp}_2\text{Re}_2(\text{CO})_4$ using the BP86/SDD method (infrared intensities in parentheses are in km/mol).

4S-5 (C_s)	4S-6 (C_1)	4S-7 (C_s)	4S-8 (C_i)
18.7 (a", 0.0)	36.0 (a, 0.2)	53.1i (a", 1.3)	37.0 (a_u , 1.5)
46.5 (a', 0.4)	48.5 (a, 0.3)	15.3i (a", 0.8)	50.7 (a_g , 0.0)
58.2 (a", 0.3)	57.1 (a, 0.2)	19.5 (a", 0.6)	69.8 (a_u , 0.3)
70.8 (a", 0.0)	69.9 (a, 0.7)	67.5 (a", 0.5)	74.6 (a_g , 0.0)
74.5 (a', 0.9)	76.6 (a, 0.8)	73.1 (a', 0.0)	80.7 (a_u , 0.7)
81.6 (a", 0.1)	84.7 (a, 0.0)	94.4 (a', 0.9)	87.8 (a_g , 0.0)
82.6 (a', 0.4)	89.8 (a, 0.1)	99.6 (a", 0.0)	89.5 (a_g , 0.0)
91.2 (a', 0.1)	92.9 (a, 0.6)	103.5 (a', 0.7)	91.3 (a_u , 1.8)
96.9 (a", 0.1)	97.1 (a, 0.1)	105.5 (a", 0.4)	114.8 (a_u , 5.3)
105.9 (a', 0.8)	103.6 (a, 0.4)	108.3 (a', 1.7)	119.8 (a_g , 0.0)
136.3 (a", 2.2)	113.4 (a, 1.0)	118.0 (a", 0.0)	124.1 (a_u , 2.8)
139.8 (a", 1.0)	128.2 (a, 2.4)	137.6 (a', 3.9)	154.8 (a_g , 0.0)
153.7 (a', 9.8)	151.1 (a, 5.3)	166.4 (a', 0.2)	159.0 (a_g , 0.0)
189.9 (a', 5.9)	163.9 (a, 2.9)	255.4 (a', 9.2)	191.4 (a_u , 26.6)
330.3 (a', 11.2)	180.5 (a, 0.4)	281.5 (a', 2.2)	242.2 (a_u , 12.7)
338.8 (a', 10.8)	220.5 (a, 6.5)	300.4 (a", 6.3)	284.3 (a_g , 0.0)
361.4 (a', 2.8)	271.1 (a, 2.1)	340.7 (a', 23.0)	298.0 (a_g , 0.0)
367.7 (a", 2.1)	319.3 (a, 0.6)	351.7 (a', 2.4)	317.0 (a_u , 5.8)
378.4 (a", 2.1)	334.7 (a, 0.9)	364.1 (a", 4.4)	398.7 (a_g , 0.0)
396.5 (a", 2.1)	351.2 (a, 2.9)	369.7 (a', 45.7)	420.6 (a_u , 11.4)
401.6 (a", 21.9)	421.9 (a, 1.2)	387.6 (a', 63.2)	448.3 (a_g , 0.0)
405.3 (a", 6.5)	446.6 (a, 1.3)	411.8 (a", 0.3)	449.9 (a_u , 20.8)
414.3 (a', 19.6)	460.4 (a, 4.0)	436.9 (a", 4.0)	476.6 (a_g , 0.0)
440.4 (a', 5.3)	498.0 (a, 1.8)	446.4 (a', 9.2)	477.1 (a_u , 20.8)
460.5 (a', 0.0)	502.5 (a, 24.6)	468.2 (a", 5.1)	492.5 (a_u , 22.5)
485.6 (a', 3.0)	509.5 (a, 12.7)	501.9 (a", 20.0)	492.5 (a_g , 0.0)
503.7 (a', 30.4)	519.3 (a, 11.7)	504.7 (a', 40.2)	524.8 (a_u , 33.9)
511.6 (a", 11.8)	533.5 (a, 9.0)	522.6 (a', 16.3)	527.4 (a_g , 0.0)
516.5 (a', 42.2)	547.0 (a, 4.7)	536.1 (a", 1.5)	527.5 (a_u , 31.0)
543.0 (a", 0.2)	557.3 (a, 1.2)	551.2 (a', 47.8)	542.1 (a_g , 0.0)
545.0 (a', 18.8)	559.5 (a, 6.7)	557.6 (a", 0.0)	590.1 (a_g , 0.0)
563.3 (a', 2.0)	580.9 (a, 1.3)	563.2 (a', 32.0)	590.6 (a_u , 16.4)
565.1 (a", 0.0)	588.0 (a, 5.1)	571.7 (a', 4.4)	596.1 (a_g , 0.0)
575.9 (a", 18.8)	589.1 (a, 10.0)	575.3 (a", 0.1)	602.9 (a_u , 8.5)
581.0 (a', 30.4)	606.9 (a, 5.2)	581.3 (a', 22.6)	635.1 (a_g , 0.0)
598.7 (a', 62.6)	608.6 (a, 15.6)	627.0 (a', 107.1)	641.5 (a_u , 4.7)
719.5 (a", 0.6)	698.1 (a, 69.9)	786.4 (a", 6.1)	742.6 (a_u , 2.7)
734.0 (a', 7.8)	765.6 (a, 9.0)	790.6 (a', 42.4)	742.7 (a_g , 0.0)
774.0 (a", 9.2)	774.0 (a, 46.3)	790.8 (a', 4.0)	771.5 (a_u , 6.2)
782.8 (a', 11.0)	784.0 (a, 5.7)	803.7 (a", 0.3)	780.2 (a_g , 0.0)

788.0 (a', 24.0)	789.1 (a, 5.4)	807.3 (a', 15.0)	797.2 (a _u , 15.2)
793.5 (a'', 0.0)	801.7 (a, 4.5)	812.7 (a', 18.6)	800.7 (a _g , 0.0)
796.3 (a', 4.5)	810.3 (a, 1.6)	816.4 (a'', 0.1)	816.0 (a _u , 23.6)
802.9 (a'', 1.7)	818.9 (a, 23.5)	818.2 (a'', 2.3)	827.8 (a _g , 0.0)
804.6 (a', 3.9)	820.8 (a, 13.8)	819.3 (a', 32.0)	845.2 (a _u , 6.4)
828.6 (a', 12.7)	853.7 (a, 1.0)	824.5 (a', 8.6)	846.8 (a _g , 0.0)
838.3 (a'', 0.2)	857.7 (a, 64.1)	856.5 (a'', 3.0)	876.2 (a _u , 5.4)
854.2 (a'', 0.3)	860.2 (a, 5.7)	856.8 (a', 28.8)	881.1 (a _g , 0.0)
860.7 (a', 8.5)	868.7 (a, 1.4)	881.4 (a'', 1.1)	905.1 (a _u , 14.6)
905.8 (a'', 5.1)	898.6 (a, 19.4)	887.1 (a', 5.0)	913.7 (a _g , 0.0)
942.3 (a', 8.2)	943.8 (a, 0.5)	968.4 (a', 5.6)	942.8 (a _g , 0.0)
970.0 (a', 8.1)	976.1 (a, 6.2)	984.4 (a', 3.8)	951.7 (a _u , 7.7)
977.7 (a'', 7.8)	979.7 (a, 3.5)	987.6 (a'', 14.8)	955.7 (a _g , 0.0)
1008.0 (a'', 12.3)	991.8 (a, 3.3)	998.8 (a'', 8.4)	961.4 (a _u , 0.6)
1020.2 (a', 4.9)	1006.6 (a, 1.0)	1038.9 (a'', 0.0)	1011.2 (a _u , 2.6)
1026.0 (a', 7.6)	1035.1 (a, 1.6)	1039.8 (a', 0.6)	1012.1 (a _g , 0.0)
1033.6 (a', 2.2)	1038.6 (a, 4.5)	1046.8 (a'', 0.8)	1032.9 (a _g , 0.0)
1037.6 (a'', 0.4)	1040.1 (a, 1.3)	1048.2 (a', 5.0)	1033.3 (a _u , 2.9)
1069.6 (a', 26.1)	1088.1 (a, 5.6)	1087.4 (a', 17.5)	1056.5 (a _u , 10.8)
1083.0 (a', 18.0)	1093.8 (a, 3.0)	1099.6 (a', 2.5)	1062.6 (a _g , 0.0)
1181.4 (a'', 0.0)	1196.4 (a, 2.0)	1220.1 (a'', 0.0)	1205.8 (a _u , 2.8)
1214.8 (a'', 0.0)	1220.8 (a, 0.0)	1226.2 (a'', 0.1)	1206.4 (a _g , 0.0)
1297.1 (a'', 0.2)	1287.9 (a, 6.7)	1347.5 (a'', 0.0)	1262.8 (a _u , 6.2)
1331.2 (a', 3.3)	1334.5 (a, 5.5)	1356.1 (a', 7.3)	1266.7 (a _g , 0.0)
1343.0 (a', 0.6)	1348.4 (a, 0.9)	1358.0 (a', 1.7)	1283.2 (a _g , 0.0)
1357.3 (a'', 0.5)	1351.2 (a, 4.3)	1361.5 (a'', 1.6)	1286.2 (a _u , 25.8)
1359.8 (a', 2.1)	1376.4 (a, 2.8)	1378.4 (a', 2.3)	1358.1 (a _g , 0.0)
1378.7 (a'', 1.4)	1390.6 (a, 5.0)	1395.0 (a'', 0.7)	1363.7 (a _u , 5.5)
1380.0 (a', 3.2)	1422.1 (a, 2.5)	1403.4 (a', 3.7)	1378.5 (a _u , 1.3)
1390.5 (a'', 1.1)	1496.5 (a, 7.0)	1411.1 (a'', 4.0)	1379.2 (a _g , 0.0)
1936.9 (a', 984.3)	1894.0 (a, 295.5)	1740.6 (a', 421.5)	1909.2 (a _g , 0.0)
1951.0(a'',1363.5)	1921.1 (a, 1461.2)	1885.7 (a', 761.4)	1910.9(a _u ,1773.1)
1955.6 (a', 494.8)	1925.2 (a, 902.8)	1942.8 (a'', 910.4)	1964.5(a _u ,2332.3)
2032.9 (a', 509.7)	2001.4 (a, 776.0)	1989.2 (a', 872.7)	1982.1 (a _g , 0.0)
2680.5 (a', 3.5)	2823.4 (a, 5.5)	3173.2 (a'', 0.2)	3084.4 (a _u , 27.6)
3166.7 (a'', 0.0)	3146.6 (a, 1.0)	3175.2 (a', 0.3)	3084.5 (a _g , 0.0)
3167.9 (a'', 2.0)	3155.7 (a, 2.2)	3175.4 (a', 0.3)	3138.2 (a _u , 0.7)
3175.8 (a', 0.0)	3171.6 (a, 0.4)	3179.3 (a'', 0.1)	3138.4 (a _g , 0.0)
3177.1 (a', 7.3)	3172.1 (a, 2.6)	3184.5 (a'', 0.0)	3151.5 (a _u , 0.8)
3187.0 (a'', 0.4)	3177.7 (a, 3.2)	3185.1 (a', 0.0)	3151.5 (a _g , 0.0)
3189.1 (a', 1.4)	3178.5 (a, 0.4)	3192.4 (a', 0.5)	3155.8 (a _g , 0.0)
3189.6 (a'', 1.4)	3185.6 (a, 0.4)	3193.7 (a', 0.4)	3155.9 (a _u , 5.5)
3190.3 (a', 2.9)	3192.5 (a, 0.3)	3209.4 (a'', 0.4)	3171.9 (a _u , 4.7)
3208.5 (a', 0.3)	3201.9 (a, 0.1)	3219.2 (a', 0.9)	3172.1 (a _g , 0.0)

Table S5. Theoretical harmonic vibrational frequencies (in cm^{-1}) for $\text{Cp}_2\text{Re}_2(\text{CO})_4$ using the BP86/SDD method (infrared intensities in parentheses are in km/mol).

4T-1 (C_{2h})	4T-2(C_{2h})	4T-3 (C_{2v})	4T-4 (C_s)
18.0 (a_u , 0.1)	20.1 (a_u , 1.5)	31.1 (a_2 , 0.0)	12.0 (a'' , 0.1)
20.8 (b_u , 3.5)	35.6 (b_g , 0.0)	36.0 (b_1 , 0.0)	41.8 (a'' , 0.0)
23.6 (b_g , 0.0)	38.6 (a_u , 0.1)	44.9 (a_1 , 2.3)	44.2 (a' , 0.3)
57.0 (a_u , 1.7)	49.5 (a_g , 0.0)	45.3 (a_2 , 0.0)	58.3 (a' , 0.1)
79.2 (a_g , 0.0)	55.0 (b_g , 0.0)	66.4 (b_2 , 0.9)	64.1 (a'' , 0.2)
84.4 (a_u , 0.0)	68.0 (b_u , 1.4)	83.9 (b_1 , 0.0)	69.4 (a'' , 0.5)
85.5 (b_u , 0.7)	68.1 (a_u , 0.3)	90.5 (a_1 , 0.1)	72.9 (a' , 0.0)
87.2 (b_g , 0.0)	83.7 (a_u , 0.3)	93.8 (b_1 , 0.4)	79.5 (a' , 0.6)
90.7 (b_u , 1.0)	86.9 (b_u , 1.7)	94.5 (a_1 , 0.3)	81.8 (a'' , 0.0)
96.6 (a_g , 0.0)	87.4 (b_g , 0.0)	95.7 (b_2 , 1.9)	89.9 (a' , 0.4)
110.0 (b_g , 0.0)	92.0 (a_g , 0.0)	111.8 (a_2 , 0.0)	92.7 (a'' , 0.0)
172.4 (b_g , 0.0)	93.8 (a_g , 0.0)	179.1 (a_1 , 0.2)	104.1 (a' , 0.5)
181.0 (a_g , 0.0)	94.1 (b_u , 1.5)	211.6 (b_2 , 0.3)	123.1 (a' , 2.1)
206.7 (b_u , 0.7)	163.7 (a_g , 0.0)	219.5 (a_2 , 0.0)	157.3 (a' , 13.0)
254.9 (b_g , 0.0)	266.4 (b_u , 5.3)	278.4 (a_2 , 0.0)	282.3 (a' , 7.2)
291.6 (b_u , 2.3)	268.7 (a_g , 0.0)	296.7 (b_2 , 0.1)	307.3 (a' , 0.8)
298.2 (a_g , 0.0)	281.3 (a_g , 0.0)	301.9 (a_1 , 2.1)	337.1 (a'' , 6.7)
303.1 (a_u , 11.9)	282.6 (b_u , 0.1)	302.6 (b_1 , 12.4)	347.5 (a'' , 0.0)
310.7 (b_g , 0.0)	301.7 (a_u , 7.5)	307.6 (a_2 , 0.0)	364.2 (a'' , 0.2)
330.4 (b_u , 4.4)	308.0 (b_g , 0.0)	334.5 (b_2 , 3.6)	365.9 (a'' , 0.3)
337.8 (a_g , 0.0)	421.6 (b_g , 0.0)	340.2 (a_1 , 2.2)	366.3 (a' , 9.3)
427.3 (b_u , 33.5)	441.7 (a_u , 1.1)	428.9 (b_1 , 2.7)	376.8 (a'' , 0.0)
433.2 (a_g , 0.0)	465.8 (b_u , 50.5)	436.9 (a_1 , 3.7)	401.8 (a' , 5.6)
445.5 (a_u , 0.1)	478.9 (a_u , 18.1)	454.4 (b_1 , 0.6)	414.5 (a' , 4.0)
446.4 (b_g , 0.0)	479.6 (b_g , 0.0)	463.4 (b_2 , 20.7)	467.0 (a' , 0.2)
477.3 (b_u , 15.2)	482.6 (a_g , 0.0)	477.2 (a_2 , 0.0)	482.6 (a'' , 0.2)
491.0 (a_g , 0.0)	500.9 (b_u , 40.9)	478.6 (a_1 , 0.3)	493.6 (a' , 6.6)
495.5 (a_u , 7.0)	510.6 (a_u , 17.3)	491.2 (a_1 , 1.5)	501.6 (a'' , 0.2)
507.9 (b_u , 42.5)	510.8 (a_g , 0.0)	496.3 (b_2 , 19.1)	504.6 (a' , 32.5)
514.2 (a_g , 0.0)	515.7 (b_g , 0.0)	541.1 (a_1 , 11.9)	515.7 (a' , 3.8)
562.8 (b_u , 2.1)	564.0 (a_u , 0.0)	550.3 (b_2 , 189.8)	528.3 (a'' , 21.2)
563.6 (a_g , 0.0)	564.2 (b_g , 0.0)	563.5 (b_2 , 5.9)	537.5 (a'' , 0.1)
566.5 (b_g , 0.0)	567.3 (b_u , 12.7)	565.0 (a_1 , 5.0)	555.0 (a' , 0.1)
566.5 (a_u , 0.1)	569.3 (a_g , 0.0)	566.0 (a_2 , 0.0)	559.3 (a' , 2.1)
577.5 (b_u , 163.2)	579.6 (b_u , 15.1)	568.0 (b_1 , 1.1)	560.1 (a'' , 0.4)
586.7 (b_g , 0.0)	590.5 (a_g , 0.0)	579.9 (b_1 , 3.5)	579.5 (a' , 70.7)
787.2 (b_u , 79.6)	774.3 (b_u , 137.5)	770.9 (b_2 , 17.9)	751.4 (a'' , 15.0)
787.9 (a_g , 0.0)	774.5 (a_g , 0.0)	776.5 (a_1 , 31.7)	772.4 (a' , 3.8)
795.2 (b_u , 56.6)	778.2 (a_u , 6.2)	793.5 (b_2 , 64.2)	779.1 (a'' , 0.6)
796.1 (a_g , 0.0)	778.4 (b_g , 0.0)	794.9 (a_1 , 14.2)	785.7 (a'' , 37.0)

805.6 (b _g , 0.0)	791.2 (b _u , 42.1)	804.1 (a ₂ , 0.0)	804.6 (a', 2.2)
805.8 (a _u , 4.7)	793.1 (a _g , 0.0)	805.0 (b ₁ , 5.2)	807.5 (a', 4.2)
809.7 (a _u , 0.0)	810.5 (b _u , 5.6)	810.1 (a ₂ , 0.0)	808.5 (a'', 22.6)
810.4 (b _u , 20.6)	812.6 (a _g , 0.0)	810.3 (b ₁ , 0.6)	811.7 (a'', 18.1)
810.7 (b _g , 0.0)	813.5 (a _u , 0.0)	810.5 (b ₂ , 12.8)	817.8 (a', 14.8)
812.3 (a _g , 0.0)	814.1 (b _g , 0.0)	813.0 (a ₁ , 8.5)	822.2 (a', 7.1)
867.5 (a _u , 2.2)	859.8 (b _u , 7.5)	867.3 (a ₂ , 0.0)	843.0 (a'', 2.7)
867.9 (b _g , 0.0)	860.0 (b _g , 0.0)	868.2 (b ₁ , 4.6)	852.6 (a', 7.6)
871.3 (b _u , 0.9)	860.5 (a _u , 0.3)	869.2 (b ₂ , 0.9)	858.5 (a'', 7.8)
871.8 (a _g , 0.0)	861.4 (a _g , 0.0)	870.0 (a ₁ , 1.8)	863.5 (a', 2.6)
979.4 (b _u , 14.8)	983.0 (a _u , 17.5)	981.1 (b ₂ , 5.3)	967.8 (a'', 0.1)
980.0 (a _g , 0.0)	983.1 (b _g , 0.0)	982.1 (a ₁ , 10.9)	970.6 (a', 3.3)
990.4 (a _u , 16.4)	992.9 (b _u , 14.7)	990.9 (a ₂ , 0.0)	978.1 (a'', 0.7)
990.7 (b _g , 0.0)	992.9 (a _g , 0.0)	991.8 (b ₁ , 15.1)	988.7 (a', 13.1)
1038.4 (b _u , 0.5)	1038.5 (a _u , 2.5)	1040.6 (a ₂ , 0.0)	1026.7 (a'', 0.1)
1039.1 (a _g , 0.0)	1039.0 (b _g , 0.0)	1040.9 (b ₂ , 0.0)	1035.0 (a', 1.3)
1040.9 (a _u , 0.1)	1042.3 (b _u , 1.2)	1042.3 (a ₁ , 0.7)	1037.5 (a'', 0.1)
1042.3 (b _g , 0.0)	1042.7 (a _g , 0.0)	1044.2 (b ₁ , 1.2)	1037.7 (a', 2.1)
1092.2 (b _u , 7.6)	1098.3 (a _g , 0.0)	1093.1 (b ₂ , 5.8)	1083.0 (a', 8.5)
1092.2 (a _g , 0.0)	1098.6 (b _u , 4.0)	1093.5 (a ₁ , 3.2)	1085.3 (a'', 15.4)
1223.3 (b _g , 0.0)	1223.3 (a _u , 0.0)	1224.5 (a ₂ , 0.0)	1217.5 (a'', 0.0)
1223.4 (a _u , 0.0)	1223.3 (b _g , 0.0)	1224.8 (b ₁ , 0.0)	1218.5 (a', 0.1)
1345.7 (b _u , 2.1)	1349.4 (b _g , 0.0)	1347.5 (b ₂ , 0.2)	1334.6 (a'', 0.0)
1346.6 (a _g , 0.0)	1349.8 (a _u , 2.4)	1348.8 (a ₁ , 2.1)	1346.6 (a', 0.4)
1348.2 (a _u , 0.0)	1358.5 (a _g , 0.0)	1351.1 (a ₂ , 0.0)	1347.6 (a'', 0.0)
1351.1 (b _g , 0.0)	1358.8 (b _u , 0.8)	1353.9 (b ₁ , 0.0)	1358.9 (a', 2.6)
1394.4 (b _u , 6.9)	1398.9 (a _u , 3.1)	1395.8 (b ₂ , 2.9)	1379.8 (a', 17.5)
1394.9 (a _g , 0.0)	1399.2 (b _g , 0.0)	1396.5 (a ₁ , 3.4)	1380.3 (a'', 1.1)
1401.7 (a _u , 6.5)	1410.8 (b _u , 3.4)	1403.6 (a ₂ , 0.0)	1397.0 (a', 7.9)
1401.8 (b _g , 0.0)	1411.4 (a _g , 0.0)	1404.1 (b ₁ , 6.4)	1397.6 (a'', 0.0)
1745.0 (a _g , 0.0)	1892.1 (b _g , 0.0)	1731.1 (b ₁ , 915.3)	1899.0(a', 1444.8)
1747.5 (a _u , 940.3)	1895.2(a _u ,1742.8)	1731.1 (a ₁ , 62.3)	1905.0(a'',1020.3)
1910.6(b _u ,1822.1)	1916.6(b _u ,1711.5)	1908.6 (b ₂ , 437.5)	1911.6 (a', 536.9)
1928.7 (a _g , 0.0)	1953.5 (a _g , 0.0)	1954.9 (a ₁ ,1320.7)	1979.7 (a', 807.4)
3173.3 (b _u , 1.2)	3172.7 (a _u , 0.2)	3173.1 (b ₂ , 1.4)	3169.9 (a'', 0.1)
3173.5 (a _g , 0.0)	3172.8 (b _g , 0.0)	3173.9 (a ₁ , 0.1)	3172.9 (a', 1.2)
3177.8 (a _u , 0.3)	3179.4 (b _u , 0.6)	3177.0 (b ₁ , 0.1)	3176.8 (a'', 0.0)
3177.8 (b _g , 0.0)	3179.5 (a _g , 0.0)	3177.1 (a ₂ , 0.0)	3177.8 (a', 2.7)
3186.9 (b _u , 0.5)	3188.2 (a _u , 0.3)	3186.7 (b ₂ , 0.2)	3186.0 (a'', 0.2)
3186.9 (a _g , 0.0)	3188.2 (b _g , 0.0)	3187.3 (a ₁ , 0.1)	3186.9 (a', 0.1)
3188.6 (a _u , 0.2)	3190.4 (b _u , 0.2)	3187.8 (a ₂ , 0.0)	3189.4 (a'', 0.3)
3188.6 (b _g , 0.0)	3190.5 (a _g , 0.0)	3187.8 (b ₁ , 0.2)	3190.2 (a', 2.2)
3198.0 (b _u , 0.1)	3204.4 (a _g , 0.0)	3197.1 (b ₂ , 0.0)	3202.6 (a'', 1.6)
3198.0 (a _g , 0.0)	3204.4 (b _u , 0.0)	3197.3 (a ₁ , 0.7)	3203.5 (a', 0.1)

Table S6. Theoretical harmonic vibrational frequencies (in cm^{-1}) for $\text{Cp}_2\text{Re}_2(\text{CO})_3$ using the BP86/SDD method (infrared intensities in parentheses are in km/mol).

3S-1 (C_{2v})	3S-2 (C_1)	3S-3 (C_1)	3T-1 (C_s)
29.5i (a ₂ , 0.0)	21.7 (a, 0.0)	27.1 (a, 0.6)	19.4i (a", 0.0)
27.5i (b ₁ , 0.0)	56.4 (a, 0.9)	34.3 (a, 0.2)	25.1 (a", 0.5)
80.1 (b ₁ , 2.4)	57.5 (a, 0.2)	46.4 (a, 3.1)	32.2 (a', 2.3)
82.8 (a ₁ , 2.2)	67.0 (a, 0.1)	67.0 (a, 0.4)	64.9 (a", 0.2)
95.4 (a ₁ , 1.5)	86.0 (a, 0.1)	71.2 (a, 2.1)	66.7 (a', 0.8)
96.8 (b ₁ , 0.8)	88.9 (a, 0.4)	83.7 (a, 0.2)	74.5 (a", 0.4)
110.6 (a ₂ , 0.0)	91.8 (a, 0.2)	86.0 (a, 0.8)	94.5 (a', 0.7)
110.6 (b ₂ , 0.0)	94.9 (a, 0.6)	100.6 (a, 0.9)	103.3 (a", 0.0)
181.7 (a ₂ , 0.0)	102.9 (a, 0.6)	112.5 (a, 0.5)	105.2 (a', 0.9)
185.5 (b ₂ , 0.0)	137.1 (a, 5.4)	129.3 (a, 0.7)	187.8 (a', 0.9)
191.0 (b ₂ , 0.2)	162.7 (a, 0.2)	175.0 (a, 3.1)	206.8 (a', 1.5)
226.3 (a ₁ , 0.0)	185.1 (a, 13.9)	204.4 (a, 4.4)	231.3 (a", 1.4)
318.4 (b ₂ , 16.7)	325.5 (a, 3.2)	300.5 (a, 6.9)	282.2 (a", 7.4)
344.2 (b ₂ , 0.0)	348.3 (a, 14.3)	310.9 (a, 5.8)	299.5 (a', 1.1)
350.7 (b ₁ , 13.8)	361.9 (a, 1.1)	321.4 (a, 10.5)	310.0 (a", 9.8)
353.7 (a ₁ , 0.0)	369.8 (a, 4.0)	345.7 (a, 5.6)	315.4 (a', 0.2)
354.6 (a ₂ , 0.0)	378.3 (a, 10.9)	354.5 (a, 6.8)	337.0 (a', 2.1)
361.9 (a ₁ , 15.2)	400.9 (a, 9.4)	369.9 (a, 5.9)	347.0 (a', 4.4)
403.5 (a ₂ , 0.0)	422.1 (a, 0.3)	379.4 (a, 15.7)	387.1 (a", 0.9)
415.0 (b ₂ , 0.0)	442.7 (a, 3.3)	455.5 (a, 9.4)	435.0 (a", 1.9)
415.2 (b ₁ , 0.0)	453.1 (a, 2.4)	463.8 (a, 45.8)	452.3 (a', 6.3)
464.1 (a ₁ , 0.0)	503.7 (a, 8.7)	470.0 (a, 28.9)	473.0 (a', 18.5)
479.6 (b ₁ , 6.6)	514.1 (a, 13.1)	477.1 (a, 14.3)	475.3 (a", 1.0)
480.4 (a ₁ , 7.3)	528.9 (a, 13.9)	489.6 (a, 20.4)	496.1 (a', 10.0)
550.6 (b ₂ , 55.5)	539.7 (a, 0.2)	516.2 (a, 28.7)	501.3 (a", 3.5)
554.2 (b ₁ , 2.0)	551.1 (a, 0.3)	536.1 (a, 30.7)	540.5 (a', 4.6)
555.5 (a ₁ , 2.3)	562.1 (a, 1.4)	552.9 (a, 1.7)	547.2 (a', 38.4)
566.1 (a ₂ , 0.0)	563.7 (a, 0.6)	557.9 (a, 5.3)	551.9 (a", 0.1)
569.6 (a ₁ , 1.4)	578.9 (a, 8.3)	565.2 (a, 4.3)	564.6 (a", 0.1)
571.8 (b ₁ , 0.6)	590.6 (a, 20.5)	571.1 (a, 13.9)	566.4 (a', 0.4)
573.6 (b ₂ , 52.3)	613.3 (a, 13.3)	575.5 (a, 5.0)	580.3 (a', 131.3)
799.5 (b ₂ , 92.2)	739.4 (a, 7.4)	764.2 (a, 18.1)	754.8 (a", 0.5)
799.5 (a ₁ , 0.0)	757.7 (a, 0.4)	781.2 (a, 54.5)	772.7 (a', 44.9)
806.8 (b ₂ , 4.7)	763.7 (a, 1.0)	785.3 (a, 4.9)	790.0 (a', 62.6)
808.5 (a ₁ , 1.1)	774.2 (a, 27.3)	795.3 (a, 1.4)	791.8 (a", 0.2)
812.2 (a ₂ , 0.0)	795.2 (a, 21.0)	797.3 (a, 15.1)	799.6 (a', 4.1)
813.0 (b ₁ , 0.1)	798.3 (a, 3.9)	804.0 (a, 3.1)	801.7 (a", 4.3)
814.3 (a ₁ , 0.1)	799.7 (a, 0.4)	808.7 (a, 5.9)	805.9 (a', 0.6)
815.1 (b ₂ , 1.3)	801.4 (a, 2.3)	810.7 (a, 4.4)	809.8 (a', 0.4)
817.8 (a ₂ , 0.0)	812.7 (a, 0.5)	811.8 (a, 1.1)	811.9 (a", 0.0)

818.3 (b ₁ , 5.8)	815.7 (a, 13.6)	820.1 (a, 8.1)	815.0 (a', 6.5)
864.4 (b ₂ , 4.0)	832.4 (a, 2.7)	845.0 (a, 3.2)	832.7 (a'', 0.0)
865.1 (a ₁ , 2.3)	840.1 (a, 12.3)	861.6 (a, 1.6)	859.6 (a', 2.3)
865.3 (b ₁ , 3.2)	846.4 (a, 1.9)	864.0 (a, 8.3)	864.2 (a'', 1.8)
865.3 (a ₂ , 0.0)	860.5 (a, 1.2)	869.1 (a, 1.0)	868.0 (a', 0.6)
985.2 (a ₂ , 0.0)	951.2 (a, 2.2)	975.9 (a, 10.9)	970.0 (a', 12.6)
985.6 (b ₁ , 16.7)	965.1 (a, 4.9)	978.9 (a, 7.7)	977.9 (a'', 12.4)
988.9 (b ₂ , 0.0)	972.0 (a, 9.2)	984.1 (a, 13.3)	983.3 (a', 7.9)
989.0 (a ₁ , 21.9)	986.5 (a, 12.6)	989.2 (a, 7.3)	991.2 (a'', 7.4)
1040.8 (b ₂ , 0.3)	1021.1 (a, 2.2)	1033.7 (a, 0.1)	1027.7 (a', 0.7)
1041.0 (a ₂ , 0.0)	1026.2 (a, 0.1)	1038.4 (a, 0.4)	1034.3 (a'', 2.0)
1041.3 (a ₁ , 0.3)	1035.3 (a, 0.3)	1040.8 (a, 0.7)	1041.9 (a', 0.9)
1041.4 (b ₁ , 0.3)	1040.5 (a, 1.1)	1041.7 (a, 0.3)	1042.4 (a'', 0.3)
1096.2 (b ₂ , 21.7)	1065.5 (a, 16.1)	1087.9 (a, 19.1)	1084.4 (a', 16.0)
1096.7 (a ₁ , 0.0)	1086.8 (a, 13.3)	1091.5 (a, 6.1)	1094.5 (a', 4.4)
1222.1 (a ₂ , 0.0)	1204.2 (a, 0.6)	1218.8 (a, 0.0)	1215.4 (a'', 0.0)
1222.1 (b ₁ , 0.0)	1218.0 (a, 0.1)	1221.6 (a, 0.0)	1224.7 (a'', 0.0)
1356.4 (b ₁ , 0.1)	1314.1 (a, 4.7)	1343.6 (a, 2.4)	1326.9 (a', 4.0)
1357.4 (a ₂ , 0.0)	1332.0 (a, 1.4)	1346.9 (a, 0.5)	1344.1 (a'', 1.5)
1358.1 (b ₂ , 3.0)	1347.9 (a, 1.1)	1352.5 (a, 1.7)	1348.8 (a', 1.1)
1358.8 (a ₁ , 0.1)	1358.9 (a, 0.3)	1356.6 (a, 0.7)	1352.9 (a'', 0.0)
1397.4 (a ₂ , 0.0)	1363.7 (a, 0.9)	1387.9 (a, 1.7)	1384.9 (a', 4.9)
1397.7 (b ₁ , 7.5)	1377.3 (a, 2.4)	1392.4 (a, 1.2)	1391.9 (a'', 0.2)
1397.9 (b ₂ , 0.0)	1382.7 (a, 3.4)	1395.8 (a, 3.5)	1396.6 (a', 3.4)
1398.1 (a ₁ , 2.5)	1396.6 (a, 3.9)	1401.8 (a, 2.8)	1404.7 (a'', 3.3)
1777.4(b ₁ ,1022.5)	1903.6 (a, 951.7)	1794.8 (a, 593.9)	1723.9 (a'', 981.5)
1778.8(a ₁ , 1035.6)	1908.7 (a, 1035.5)	1846.1 (a, 547.3)	1733.2 (a', 109.3)
1804.8 (a ₁ , 1.2)	1989.2 (a, 707.1)	1963.1 (a, 1021.1)	1922.9 (a', 793.3)
3174.7 (b ₂ , 0.6)	3087.5 (a, 5.3)	3168.4 (a, 0.1)	3164.3 (a', 0.0)
3174.8 (a ₁ , 0.0)	3164.4 (a, 1.1)	3174.4 (a, 0.0)	3172.8 (a'', 0.0)
3175.3 (b ₁ , 0.0)	3167.0 (a, 0.5)	3176.7 (a, 0.3)	3173.4 (a', 0.6)
3175.4 (a ₂ , 0.0)	3168.2 (a, 0.8)	3178.2 (a, 0.3)	3177.5 (a'', 0.2)
3186.3 (a ₂ , 0.0)	3176.2 (a, 1.2)	3181.8 (a, 0.5)	3181.9 (a', 0.0)
3186.4 (b ₁ , 0.0)	3180.6 (a, 1.6)	3187.9 (a, 0.1)	3186.9 (a', 0.1)
3186.7 (b ₂ , 0.0)	3182.9 (a, 1.9)	3188.1 (a, 0.0)	3188.1 (a'', 0.1)
3186.7 (a ₁ , 0.2)	3186.1 (a, 3.9)	3196.1 (a, 0.1)	3190.8 (a'', 0.5)
3195.7 (b ₂ , 0.3)	3186.7 (a, 0.8)	3197.0 (a, 0.0)	3196.5 (a', 0.4)
3195.9 (a ₁ , 0.0)	3196.9 (a, 0.3)	3205.6 (a, 0.1)	3197.8 (a', 0.0)

Table S7. Theoretical harmonic vibrational frequencies (in cm^{-1}) for $\text{Cp}_2\text{Re}_2(\text{CO})_3$ using the BP86/SDD method (infrared intensities in parentheses are in km/mol).

3S-4 (C_1)	3S-5 (C_1)	3S-6 (C_1)	3T-2 (C_2)
21.0 (a, 0.1)	44.2 (a, 0.7)	45.0 (a", 0.6)	29.0 (b, 0.6)
38.8 (a, 0.9)	46.3 (a, 0.2)	53.6 (a', 1.1)	30.0 (a, 0.1)
73.0 (a, 0.3)	59.9 (a, 1.4)	76.4 (a', 2.3)	40.9 (b, 1.7)
73.3 (a, 0.3)	66.2 (a, 0.2)	77.4 (a", 0.4)	45.1 (a, 1.7)
80.1 (a, 0.4)	85.9 (a, 1.2)	81.7 (a", 1.3)	72.9 (a, 0.2)
84.7 (a, 0.4)	92.3 (a, 0.7)	94.2 (a', 0.7)	77.9 (b, 0.0)
93.8 (a, 0.9)	94.8 (a, 0.5)	103.6 (a", 0.0)	80.6 (a, 0.3)
100.9 (a, 1.0)	101.9 (a, 0.2)	120.9 (a', 1.4)	85.9 (b, 0.5)
106.2 (a, 0.9)	108.8 (a, 2.7)	151.0 (a", 0.5)	98.0 (a, 0.5)
115.7 (a, 0.1)	134.7 (a, 0.4)	156.0 (a', 5.8)	105.5 (b, 1.3)
178.4 (a, 3.2)	169.3 (a, 2.0)	177.7 (a', 5.7)	187.8 (a, 0.0)
186.3 (a, 7.2)	204.8 (a, 0.8)	226.5 (a', 5.7)	197.8 (b, 1.8)
304.6 (a, 6.9)	215.6 (a, 1.4)	270.7 (a", 5.2)	270.8 (a, 0.1)
317.2 (a, 5.2)	246.2 (a, 1.3)	316.1 (a', 2.1)	279.2 (b, 3.1)
344.4 (a, 14.0)	291.4 (a, 9.0)	332.4 (a", 7.2)	296.7 (a, 5.3)
386.6 (a, 3.8)	307.8 (a, 0.9)	349.6 (a', 10.2)	297.1 (b, 0.9)
387.8 (a, 2.4)	332.7 (a, 2.8)	400.4 (a", 0.8)	318.5 (b, 4.2)
391.9 (a, 2.0)	340.7 (a, 0.6)	422.4 (a', 1.5)	328.8 (a, 1.0)
435.8 (a, 0.7)	408.7 (a, 29.8)	445.2 (a', 4.2)	380.0 (b, 9.7)
464.0 (a, 61.2)	439.8 (a, 11.0)	472.8 (a", 1.7)	454.2 (a, 0.0)
480.8 (a, 10.9)	463.8 (a, 7.1)	493.0 (a', 17.1)	480.5 (b, 20.5)
498.9 (a, 12.9)	475.7 (a, 1.6)	505.9 (a", 11.1)	485.5 (a, 0.0)
504.3 (a, 15.6)	491.4 (a, 14.5)	520.0 (a', 18.5)	496.8 (a, 14.0)
509.9 (a, 0.5)	520.4 (a, 6.5)	524.3 (a", 10.7)	507.3 (b, 13.8)
531.5 (a, 50.7)	539.1 (a, 4.7)	525.1 (a', 8.2)	517.6 (b, 90.2)
540.8 (a, 14.5)	542.7 (a, 1.0)	538.5 (a', 1.8)	521.2 (a, 1.1)
549.9 (a, 0.2)	559.0 (a, 2.7)	586.0 (a", 0.9)	537.6 (b, 5.2)
551.5 (a, 0.2)	561.5 (a, 4.7)	596.4 (a', 1.0)	553.3 (a, 1.4)
559.1 (a, 4.1)	580.8 (a, 5.2)	614.4 (a', 0.2)	555.6 (b, 0.7)
567.3 (a, 8.5)	588.9 (a, 1.2)	615.3 (a", 0.7)	558.5 (a, 0.0)
590.7 (a, 32.4)	610.8 (a, 1.6)	628.3 (a', 0.1)	563.0 (b, 9.9)
698.9 (a, 6.5)	727.8 (a, 81.8)	738.6 (a", 0.9)	766.2 (b, 20.8)
707.5 (a, 9.3)	730.1 (a, 10.3)	748.4 (a", 4.5)	767.4 (a, 0.5)
765.2 (a, 22.0)	770.9 (a, 45.1)	755.3 (a', 4.0)	776.3 (a, 1.8)
774.2 (a, 4.1)	779.6 (a, 1.9)	763.4 (a", 0.1)	777.0 (b, 122.2)
782.1 (a, 9.9)	782.9 (a, 45.8)	766.3 (a', 1.1)	800.5 (b, 7.2)
790.3 (a, 3.0)	791.4 (a, 3.5)	780.1 (a', 0.7)	803.0 (a, 1.1)
799.1 (a, 3.5)	808.4 (a, 3.0)	796.1 (a", 7.5)	805.9 (a, 0.0)
800.7 (a, 11.6)	811.5 (a, 5.9)	812.9 (a", 7.4)	806.3 (b, 0.8)
812.2 (a, 5.7)	812.6 (a, 1.8)	813.7 (a', 14.2)	811.9 (b, 12.3)

814.4 (a, 12.3)	822.4 (a, 1.4)	822.5 (a', 5.0)	812.3 (a, 3.4)
840.9 (a, 12.1)	855.7 (a, 1.0)	850.5 (a", 0.0)	855.2 (b, 2.6)
846.0 (a, 0.1)	871.9 (a, 1.3)	862.4 (a', 3.2)	855.9 (a, 1.3)
849.0 (a, 2.7)	873.0 (a, 7.9)	874.2 (a", 0.0)	871.4 (b, 3.0)
862.8 (a, 1.8)	876.7 (a, 3.7)	887.7 (a', 0.9)	871.9 (a, 4.2)
953.8 (a, 1.5)	943.7 (a, 1.7)	913.9 (a', 17.6)	981.3 (b, 11.2)
959.4 (a, 13.6)	974.3 (a, 6.6)	918.0 (a", 0.4)	981.9 (a, 7.9)
967.0 (a, 8.7)	984.4 (a, 6.5)	963.1 (a", 3.0)	989.6 (b, 8.4)
979.7 (a, 13.0)	990.7 (a, 5.2)	977.7 (a', 0.8)	989.8 (a, 10.2)
1021.6 (a, 4.3)	996.9 (a, 1.4)	993.3 (a', 4.2)	1036.6 (b, 0.3)
1027.1 (a, 0.1)	1030.5 (a, 0.1)	994.9 (a", 1.9)	1037.3 (a, 0.1)
1033.4 (a, 0.1)	1039.2 (a, 0.3)	1009.6 (a", 3.1)	1041.0 (b, 0.5)
1037.6 (a, 0.8)	1043.8 (a, 1.1)	1016.5 (a', 0.3)	1041.4 (a, 0.3)
1061.5 (a, 8.5)	1078.1 (a, 5.1)	1046.2 (a", 8.2)	1091.3 (b, 9.8)
1076.3 (a, 25.1)	1097.6 (a, 2.6)	1050.5 (a', 1.8)	1091.6 (a, 0.2)
1210.4 (a, 0.0)	1210.7 (a, 0.7)	1204.3 (a", 0.0)	1223.3 (b, 0.0)
1212.0 (a, 0.3)	1225.1 (a, 0.0)	1204.8 (a', 0.7)	1223.4 (a, 0.0)
1297.0 (a, 11.0)	1280.7 (a, 1.5)	1267.6 (a", 0.2)	1342.2 (b, 2.2)
1333.0 (a, 3.1)	1309.1 (a, 3.3)	1276.6 (a', 5.2)	1345.0 (a, 0.0)
1341.3 (a, 0.3)	1341.9 (a, 2.7)	1299.1 (a", 4.4)	1349.5 (b, 0.1)
1348.4 (a, 0.0)	1344.5 (a, 1.7)	1307.9 (a', 13.1)	1352.0 (a, 0.1)
1364.3 (a, 2.5)	1355.7 (a, 1.8)	1309.6 (a", 2.6)	1393.1 (b, 2.7)
1368.9 (a, 4.1)	1398.3 (a, 3.8)	1318.5 (a', 3.9)	1393.9 (a, 5.0)
1379.8 (a, 3.1)	1415.4 (a, 4.5)	1375.5 (a', 4.6)	1401.0 (b, 5.8)
1384.1 (a, 0.5)	1509.4 (a, 3.6)	1375.7 (a", 2.7)	1401.2 (a, 2.6)
1824.9 (a, 376.8)	1882.8 (a, 460.0)	1889.2 (a', 955.2)	1776.7 (a, 558.0)
1935.6 (a, 928.6)	1897.9 (a, 1381.4)	1919.7(a', 1609.7)	1885.9 (b, 1895.3)
1982.8 (a, 1230.3)	1964.8 (a, 1058.6)	1954.6 (a', 759.7)	1904.3 (a, 1.9)
3141.8 (a, 3.1)	3074.5 (a, 2.8)	3121.0 (a", 3.5)	3168.1 (b, 0.3)
3146.6 (a, 2.5)	3104.6 (a, 2.2)	3121.4 (a', 2.3)	3168.2 (a, 0.0)
3160.7 (a, 3.0)	3136.0 (a, 3.4)	3128.9 (a", 2.4)	3177.1 (b, 0.7)
3171.1 (a, 0.7)	3147.7 (a, 0.4)	3129.9 (a', 0.2)	3177.2 (a, 0.0)
3175.6 (a, 0.8)	3160.1 (a, 10.2)	3136.1 (a", 0.5)	3185.7 (a, 0.0)
3178.5 (a, 0.8)	3170.5 (a, 1.2)	3136.4 (a', 4.6)	3185.7 (b, 0.5)
3181.2 (a, 0.0)	3178.8 (a, 0.5)	3153.0 (a", 3.0)	3190.1 (b, 1.0)
3182.3 (a, 0.7)	3189.0 (a, 0.1)	3153.5 (a', 4.6)	3190.2 (a, 0.0)
3191.5 (a, 0.9)	3190.8 (a, 0.5)	3159.4 (a", 2.0)	3197.8 (b, 0.1)
3199.7 (a, 0.1)	3200.5 (a, 0.1)	3160.0 (a', 0.0)	3197.8 (a, 0.0)

Table S8. Theoretical harmonic vibrational frequencies (in cm^{-1}) for $\text{Cp}_2\text{Re}_2(\text{CO})_2$ using the BP86/SDD method (infrared intensities in parentheses are in km/mol).

2S-1 (C_1)	2S-2 (C_s)	2S-3 (C_{2v})	2S-4 (C_2)	2S-5 (C_1)
24.8 (a, 0.2)	31.0i (a", 0.3)	39.3 (b ₂ , 0.5)	34.1 (b, 0.1)	48.6 (a, 2.1)
32.1 (a, 0.1)	24.6 (a", 0.0)	60.8 (a ₂ , 0.0)	39.7 (a, 0.1)	78.9 (a, 1.6)
47.5 (a, 2.3)	45.0 (a', 2.5)	74.1 (b ₁ , 0.9)	45.9 (b, 0.4)	85.1 (a, 0.8)
79.9 (a, 0.7)	81.6 (a", 0.9)	86.0 (a ₁ , 0.3)	47.3 (a, 0.5)	95.8 (a, 0.7)
91.8 (a, 2.1)	93.7 (a', 1.7)	115.9 (a ₂ , 0.0)	52.7 (b, 0.2)	109.4 (a, 2.3)
116.2 (a, 0.2)	112.8 (a", 0.5)	120.4 (b ₂ , 1.3)	71.5 (a, 0.4)	137.3 (a, 4.0)
120.3 (a, 0.4)	120.0 (a', 0.1)	144.7 (b ₂ , 3.6)	83.4 (b, 0.8)	158.5 (a, 0.8)
126.9 (a, 0.1)	122.0 (a", 0.3)	169.8 (b ₁ , 0.1)	99.3 (a, 0.0)	175.5 (a, 5.6)
194.3 (a, 0.3)	195.4 (a', 0.3)	183.4 (a ₁ , 2.9)	110.8 (a, 0.6)	190.1 (a, 0.7)
218.7 (a, 0.2)	219.7 (a', 0.2)	211.0 (a ₁ , 15.5)	214.3 (a, 0.2)	244.3 (a, 5.6)
282.5 (a, 2.7)	280.5 (a', 2.5)	335.8 (a ₁ , 28.2)	219.1 (b, 2.2)	306.5 (a, 4.4)
298.8 (a, 1.5)	301.6 (a", 1.3)	344.4 (b ₁ , 13.1)	255.7 (a, 4.9)	334.7 (a, 7.7)
310.4 (a, 3.7)	309.9 (a', 3.6)	368.0 (a ₂ , 0.0)	291.4 (b, 1.9)	346.4 (a, 7.7)
333.4 (a, 5.3)	338.0 (a', 5.2)	375.7 (b ₁ , 4.5)	309.6 (a, 1.0)	358.1 (a, 0.7)
349.0 (a, 3.9)	345.6 (a", 0.3)	394.7 (b ₂ , 10.9)	319.1 (b, 6.3)	405.1 (a, 13.2)
351.5 (a, 5.6)	349.2 (a", 7.5)	411.9 (a ₁ , 1.9)	327.9 (a, 2.9)	449.1 (a, 18.0)
354.8 (a, 1.3)	349.7 (a', 1.9)	416.4 (b ₂ , 1.6)	419.0 (b, 25.8)	482.6 (a, 4.1)
454.0 (a, 1.8)	450.7 (a", 1.7)	488.9 (a ₂ , 0.0)	458.4 (a, 8.6)	491.5 (a, 9.3)
464.0 (a, 3.4)	461.4 (a', 3.7)	509.7 (a ₁ , 1.3)	469.2 (b, 42.1)	494.8 (a, 16.1)
485.7 (a, 7.3)	486.9 (a", 3.3)	513.2 (b ₁ , 7.2)	486.1 (a, 0.5)	502.8 (a, 6.3)
527.5 (a, 28.6)	524.7 (a', 32.9)	535.2 (b ₂ , 10.2)	519.1 (a, 3.9)	519.0 (a, 12.1)
552.4 (a, 10.2)	553.0 (a', 4.8)	549.6 (b ₂ , 1.3)	522.2 (b, 1.9)	542.4 (a, 8.0)
555.3 (a, 1.5)	553.6 (a', 8.2)	555.3 (a ₂ , 0.0)	542.9 (b, 1.5)	549.7 (a, 9.6)
557.6 (a, 0.1)	558.9 (a', 0.0)	581.2 (b ₁ , 7.5)	544.6 (a, 0.9)	564.1 (a, 4.5)
560.2 (a, 0.0)	559.1 (a", 0.1)	585.7 (a ₁ , 7.8)	569.9 (b, 1.7)	620.1 (a, 6.7)
563.2 (a, 2.6)	562.2 (a", 0.3)	610.5 (a ₁ , 4.3)	571.9 (a, 0.0)	631.2 (a, 9.4)
774.5 (a, 50.5)	771.4 (a', 48.9)	751.5 (a ₂ , 0.0)	753.8 (b, 67.0)	735.2 (a, 9.7)
776.8 (a, 11.1)	776.7 (a', 17.2)	752.7 (b ₁ , 14.4)	755.5 (a, 8.9)	737.6 (a, 6.9)
779.2 (a, 6.7)	779.8 (a", 2.3)	781.2 (a ₂ , 0.0)	760.8 (b, 44.0)	760.6 (a, 7.4)
789.5 (a, 23.1)	790.8 (a', 38.2)	784.9 (b ₂ , 10.5)	775.1 (a, 12.2)	766.0 (a, 6.9)
791.0 (a, 11.7)	791.7 (a', 1.0)	785.0 (a ₁ , 3.4)	785.7 (b, 15.9)	782.5 (a, 7.5)
792.8 (a, 2.3)	792.3 (a", 2.3)	794.7 (b ₁ , 45.3)	790.0 (a, 1.6)	790.3 (a, 12.6)
806.1 (a, 5.0)	803.2 (a", 0.0)	804.6 (b ₂ , 0.0)	798.7 (b, 2.6)	798.5 (a, 9.3)
810.9 (a, 4.4)	810.1 (a', 5.2)	805.9 (a ₁ , 16.9)	799.2 (a, 2.5)	806.0 (a, 0.2)
811.6 (a, 1.5)	811.4 (a", 1.4)	808.6 (b ₁ , 0.1)	809.8 (b, 11.3)	832.5 (a, 0.5)
813.8 (a, 0.2)	814.1 (a', 0.3)	831.0 (a ₁ , 0.2)	810.7 (a, 1.1)	842.1 (a, 9.9)
844.3 (a, 0.1)	842.9 (a", 0.3)	833.0 (a ₂ , 0.0)	833.2 (b, 1.3)	849.8 (a, 20.0)
846.4 (a, 3.5)	847.3 (a", 4.0)	850.5 (b ₂ , 0.1)	839.3 (a, 0.1)	855.3 (a, 8.5)
852.2 (a, 0.9)	850.8 (a', 1.6)	863.3 (a ₂ , 0.0)	851.3 (b, 10.1)	877.1 (a, 8.3)
856.9 (a, 2.4)	858.0 (a', 2.8)	883.3 (b ₂ , 22.5)	853.4 (a, 0.5)	900.5 (a, 9.5)

977.7 (a, 8.7)	978.8 (a", 0.0)	947.2 (b ₁ , 1.3)	976.7 (b, 12.9)	917.5 (a, 18.0)
979.8 (a, 9.8)	979.6 (a", 17.5)	950.2 (a ₁ , 1.0)	978.0 (a, 11.0)	932.4 (a, 6.9)
983.6 (a, 19.2)	983.7 (a', 16.9)	984.4 (b ₁ , 44.3)	986.2 (b, 15.1)	943.7 (a, 12.3)
986.0 (a, 9.4)	986.9 (a', 11.8)	1001.4 (a ₁ , 5.4)	988.0 (a, 8.1)	966.3 (a, 32.4)
1033.2 (a, 1.1)	1033.2 (a', 0.9)	1004.0 (a ₂ , 0.0)	1034.1 (b, 2.6)	992.5 (a, 2.2)
1036.9 (a, 0.2)	1037.1 (a", 0.3)	1012.0 (b ₂ , 15.7)	1036.1 (a, 0.8)	1010.0 (a, 2.8)
1038.5 (a, 0.6)	1038.1 (a', 0.1)	1029.3 (b ₁ , 0.8)	1041.7 (b, 3.3)	1021.9 (a, 11.4)
1040.3 (a, 0.1)	1039.7 (a", 0.0)	1035.4 (a ₁ , 0.0)	1042.3 (a, 0.0)	1034.8 (a, 9.4)
1086.8 (a, 10.0)	1087.2 (a', 9.9)	1063.6 (a ₁ , 19.8)	1091.5 (a, 2.2)	1039.8 (a, 6.8)
1089.9 (a, 11.1)	1090.5 (a', 10.5)	1067.2 (b ₁ , 21.9)	1091.5 (b, 8.2)	1061.1 (a, 12.7)
1218.8 (a, 0.0)	1219.0 (a", 0.0)	1179.5 (a ₂ , 0.0)	1220.8 (b, 0.0)	1151.2 (a, 2.0)
1219.3 (a, 0.0)	1219.8 (a", 0.0)	1182.4 (b ₂ , 2.0)	1221.2 (a, 0.0)	1195.6 (a, 0.4)
1343.7 (a, 1.8)	1345.1 (a', 0.5)	1278.3 (a ₂ , 0.0)	1339.3 (b, 1.2)	1235.3 (a, 0.6)
1344.4 (a, 0.5)	1347.4 (a", 1.2)	1290.8 (b ₂ , 1.9)	1341.3 (a, 0.2)	1265.3 (a, 5.3)
1350.1 (a, 1.0)	1348.4 (a', 0.2)	1333.5 (b ₁ , 0.3)	1346.0 (b, 7.5)	1278.5 (a, 6.2)
1354.6 (a, 0.1)	1354.0 (a", 0.1)	1343.2 (a ₁ , 0.4)	1347.5 (a, 0.2)	1316.9 (a, 3.0)
1387.9 (a, 2.3)	1387.9 (a", 3.2)	1360.3 (b ₁ , 0.0)	1388.7 (b, 3.7)	1336.8 (a, 11.1)
1393.0 (a, 1.9)	1392.6 (a', 1.5)	1369.4 (a ₁ , 7.6)	1390.3 (a, 4.7)	1351.3 (a, 2.3)
1394.2 (a, 2.3)	1397.2 (a', 1.5)	1372.6 (a ₂ , 0.0)	1416.8 (b, 0.6)	1366.9 (a, 1.0)
1401.5 (a, 1.5)	1398.8 (a", 2.2)	1377.7 (b ₂ , 4.9)	1417.9 (a, 0.1)	1392.3 (a, 2.4)
1758.8 (a, 1095.7)	1756.4(a", 1104.7)	1876.7(b ₂ , 1127.2)	1907.0 (b, 514.8)	1870.8 (a, 1216.9)
1767.8 (a, 179.7)	1766.0 (a', 177.8)	1928.3(a ₁ , 1053.6)	1949.7 (a, 1149.6)	1917.0 (a, 943.1)
3166.1 (a, 0.8)	3165.0 (a', 0.8)	2391.7 (b ₁ , 2.6)	3166.0 (b, 1.0)	2197.5 (a, 26.9)
3168.6 (a, 0.1)	3167.8 (a", 0.0)	2408.3 (a ₁ , 21.2)	3166.2 (a, 0.1)	3026.1 (a, 12.2)
3174.7 (a, 0.7)	3173.7 (a', 0.8)	3168.0 (a ₂ , 0.0)	3174.4 (a, 0.1)	3119.8 (a, 6.4)
3178.5 (a, 0.0)	3179.5 (a", 0.0)	3168.2 (b ₂ , 1.4)	3174.5 (b, 0.6)	3139.2 (a, 0.5)
3182.9 (a, 0.2)	3181.9 (a', 0.2)	3177.7 (b ₁ , 0.3)	3184.1 (a, 0.5)	3154.6 (a, 5.3)
3185.3 (a, 0.0)	3184.5 (a", 0.0)	3177.9 (a ₁ , 1.2)	3184.2 (b, 0.2)	3165.2 (a, 3.8)
3186.5 (a, 0.0)	3187.4 (a', 0.0)	3191.5 (a ₂ , 0.0)	3185.6 (a, 0.2)	3172.8 (a, 0.2)
3190.7 (a, 0.0)	3190.9 (a", 0.0)	3191.7 (b ₂ , 0.1)	3185.6 (b, 0.1)	3181.0 (a, 0.1)
3194.6 (a, 0.0)	3193.8 (a', 0.0)	3194.0 (a ₁ , 0.2)	3197.3 (a, 0.0)	3187.9 (a, 0.3)
3198.5 (a, 0.0)	3198.9 (a', 0.0)	3194.3 (b ₁ , 0.4)	3197.3 (b, 0.7)	3197.0 (a, 0.4)

Table S9. Theoretical harmonic vibrational frequencies (in cm^{-1}) for $\text{Cp}_2\text{Re}_2(\text{CO})_2$ using the BP86/SDD method (infrared intensities in parentheses are in km/mol).

2T-1 (C_{2v})	2T-2 (C_2)	2T-3 (C_1)	2T-4 (C_1)
24.9 (a ₂ , 0.0)	33.1 (a, 2.1)	18.1 (a, 0.0)	38.0 (a, 2.0)
28.9 (b ₁ , 0.0)	44.1 (a, 0.0)	42.4 (a, 0.5)	58.8 (a, 1.7)
61.1 (a ₁ , 4.4)	48.1 (b, 2.4)	53.5 (a, 0.1)	74.2 (a, 0.3)
86.7 (b ₁ , 1.2)	54.8 (b, 0.7)	64.6 (a, 0.4)	89.9 (a, 1.8)
97.9 (a ₁ , 0.7)	59.6 (b, 0.2)	83.2 (a, 0.2)	94.8 (a, 0.6)
103.9 (b ₂ , 1.3)	68.7 (a, 0.2)	95.1 (a, 0.2)	129.4 (a, 0.3)
111.3 (a ₂ , 0.0)	97.6 (a, 0.2)	101.1 (a, 0.9)	133.9 (a, 2.8)
201.3 (a ₂ , 0.0)	125.2 (a, 0.5)	137.8 (a, 5.0)	164.8 (a, 2.4)
207.4 (a ₁ , 0.0)	133.5 (b, 0.2)	140.5 (a, 0.7)	178.7 (a, 1.2)
208.2 (b ₂ , 0.2)	200.5 (a, 0.0)	177.6 (a, 6.9)	207.7 (a, 4.1)
299.3 (b ₂ , 6.4)	260.5 (b, 0.2)	321.8 (a, 0.3)	283.6 (a, 3.7)
318.2 (a ₁ , 0.8)	272.6 (a, 0.2)	341.1 (a, 12.0)	299.1 (a, 1.2)
318.7 (a ₂ , 0.0)	302.3 (b, 2.5)	354.4 (a, 2.2)	334.1 (a, 6.7)
340.2 (b ₁ , 15.6)	308.5 (a, 0.4)	366.5 (a, 7.7)	346.9 (a, 3.4)
342.4 (a ₁ , 5.4)	329.6 (b, 0.1)	376.2 (a, 5.7)	393.0 (a, 4.8)
343.9 (b ₂ , 0.6)	335.5 (a, 7.2)	380.7 (a, 0.2)	399.6 (a, 0.5)
389.8 (a ₂ , 0.0)	436.9 (a, 2.5)	391.3 (a, 12.2)	467.8 (a, 19.7)
443.6 (b ₁ , 0.3)	455.6 (b, 11.6)	429.2 (a, 0.0)	478.8 (a, 10.5)
476.4 (a ₁ , 1.2)	472.6 (b, 37.1)	463.0 (a, 8.3)	491.5 (a, 3.2)
496.6 (b ₁ , 4.4)	503.6 (a, 1.2)	493.7 (a, 3.8)	507.7 (a, 5.6)
536.6 (b ₂ , 32.1)	507.5 (a, 4.2)	505.8 (a, 21.5)	515.0 (a, 6.1)
539.5 (a ₁ , 4.6)	521.1 (b, 0.7)	535.0 (a, 1.0)	534.7 (a, 20.0)
551.3 (a ₂ , 0.0)	550.5 (a, 0.2)	545.7 (a, 0.6)	546.0 (a, 9.8)
552.3 (b ₁ , 0.2)	551.6 (b, 2.1)	559.2 (a, 0.3)	594.6 (a, 2.4)
558.7 (b ₂ , 0.2)	564.0 (b, 1.1)	564.0 (a, 0.1)	621.5 (a, 0.9)
566.1 (a ₁ , 1.4)	565.6 (a, 0.9)	580.4 (a, 14.3)	637.6 (a, 1.2)
781.5 (b ₂ , 83.9)	770.1 (b, 65.7)	711.5 (a, 2.6)	718.8 (a, 4.6)
782.0 (a ₁ , 13.5)	770.3 (a, 0.6)	748.2 (a, 2.5)	731.9 (a, 8.2)
787.5 (a ₂ , 0.0)	772.9 (a, 9.8)	759.5 (a, 0.3)	750.4 (a, 10.7)
787.6 (b ₁ , 2.5)	772.9 (b, 45.7)	773.6 (a, 28.3)	768.4 (a, 8.6)
797.8 (a ₁ , 4.8)	786.9 (b, 10.4)	795.5 (a, 21.8)	775.1 (a, 3.1)
797.9 (b ₂ , 0.8)	789.2 (a, 0.9)	798.5 (a, 2.3)	791.3 (a, 14.7)
807.2 (b ₁ , 0.2)	802.9 (b, 0.7)	798.8 (a, 2.9)	798.9 (a, 3.1)
807.7 (b ₂ , 0.1)	804.4 (a, 0.1)	800.1 (a, 0.5)	805.2 (a, 0.5)
808.9 (a ₂ , 0.0)	809.5 (a, 0.1)	809.5 (a, 4.6)	828.7 (a, 7.3)
812.3 (a ₁ , 0.1)	810.2 (b, 0.7)	813.4 (a, 12.8)	835.7 (a, 3.2)
843.1 (b ₁ , 3.1)	832.7 (a, 0.4)	830.6 (a, 0.4)	851.1 (a, 4.2)
844.0 (a ₂ , 0.0)	835.2 (b, 1.1)	840.7 (a, 12.3)	857.9 (a, 6.0)
853.9 (b ₂ , 0.3)	855.8 (a, 0.0)	849.2 (a, 1.0)	869.2 (a, 7.7)
854.4 (a ₁ , 0.0)	856.5 (b, 2.6)	859.2 (a, 3.7)	907.0 (a, 7.3)

980.1 (b ₁ , 19.6)	974.6 (b, 19.8)	944.8 (a, 4.2)	917.0 (a, 6.0)
980.2 (a ₂ , 0.0)	975.0 (a, 0.3)	960.3 (a, 6.8)	937.9 (a, 0.2)
981.8 (a ₁ , 20.0)	986.0 (b, 0.1)	970.9 (a, 8.5)	951.0 (a, 1.1)
981.9 (b ₂ , 0.3)	986.1 (a, 25.8)	985.9 (a, 11.9)	982.0 (a, 2.1)
1034.7 (b ₂ , 0.8)	1033.2 (a, 0.1)	1012.7 (a, 0.9)	998.8 (a, 14.2)
1035.2 (a ₁ , 0.0)	1033.6 (b, 0.1)	1028.2 (a, 0.2)	1004.8 (a, 6.9)
1036.0 (b ₁ , 1.6)	1040.5 (b, 0.3)	1035.0 (a, 0.3)	1016.7 (a, 9.5)
1036.6 (a ₂ , 0.0)	1041.1 (a, 1.3)	1036.6 (a, 0.2)	1031.8 (a, 6.6)
1088.4 (b ₂ , 28.6)	1089.0 (b, 17.9)	1057.0 (a, 19.3)	1038.8 (a, 0.8)
1088.8 (a ₁ , 0.0)	1089.3 (a, 0.9)	1083.3 (a, 10.3)	1058.4 (a, 8.5)
1217.7 (a ₂ , 0.0)	1218.3 (a, 0.0)	1203.0 (a, 0.3)	1172.8 (a, 0.7)
1217.7 (b ₁ , 0.0)	1218.4 (b, 0.0)	1218.1 (a, 0.1)	1191.7 (a, 0.1)
1346.5 (b ₁ , 2.6)	1336.1 (a, 0.0)	1305.2 (a, 5.5)	1242.2 (a, 2.9)
1346.7 (a ₁ , 0.0)	1337.9 (b, 0.3)	1321.0 (a, 2.1)	1253.0 (a, 1.3)
1348.2 (b ₂ , 2.5)	1347.3 (b, 2.8)	1344.5 (a, 0.4)	1264.4 (a, 3.9)
1348.2 (a ₂ , 0.0)	1348.1 (a, 0.5)	1352.9 (a, 0.2)	1301.0 (a, 3.6)
1390.4 (b ₁ , 1.3)	1388.0 (a, 0.4)	1359.2 (a, 0.7)	1337.9 (a, 0.9)
1391.1 (a ₂ , 0.0)	1388.1 (b, 5.4)	1375.5 (a, 1.2)	1339.0 (a, 6.7)
1392.2 (b ₂ , 0.1)	1408.5 (b, 2.5)	1380.2 (a, 2.0)	1362.6 (a, 4.4)
1392.5 (a ₁ , 6.3)	1408.7 (a, 1.4)	1391.1 (a, 6.2)	1385.4 (a, 1.1)
1746.2(b ₁ , 1102.0)	1823.2 (b, 1106.6)	1844.9 (a, 1380.2)	1861.2 (a, 1605.4)
1753.7 (a ₁ , 124.3)	1832.2 (a, 214.9)	1912.9 (a, 923.3)	1916.7 (a, 983.0)
3169.0 (b ₂ , 0.0)	3169.9 (b, 0.0)	3115.3 (a, 0.4)	2420.6 (a, 3.2)
3169.1 (a ₁ , 0.2)	3169.9 (a, 0.0)	3128.3 (a, 1.9)	3094.1 (a, 2.9)
3177.5 (b ₁ , 0.0)	3175.1 (b, 0.1)	3163.4 (a, 0.4)	3125.3 (a, 6.6)
3177.5 (a ₂ , 0.0)	3175.1 (a, 0.0)	3166.0 (a, 0.3)	3143.4 (a, 0.1)
3185.4 (b ₂ , 0.1)	3183.6 (a, 0.1)	3167.8 (a, 1.5)	3157.7 (a, 3.6)
3185.5 (a ₁ , 0.1)	3183.6 (b, 0.2)	3178.3 (a, 1.7)	3164.4 (a, 3.3)
3188.2 (a ₂ , 0.0)	3186.8 (b, 0.8)	3180.9 (a, 2.4)	3177.9 (a, 0.1)
3188.2 (b ₁ , 0.1)	3186.9 (a, 0.1)	3183.7 (a, 3.7)	3185.5 (a, 0.0)
3196.3 (b ₂ , 0.2)	3195.6 (b, 0.1)	3187.4 (a, 1.1)	3194.6 (a, 0.2)
3196.4 (a ₁ , 0.0)	3195.6 (a, 0.0)	3194.9 (a, 0.2)	3198.6 (a, 0.4)

Table S10. 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	-1.379756	2.597940	1.025533
2	6	0	-0.260841	3.461977	0.879398
3	6	0	0.000000	3.627077	-0.523396
4	6	0	-0.990102	2.870561	-1.235053
5	6	0	-1.832517	2.233302	-0.284998
6	1	0	-1.811591	2.271793	1.963266
7	1	0	0.300106	3.914799	1.687704
8	1	0	0.759961	4.261923	-0.960565
9	1	0	-1.077990	2.789103	-2.311573
10	1	0	-2.673177	1.590269	-0.511036
11	75	0	0.367718	1.444969	-0.007165
12	75	0	-0.367718	-1.444969	-0.007165
13	6	0	1.379756	-2.597940	1.025533
14	6	0	0.260841	-3.461977	0.879398
15	6	0	1.832517	-2.233302	-0.284998
16	1	0	1.811591	-2.271793	1.963266
17	6	0	0.000000	-3.627077	-0.523396
18	1	0	-0.300106	-3.914799	1.687704
19	6	0	0.990102	-2.870561	-1.235053
20	1	0	2.673177	-1.590269	-0.511036
21	1	0	-0.759961	-4.261923	-0.960565
22	1	0	1.077990	-2.789103	-2.311573
23	6	0	2.083620	1.493794	0.823365
24	6	0	1.291020	0.737992	-1.542048
25	6	0	-1.291020	-0.737992	-1.542048
26	6	0	-2.083620	-1.493794	0.823365
27	8	0	3.123777	1.583118	1.338574
28	8	0	1.854382	0.391225	-2.499215
29	8	0	-1.854382	-0.391225	-2.499215
30	8	0	-3.123777	-1.583118	1.338574
31	6	0	0.000000	0.000000	1.476131
32	8	0	0.000000	0.000000	2.667387

Table S11. 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	1.491813	-2.591096	1.159613
2	6	0	0.491033	-3.515200	0.714716
3	6	0	0.491033	-3.515200	-0.714716
4	6	0	1.491813	-2.591096	-1.159613
5	6	0	2.087238	-2.013802	0.000000
6	1	0	1.735595	-2.359709	2.188425
7	1	0	-0.134470	-4.131009	1.348812
8	1	0	-0.134470	-4.131009	-1.348812
9	1	0	1.735595	-2.359709	-2.188425
10	1	0	2.862395	-1.256665	0.000000
11	75	0	-0.190652	-1.474028	0.000000
12	75	0	0.213101	1.504159	0.000000
13	6	0	-0.812732	3.231200	-1.156953
14	6	0	-1.841434	2.337574	-0.712302
15	6	0	-0.179135	3.774024	0.000000
16	1	0	-0.563533	3.457727	-2.186033
17	6	0	-1.841434	2.337574	0.712302
18	1	0	-2.504801	1.764404	-1.348336
19	6	0	-0.812732	3.231200	1.156953
20	1	0	0.638123	4.484835	0.000000
21	1	0	-2.504801	1.764404	1.348336
22	1	0	-0.563533	3.457727	2.186033
23	6	0	-1.613302	-1.372474	1.274907
24	6	0	-1.613302	-1.372474	-1.274907
25	6	0	0.418380	0.355545	1.575456
26	6	0	0.418380	0.355545	-1.575456
27	8	0	-2.476644	-1.382882	2.056308
28	8	0	-2.476644	-1.382882	-2.056308
29	8	0	0.596759	0.125962	2.715379
30	8	0	0.596759	0.125962	-2.715379
31	6	0	2.111660	1.705330	0.000000
32	8	0	3.263095	1.877508	0.000000

Table S12. 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	3.070114	-0.565411	-1.501316
2	6	0	3.751293	-0.111354	-0.327500
3	6	0	3.421592	-0.993688	0.741644
4	6	0	2.545891	-2.012634	0.230554
5	6	0	2.325010	-1.734662	-1.144604
6	1	0	3.102368	-0.109820	-2.482560
7	1	0	4.412042	0.744063	-0.262866
8	1	0	3.785735	-0.918127	1.758942
9	1	0	2.151627	-2.851611	0.789745
10	1	0	1.700005	-2.304739	-1.820144
11	75	0	1.513092	0.087024	0.070047
12	75	0	-1.507480	0.001936	-0.050526
13	6	0	-1.401933	-2.177527	0.834169
14	6	0	-2.400388	-1.446270	1.527636
15	6	0	-1.781374	-2.263006	-0.547722
16	1	0	-0.505960	-2.594737	1.273370
17	6	0	-3.407579	-1.057583	0.580900
18	1	0	-2.394044	-1.211649	2.584943
19	6	0	-3.021078	-1.585896	-0.698233
20	1	0	-1.232404	-2.762948	-1.335333
21	1	0	-4.327705	-0.532534	0.803249
22	1	0	-3.576444	-1.480530	-1.622256
23	6	0	1.568747	1.997247	-0.000268
24	8	0	1.694825	3.151261	-0.060546
25	6	0	0.080013	0.089831	-1.452440
26	8	0	0.148039	-0.016262	-2.638945
27	6	0	-1.482406	1.551540	1.091766
28	8	0	-1.551629	2.468797	1.797920
29	6	0	-2.189506	1.240294	-1.338440
30	6	0	0.797993	0.129487	1.862916
31	8	0	-2.656879	1.949933	-2.128503
32	8	0	0.516335	0.069820	2.991886

Table S13. Theoretical Cartesian coordinates (in Å) for the structure **5S-4** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.111069	-0.940973	1.856278
2	6	0	-1.236157	-1.436257	2.860742
3	6	0	-0.765150	-0.331763	3.640099
4	6	0	-1.377902	0.858112	3.114604
5	6	0	-2.189297	0.482261	2.010454
6	1	0	-2.643802	-1.539614	1.130995
7	1	0	-0.962874	-2.474491	3.007032
8	1	0	-0.121802	-0.390626	4.508746
9	1	0	-1.244100	1.864845	3.490249
10	1	0	-2.771513	1.162485	1.402197
11	75	0	0.041541	-0.011840	1.546924
12	75	0	0.041541	-0.011840	-1.546924
13	6	0	-1.377902	0.858112	-3.114604
14	6	0	-0.765150	-0.331763	-3.640099
15	6	0	-2.189297	0.482261	-2.010454
16	1	0	-1.244100	1.864845	-3.490249
17	6	0	-1.236157	-1.436257	-2.860742
18	1	0	-0.121802	-0.390626	-4.508746
19	6	0	-2.111069	-0.940973	-1.856278
20	1	0	-2.771513	1.162485	-1.402197
21	1	0	-0.962874	-2.474491	-3.007032
22	1	0	-2.643802	-1.539614	-1.130995
23	6	0	1.409511	-1.359358	1.366717
24	6	0	1.479654	1.158334	1.997080
25	6	0	1.409511	-1.359358	-1.366717
26	6	0	1.479654	1.158334	-1.997080
27	8	0	2.202478	-2.203026	1.441310
28	8	0	2.322077	1.878801	2.345421
29	8	0	2.202478	-2.203026	-1.441310
30	8	0	2.322077	1.878801	-2.345421
31	6	0	-0.199903	1.388342	0.000000
32	8	0	-0.556441	2.528006	0.000000

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

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.110733	-0.726133	-1.130680
2	6	0	-1.703106	-1.170984	-2.414000
3	6	0	-1.451140	0.000000	-3.207387
4	6	0	-1.703106	1.170984	-2.414000
5	6	0	-2.110733	0.726133	-1.130680
6	1	0	-2.440624	-1.375748	-0.334051
7	1	0	-1.638450	-2.199505	-2.744033
8	1	0	-1.150562	0.000000	-4.246284
9	1	0	-1.638450	2.199505	-2.744033
10	1	0	-2.440624	1.375748	-0.334051
11	6	0	1.703106	1.170984	-2.414000
12	6	0	1.451140	0.000000	-3.207387
13	6	0	2.110733	0.726133	-1.130680
14	1	0	1.638450	2.199505	-2.744033
15	6	0	1.703106	-1.170984	-2.414000
16	1	0	1.150562	0.000000	-4.246284
17	6	0	2.110733	-0.726133	-1.130680
18	1	0	2.440624	1.375748	-0.334051
19	1	0	1.638450	-2.199505	-2.744033
20	1	0	2.440624	-1.375748	-0.334051
21	75	0	0.000000	0.000000	1.606786
22	75	0	0.000000	0.000000	-1.528514
23	6	0	1.986599	0.000000	1.776132
24	6	0	0.000000	-1.934972	1.118497
25	6	0	0.000000	1.934972	1.118497
26	6	0	-1.986599	0.000000	1.776132
27	8	0	3.123361	0.000000	1.968427
28	8	0	0.000000	3.054350	0.830470
29	8	0	-3.123361	0.000000	1.968427
30	8	0	0.000000	-3.054350	0.830470
31	6	0	0.000000	0.000000	3.550682
32	8	0	0.000000	0.000000	4.709201

Table S15. Theoretical Cartesian coordinates (in Å) for the structure **5S-6** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.271025	-2.225335	-0.321827
2	6	0	-2.251708	-1.911471	1.068353
3	6	0	-3.230989	-0.907167	1.325954
4	6	0	-3.855387	-0.578037	0.074598
5	6	0	-3.259626	-1.390756	-0.934550
6	1	0	-1.656391	-2.963888	-0.820116
7	1	0	-1.596487	-2.349371	1.811125
8	1	0	-3.459978	-0.475159	2.291618
9	1	0	-4.657639	0.133890	-0.072433
10	1	0	-3.511946	-1.374525	-1.987997
11	75	0	-1.658675	0.028347	-0.082949
12	75	0	1.299541	0.249137	-0.253649
13	6	0	3.596799	0.442263	-0.072099
14	6	0	2.983112	0.226121	1.225218
15	6	0	4.181991	-0.800458	-0.458781
16	1	0	3.910409	1.400770	-0.473385
17	6	0	3.235441	-1.150075	1.565369
18	1	0	2.827813	0.989912	1.980550
19	6	0	3.994083	-1.755643	0.559010
20	1	0	4.678454	-0.978755	-1.408764
21	1	0	2.847243	-1.634227	2.456409
22	1	0	4.254447	-2.806223	0.499489
23	6	0	-0.567504	0.451555	-1.574236
24	6	0	-2.005024	1.875540	0.267495
25	6	0	1.304634	-1.703483	-0.599002
26	6	0	1.299599	2.208111	0.047647
27	8	0	0.317412	0.641193	-2.368248
28	8	0	-2.309209	2.975548	0.489760
29	8	0	1.238040	-2.834026	-0.828857
30	8	0	1.341052	3.345110	0.231998
31	6	0	-0.083202	0.051137	1.306006
32	8	0	0.021699	-0.096264	2.487029

Table S16. Theoretical Cartesian coordinates (in Å) for the structure **5S-7** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.160522	1.684810	0.859917
2	6	0	0.721189	2.142624	2.114975
3	6	0	-0.721189	2.142624	2.114975
4	6	0	-1.160522	1.684810	0.859917
5	6	0	0.000000	1.642098	-0.109506
6	1	0	2.203191	1.639995	0.568226
7	1	0	1.348088	2.391530	2.963785
8	1	0	-1.348088	2.391530	2.963785
9	1	0	-2.203191	1.639995	0.568226
10	1	0	0.000000	2.535091	-0.750290
11	6	0	-0.721189	-2.142624	2.114975
12	6	0	0.721189	-2.142624	2.114975
13	6	0	-1.160522	-1.684810	0.859917
14	1	0	-1.348088	-2.391530	2.963785
15	6	0	1.160522	-1.684810	0.859917
16	1	0	1.348088	-2.391530	2.963785
17	6	0	0.000000	-1.642098	-0.109506
18	1	0	-2.203191	-1.639995	0.568226
19	1	0	2.203191	-1.639995	0.568226
20	1	0	0.000000	-2.535091	-0.750290
21	75	0	0.000000	0.000000	-1.753734
22	75	0	0.000000	0.000000	1.808730
23	6	0	0.000000	0.000000	3.692089
24	6	0	0.000000	-1.403750	-3.113482
25	6	0	1.990993	0.000000	-1.712259
26	6	0	-1.990993	0.000000	-1.712259
27	6	0	0.000000	1.403750	-3.113482
28	8	0	0.000000	-2.235514	-3.920922
29	8	0	-3.144894	0.000000	-1.701755
30	8	0	0.000000	2.235514	-3.920922
31	8	0	3.144894	0.000000	-1.701755
32	8	0	0.000000	0.000000	4.860466

Table S17. Theoretical Cartesian coordinates (in Å) for the structure **5S-8** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.093798	0.704414	0.790913
2	6	0	1.926144	1.134541	-0.624945
3	6	0	2.197686	0.000000	-1.467130
4	6	0	1.926144	-1.134541	-0.624945
5	6	0	2.093798	-0.704414	0.790913
6	1	0	2.566975	1.314836	1.551926
7	1	0	2.065603	2.166517	-0.929627
8	1	0	2.624437	0.000000	-2.463190
9	1	0	2.065603	-2.166517	-0.929627
10	1	0	2.566975	-1.314836	1.551926
11	6	0	-1.926144	-1.134541	-0.624945
12	6	0	-2.197686	0.000000	-1.467130
13	6	0	-2.093798	-0.704414	0.790913
14	1	0	-2.065603	-2.166517	-0.929627
15	6	0	-1.926144	1.134541	-0.624945
16	1	0	-2.624437	0.000000	-2.463190
17	6	0	-2.093798	0.704414	0.790913
18	1	0	-2.566975	-1.314836	1.551926
19	1	0	-2.065603	2.166517	-0.929627
20	1	0	-2.566975	1.314836	1.551926
21	75	0	0.000000	0.000000	1.478943
22	75	0	0.000000	0.000000	-1.398324
23	6	0	0.000000	-1.312527	-2.840410
24	6	0	0.000000	1.995843	1.582761
25	6	0	0.000000	-1.995843	1.582761
26	6	0	0.000000	0.000000	3.393438
27	8	0	0.000000	3.144696	1.705701
28	8	0	0.000000	-3.144696	1.705701
29	8	0	0.000000	0.000000	4.562873
30	8	0	0.000000	-2.096376	-3.690621
31	6	0	0.000000	1.312527	-2.840410
32	8	0	0.000000	2.096376	-3.690621

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	-0.911549	2.977623	0.040130
2	6	0	-0.911980	2.998382	1.472587
3	6	0	0.454920	3.023913	1.909660
4	6	0	1.277684	2.958581	0.747833
5	6	0	0.427900	2.960502	-0.415127
6	1	0	-1.794395	2.944199	-0.586980
7	1	0	-1.787252	3.050364	2.107589
8	1	0	0.801679	3.083683	2.933311
9	1	0	2.360853	2.961134	0.739539
10	1	0	0.755193	2.935045	-1.446884
11	75	0	0.097024	1.016099	0.891587
12	75	0	-0.097024	-1.016099	-0.891587
13	6	0	0.911549	-2.977623	-0.040130
14	6	0	-0.427900	-2.960502	0.415127
15	6	0	0.911980	-2.998382	-1.472587
16	1	0	1.794395	-2.944199	0.586980
17	6	0	-1.277684	-2.958581	-0.747833
18	1	0	-0.755193	-2.935045	1.446884
19	6	0	-0.454920	-3.023913	-1.909660
20	1	0	1.787252	-3.050364	-2.107589
21	1	0	-2.360853	-2.961134	-0.739539
22	1	0	-0.801679	-3.083683	-2.933311
23	6	0	-0.150525	0.019089	2.485824
24	8	0	-0.273062	-0.557179	3.494874
25	6	0	0.150525	-0.019089	-2.485824
26	8	0	0.273062	0.557179	-3.494874
27	6	0	1.712127	0.019593	0.648002
28	6	0	-1.712127	-0.019593	-0.648002
29	8	0	2.808075	-0.400171	0.623362
30	8	0	-2.808075	0.400171	-0.623362

Table S19. Theoretical Cartesian coordinates (in Å) for the structure **4S-2** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.741928	2.211053	0.708236
2	6	0	-0.641957	3.017239	1.149600
3	6	0	0.010699	3.552562	0.000000
4	6	0	-0.641957	3.017239	-1.149600
5	6	0	-1.741928	2.211053	-0.708236
6	1	0	-2.444200	1.693459	1.348668
7	1	0	-0.388563	3.227888	2.181394
8	1	0	0.861654	4.221620	0.000000
9	1	0	-0.388563	3.227888	-2.181394
10	1	0	-2.444200	1.693459	-1.348668
11	75	0	0.328605	1.244975	0.000000
12	75	0	-0.328605	-1.244975	0.000000
13	6	0	1.741928	-2.211053	-0.708236
14	6	0	1.741928	-2.211053	0.708236
15	6	0	0.641957	-3.017239	-1.149600
16	1	0	2.444200	-1.693459	-1.348668
17	6	0	0.641957	-3.017239	1.149600
18	1	0	2.444200	-1.693459	1.348668
19	6	0	-0.010699	-3.552562	0.000000
20	1	0	0.388563	-3.227888	-2.181394
21	1	0	0.388563	-3.227888	2.181394
22	1	0	-0.861654	-4.221620	0.000000
23	6	0	1.741928	0.965092	1.245211
24	8	0	2.620294	0.841490	2.004195
25	6	0	-1.741928	-0.965092	-1.245211
26	8	0	-2.620294	-0.841490	-2.004195
27	6	0	1.741928	0.965092	-1.245211
28	6	0	-1.741928	-0.965092	1.245211
29	8	0	2.620294	0.841490	-2.004195
30	8	0	-2.620294	-0.841490	2.004195

Table S20. Theoretical Cartesian coordinates (in Å) for the structure **4S-3** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.067186	3.096854	-0.943307
2	6	0	0.971338	2.074209	-1.941450
3	6	0	-0.396008	1.842767	-2.232206
4	6	0	-1.166129	2.713969	-1.384826
5	6	0	-0.268483	3.512832	-0.619192
6	1	0	1.982372	3.517089	-0.545909
7	1	0	1.812417	1.551169	-2.381846
8	1	0	-0.793025	1.144839	-2.957539
9	1	0	-2.246691	2.788214	-1.368175
10	1	0	-0.544529	4.296303	0.074935
11	75	0	-0.037564	1.348531	0.052555
12	75	0	0.037564	-1.348531	0.052555
13	6	0	-0.971338	-2.074209	-1.941450
14	6	0	0.396008	-1.842767	-2.232206
15	6	0	-1.067186	-3.096854	-0.943307
16	1	0	-1.812417	-1.551169	-2.381846
17	6	0	1.166129	-2.713969	-1.384826
18	1	0	0.793025	-1.144839	-2.957539
19	6	0	0.268483	-3.512832	-0.619192
20	1	0	-1.982372	-3.517089	-0.545909
21	1	0	2.246691	-2.788214	-1.368175
22	1	0	0.544529	-4.296303	0.074935
23	6	0	1.693648	-0.555935	0.620638
24	8	0	2.804068	-0.305315	0.898086
25	6	0	0.268483	1.784134	1.876280
26	8	0	0.439041	2.134115	2.974578
27	6	0	-1.693648	0.555935	0.620638
28	6	0	-0.268483	-1.784134	1.876280
29	8	0	-2.804068	0.305315	0.898086
30	8	0	-0.439041	-2.134115	2.974578

Table S21. Theoretical Cartesian coordinates (in Å) for the structure **4S-4** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.510372	-0.782163	2.890183
2	6	0	-0.297222	-0.492009	3.580558
3	6	0	-0.025372	0.910437	3.413775
4	6	0	-1.061094	1.461154	2.602931
5	6	0	-2.001587	0.424230	2.298769
6	1	0	-1.973495	-1.757736	2.804696
7	1	0	0.296191	-1.194934	4.151287
8	1	0	0.819689	1.453794	3.817526
9	1	0	-1.122435	2.494265	2.283300
10	1	0	-2.912526	0.529273	1.723768
11	75	0	0.052813	-0.070176	1.367945
12	75	0	0.052813	-0.070176	-1.367945
13	6	0	-1.061094	1.461154	-2.602931
14	6	0	-0.025372	0.910437	-3.413775
15	6	0	-2.001587	0.424230	-2.298769
16	1	0	-1.122435	2.494265	-2.283300
17	6	0	-0.297222	-0.492009	-3.580558
18	1	0	0.819689	1.453794	-3.817526
19	6	0	-1.510372	-0.782163	-2.890183
20	1	0	-2.912526	0.529273	-1.723768
21	1	0	0.296191	-1.194934	-4.151287
22	1	0	-1.973495	-1.757736	-2.804696
23	6	0	1.939101	-0.460009	1.488168
24	8	0	3.057185	-0.686290	1.707894
25	6	0	-0.963806	-1.262394	0.000000
26	8	0	-1.859165	-2.049486	0.000000
27	6	0	0.505826	1.457472	0.000000
28	6	0	1.939101	-0.460009	-1.488168
29	8	0	0.756007	2.617939	0.000000
30	8	0	3.057185	-0.686290	-1.707894

Table S22. Theoretical Cartesian coordinates (in Å) for the structure **4S-5** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.910075	-1.039623	1.186736
2	6	0	-1.933721	-2.387567	0.719914
3	6	0	-1.933721	-2.387567	-0.719914
4	6	0	-1.910075	-1.039623	-1.186736
5	6	0	-1.852497	-0.205043	0.000000
6	1	0	-1.992317	-0.704585	2.211794
7	1	0	-1.952978	-3.269499	1.348190
8	1	0	-1.952978	-3.269499	-1.348190
9	1	0	-1.992317	-0.704585	-2.211794
10	1	0	-2.082287	0.900026	0.000000
11	6	0	1.281965	-3.019331	-0.721001
12	6	0	1.281965	-3.019331	0.721001
13	6	0	1.847051	-1.779408	-1.167248
14	1	0	0.948499	-3.828303	-1.358963
15	6	0	1.847051	-1.779408	1.167248
16	1	0	0.948499	-3.828303	1.358963
17	6	0	2.200825	-1.031683	0.000000
18	1	0	2.018333	-1.487414	-2.194748
19	1	0	2.018333	-1.487414	2.194748
20	1	0	2.707588	-0.077918	0.000000
21	75	0	-0.090521	1.458021	0.000000
22	75	0	-0.059741	-1.430257	0.000000
23	6	0	1.650072	2.254680	0.000000
24	6	0	0.044245	1.246545	1.982552
25	6	0	0.044245	1.246545	-1.982552
26	6	0	-0.868148	3.231934	0.000000
27	8	0	2.724540	2.693062	0.000000
28	8	0	0.193067	1.137002	-3.120362
29	8	0	-1.377403	4.273994	0.000000
30	8	0	0.193067	1.137002	3.120362

Table S23. Theoretical Cartesian coordinates (in Å) for the structure **4S-6** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.002509	2.697511	-0.582169
2	6	0	-0.195992	1.907661	0.374260
3	6	0	-1.054011	1.611069	1.504386
4	6	0	-2.372888	1.788379	1.022725
5	6	0	-2.303073	2.622091	-0.189902
6	1	0	-0.612669	3.164124	-1.480136
7	1	0	0.878038	2.148865	0.548065
8	1	0	-0.742729	1.408968	2.520785
9	1	0	-3.264016	1.643648	1.624623
10	1	0	-3.163424	3.010286	-0.724038
11	6	0	-2.914213	-1.557772	-0.370319
12	6	0	-1.670945	-2.148524	-0.770905
13	6	0	-3.127898	-0.404279	-1.202895
14	1	0	-3.608706	-1.964081	0.353331
15	6	0	-1.092682	-1.321536	-1.784162
16	1	0	-1.240988	-3.059019	-0.372647
17	6	0	-2.025184	-0.258206	-2.061517
18	1	0	-3.981548	0.260096	-1.150295
19	1	0	-0.195299	-1.536435	-2.347900
20	1	0	-1.873531	0.542024	-2.775287
21	75	0	1.398893	0.100189	-0.061158
22	75	0	-1.220111	-0.172168	0.203390
23	6	0	2.063432	-1.630736	-0.489512
24	6	0	2.456024	0.877922	-1.452192
25	6	0	2.872320	0.348406	1.138038
26	8	0	2.424188	-2.697463	-0.773726
27	8	0	3.029017	1.344263	-2.349926
28	8	0	3.709283	0.490829	1.930600
29	6	0	-0.633045	-1.086084	1.745734
30	8	0	-0.362465	-1.749558	2.673882

Table S24. Theoretical Cartesian coordinates (in Å) for the structure **4S-7** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.387547	-2.754350	1.153324
2	6	0	0.892437	-3.445921	0.000000
3	6	0	1.387547	-2.754350	-1.153324
4	6	0	2.162011	-1.648542	-0.718617
5	6	0	2.162011	-1.648542	0.718617
6	1	0	1.204161	-3.033493	2.183898
7	1	0	0.302854	-4.353846	0.000000
8	1	0	1.204161	-3.033493	-2.183898
9	1	0	2.696659	-0.963307	-1.360271
10	1	0	2.696659	-0.963307	1.360271
11	75	0	-0.090313	-1.396478	0.000000
12	75	0	0.078022	1.465742	0.000000
13	6	0	0.645596	3.511383	-0.717662
14	6	0	-0.676726	3.197724	-1.166638
15	6	0	0.645596	3.511383	0.717662
16	1	0	1.500184	3.696324	-1.356160
17	6	0	-1.500224	3.055042	0.000000
18	1	0	-1.004702	3.151110	-2.197089
19	6	0	-0.676726	3.197724	1.166638
20	1	0	1.500184	3.696324	1.356160
21	1	0	-2.551886	2.798942	0.000000
22	1	0	-1.004702	3.151110	2.197089
23	6	0	-1.564395	0.281188	0.000000
24	8	0	-2.755191	0.300508	0.000000
25	6	0	-1.371456	-1.771419	-1.372444
26	6	0	-1.371456	-1.771419	1.372444
27	6	0	1.993193	1.108992	0.000000
28	8	0	-2.096820	-2.077114	-2.223381
29	8	0	-2.096820	-2.077114	2.223381
30	8	0	3.159893	1.134405	0.000000

Table S25. Theoretical Cartesian coordinates (in Å) for the structure **4S-8** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.591117	-2.467848	-1.168975
2	6	0	-0.545602	-2.231105	0.235019
3	6	0	0.859071	-1.902006	0.641697
4	6	0	1.417244	-1.378446	-0.599698
5	6	0	0.530902	-1.781094	-1.716957
6	1	0	-1.355822	-2.993265	-1.729105
7	1	0	-1.296158	-2.590205	0.931311
8	1	0	1.424131	-2.573084	1.286485
9	1	0	2.478584	-1.252357	-0.788804
10	1	0	0.862895	-1.830825	-2.748089
11	6	0	0.545602	2.231105	-0.235019
12	6	0	0.591117	2.467848	1.168975
13	6	0	-0.859071	1.902006	-0.641697
14	1	0	1.296158	2.590205	-0.931311
15	6	0	-0.530902	1.781094	1.716957
16	1	0	1.355822	2.993265	1.729105
17	6	0	-1.417244	1.378446	0.599698
18	1	0	-1.424131	2.573084	-1.286485
19	1	0	-0.862895	1.830825	2.748089
20	1	0	-2.478584	1.252357	0.788804
21	75	0	-0.883368	-0.220423	-1.072580
22	75	0	0.883368	0.220423	1.072580
23	6	0	2.730875	0.539668	1.361183
24	6	0	-0.891208	0.491985	-2.872486
25	6	0	-2.730875	-0.539668	-1.361183
26	8	0	-0.894893	0.946097	-3.938563
27	8	0	-3.866875	-0.763721	-1.501008
28	8	0	3.866875	0.763721	1.501008
29	6	0	0.891208	-0.491985	2.872486
30	8	0	0.894893	-0.946097	3.938563

Table S26.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	0.000000	3.089989	1.155818
2	6	0	1.349657	3.226585	0.721074
3	6	0	1.349657	3.226585	-0.721074
4	6	0	0.000000	3.089989	-1.155818
5	6	0	-0.840365	3.018829	0.000000
6	1	0	-0.329662	3.039215	2.186459
7	1	0	2.215675	3.333573	1.361659
8	1	0	2.215675	3.333573	-1.361659
9	1	0	-0.329662	3.039215	-2.186459
10	1	0	-1.918361	2.912465	0.000000
11	75	0	0.599210	1.186344	0.000000
12	75	0	-0.599210	-1.186344	0.000000
13	6	0	0.000000	-3.089989	-1.155818
14	6	0	0.840365	-3.018829	0.000000
15	6	0	-1.349657	-3.226585	-0.721074
16	1	0	0.329662	-3.039215	-2.186459
17	6	0	0.000000	-3.089989	1.155818
18	1	0	1.918361	-2.912465	0.000000
19	6	0	-1.349657	-3.226585	0.721074
20	1	0	-2.215675	-3.333573	-1.361659
21	1	0	0.329662	-3.039215	2.186459
22	1	0	-2.215675	-3.333573	1.361659
23	6	0	2.358934	0.422993	0.000000
24	8	0	3.456595	0.033766	0.000000
25	6	0	-2.358934	-0.422993	0.000000
26	8	0	-3.456595	-0.033766	0.000000
27	6	0	0.000000	0.000000	-1.612953
28	6	0	0.000000	0.000000	1.612953
29	8	0	0.000000	0.000000	-2.802424
30	8	0	0.000000	0.000000	2.802424

Table S27.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	-2.073545	-2.139320	0.000000
2	6	0	-1.419117	-2.656048	1.157879
3	6	0	-0.352528	-3.505716	0.711036
4	6	0	-0.352528	-3.505716	-0.711036
5	6	0	-1.419117	-2.656048	-1.157879
6	1	0	-2.921320	-1.465326	0.000000
7	1	0	-1.691920	-2.457122	2.186647
8	1	0	0.330782	-4.055924	1.345981
9	1	0	0.330782	-4.055924	-1.345981
10	1	0	-1.691920	-2.457122	-2.186647
11	6	0	0.352528	3.505716	-0.711036
12	6	0	1.419117	2.656048	-1.157879
13	6	0	0.352528	3.505716	0.711036
14	1	0	-0.330782	4.055924	-1.345981
15	6	0	2.073545	2.139320	0.000000
16	1	0	1.691920	2.457122	-2.186647
17	6	0	1.419117	2.656048	1.157879
18	1	0	-0.330782	4.055924	1.345981
19	1	0	2.921320	1.465326	0.000000
20	1	0	1.691920	2.457122	2.186647
21	75	0	-0.120853	1.333160	0.000000
22	75	0	0.120853	-1.333160	0.000000
23	6	0	1.419117	-0.926390	-1.350164
24	6	0	-1.419117	0.926390	1.350164
25	6	0	-1.419117	0.926390	-1.350164
26	8	0	-2.203835	0.749741	2.194658
27	8	0	-2.203835	0.749741	-2.194658
28	8	0	2.203835	-0.749741	-2.194658
29	6	0	1.419117	-0.926390	1.350164
30	8	0	2.203835	-0.749741	2.194658

Table S28. Theoretical Cartesian coordinates (in Å) for the structure **4T-3** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.156430	2.692004	-1.411965
2	6	0	-0.721141	3.481179	-0.310133
3	6	0	0.721141	3.481179	-0.310133
4	6	0	1.156430	2.692004	-1.411965
5	6	0	0.000000	2.211229	-2.105103
6	1	0	-2.187427	2.482107	-1.669306
7	1	0	-1.361868	4.003107	0.389191
8	1	0	1.361868	4.003107	0.389191
9	1	0	2.187427	2.482107	-1.669306
10	1	0	0.000000	1.595655	-2.995889
11	75	0	0.000000	1.336678	0.047709
12	75	0	0.000000	-1.336678	0.047709
13	6	0	1.156430	-2.692004	-1.411965
14	6	0	0.721141	-3.481179	-0.310133
15	6	0	0.000000	-2.211229	-2.105103
16	1	0	2.187427	-2.482107	-1.669306
17	6	0	-0.721141	-3.481179	-0.310133
18	1	0	1.361868	-4.003107	0.389191
19	6	0	-1.156430	-2.692004	-1.411965
20	1	0	0.000000	-1.595655	-2.995889
21	1	0	-1.361868	-4.003107	0.389191
22	1	0	-2.187427	-2.482107	-1.669306
23	6	0	0.000000	1.579335	1.960938
24	8	0	0.000000	1.829275	3.094969
25	6	0	-1.598671	0.000000	0.002588
26	8	0	-2.779842	0.000000	-0.158402
27	6	0	1.598671	0.000000	0.002588
28	6	0	0.000000	-1.579335	1.960938
29	8	0	2.779842	0.000000	-0.158402
30	8	0	0.000000	-1.829275	3.094969

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

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.964001	-1.219400	2.112459
2	6	0	0.890134	-2.594966	1.766756
3	6	0	-0.498781	-2.911248	1.578051
4	6	0	-1.274056	-1.719189	1.783874
5	6	0	-0.359033	-0.670101	2.131781
6	1	0	1.875306	-0.662199	2.292690
7	1	0	1.721951	-3.284336	1.697904
8	1	0	-0.893983	-3.889735	1.334864
9	1	0	-2.353209	-1.639179	1.765058
10	1	0	-0.629147	0.318221	2.474313
11	6	0	-1.274056	-1.719189	-1.783874
12	6	0	-0.498781	-2.911248	-1.578051
13	6	0	-0.359033	-0.670101	-2.131781
14	1	0	-2.353209	-1.639179	-1.765058
15	6	0	0.890134	-2.594966	-1.766756
16	1	0	-0.893983	-3.889735	-1.334864
17	6	0	0.964001	-1.219400	-2.112459
18	1	0	-0.629147	0.318221	-2.474313
19	1	0	1.721951	-3.284336	-1.697904
20	1	0	1.875306	-0.662199	-2.292690
21	75	0	-0.013296	1.492090	0.000000
22	75	0	0.044353	-1.475076	0.000000
23	6	0	0.053678	2.792417	-1.403908
24	6	0	1.959998	1.273653	0.000000
25	6	0	-2.001613	1.391902	0.000000
26	6	0	0.053678	2.792417	1.403908
27	8	0	0.095311	3.605834	-2.237556
28	8	0	-3.158102	1.280692	0.000000
29	8	0	0.095311	3.605834	2.237556
30	8	0	3.113389	1.122002	0.000000

Table S30. 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	6	0	0.714948	3.136121	0.982204
2	6	0	1.156590	3.129657	-0.376881
3	6	0	0.000000	3.134072	-1.217595
4	6	0	-1.156590	3.129657	-0.376881
5	6	0	-0.714948	3.136121	0.982204
6	1	0	1.348320	3.120938	1.860387
7	1	0	2.185462	3.105570	-0.714285
8	1	0	0.000000	3.117262	-2.300399
9	1	0	-2.185462	3.105570	-0.714285
10	1	0	-1.348320	3.120938	1.860387
11	75	0	0.000000	1.213332	0.001091
12	75	0	0.000000	-1.213332	0.001091
13	6	0	-1.156590	-3.129657	-0.376881
14	6	0	0.000000	-3.134072	-1.217595
15	6	0	-0.714948	-3.136121	0.982204
16	1	0	-2.185462	-3.105570	-0.714285
17	6	0	1.156590	-3.129657	-0.376881
18	1	0	0.000000	-3.117262	-2.300399
19	6	0	0.714948	-3.136121	0.982204
20	1	0	-1.348320	-3.120938	1.860387
21	1	0	2.185462	-3.105570	-0.714285
22	1	0	1.348320	-3.120938	1.860387
23	6	0	1.471208	0.000000	-0.849417
24	8	0	2.496412	0.000000	-1.447627
25	6	0	0.000000	0.000000	1.699835
26	8	0	0.000000	0.000000	2.886512
27	6	0	-1.471208	0.000000	-0.849417
28	8	0	-2.496412	0.000000	-1.447627

Table S31. 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	6	0	1.591533	-1.858616	1.232618
2	6	0	2.543790	-1.895418	0.166624
3	6	0	1.850070	-1.921176	-1.089083
4	6	0	0.443497	-2.017446	-0.810494
5	6	0	0.280389	-1.963674	0.630653
6	1	0	1.802801	-1.878305	2.293820
7	1	0	3.619435	-1.845839	0.285348
8	1	0	2.301087	-1.973603	-2.071489
9	1	0	-0.317441	-2.265375	-1.540710
10	1	0	-0.630589	-2.192858	1.184952
11	6	0	2.431959	1.576443	-1.095492
12	6	0	3.005154	1.363564	0.203102
13	6	0	1.104790	2.054222	-0.904288
14	1	0	2.930962	1.443490	-2.046715
15	6	0	2.023005	1.683191	1.199053
16	1	0	4.010463	1.011222	0.398549
17	6	0	0.844187	2.117622	0.508082
18	1	0	0.420701	2.345869	-1.689852
19	1	0	2.165935	1.670414	2.271719
20	1	0	-0.041121	2.530689	0.973987
21	75	0	-1.305551	-0.037204	-0.004068
22	75	0	1.326049	-0.054459	-0.012247
23	6	0	-2.102169	1.441798	-0.873815
24	6	0	-2.305495	0.333209	1.575447
25	6	0	-2.749785	-1.108153	-0.659164
26	8	0	-2.528443	2.388177	-1.403860
27	8	0	-3.561095	-1.829556	-1.080973
28	8	0	-2.856105	0.590833	2.567905

Table S32. Theoretical Cartesian coordinates (in Å) for the structure **3S-3** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.845511	-0.578839	-2.073332
2	6	0	2.185705	0.790718	-1.852566
3	6	0	3.166250	0.856732	-0.823702
4	6	0	3.453845	-0.482159	-0.397083
5	6	0	2.624262	-1.361827	-1.156537
6	1	0	1.149203	-0.954144	-2.810215
7	1	0	1.741733	1.641525	-2.355211
8	1	0	3.619345	1.762069	-0.439501
9	1	0	4.169510	-0.775451	0.360085
10	1	0	2.606512	-2.441554	-1.072257
11	75	0	1.231617	-0.056612	0.097420
12	75	0	-1.269880	-0.037222	-0.067158
13	6	0	-3.235819	-0.408833	0.933472
14	6	0	-3.276448	0.889695	0.331676
15	6	0	-3.081994	-1.361185	-0.126974
16	1	0	-3.356583	-0.628328	1.986373
17	6	0	-3.103235	0.740118	-1.084497
18	1	0	-3.382990	1.827423	0.861848
19	6	0	-2.960147	-0.656855	-1.372698
20	1	0	-2.979676	-2.432541	0.005208
21	1	0	-3.075207	1.542444	-1.810341
22	1	0	-2.855731	-1.095900	-2.356644
23	6	0	0.461320	-1.575773	0.995426
24	6	0	-0.553341	1.733180	-0.044312
25	6	0	1.449801	0.766271	1.836378
26	8	0	0.197421	-2.593927	1.514350
27	8	0	1.638406	1.252660	2.870468
28	8	0	-0.413412	2.901835	-0.088630

Table S33. Theoretical Cartesian coordinates (in Å) for the structure **3S-4** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.752732	-1.942830	1.099684
2	6	0	-2.615695	-1.901083	-0.038091
3	6	0	-1.787995	-1.884202	-1.205382
4	6	0	-0.413018	-2.011546	-0.807475
5	6	0	-0.384330	-2.041725	0.647902
6	1	0	-2.068589	-1.970913	2.135306
7	1	0	-3.696973	-1.868253	-0.019673
8	1	0	-2.137152	-1.846908	-2.229979
9	1	0	0.409898	-2.220468	-1.483160
10	1	0	0.455429	-2.312736	1.281660
11	75	0	-1.303827	-0.025363	0.007520
12	75	0	1.278651	-0.082317	-0.004641
13	6	0	3.161409	-0.430508	-1.125523
14	6	0	3.052226	0.957706	-0.788526
15	6	0	3.238078	-1.159987	0.110435
16	1	0	3.248617	-0.836828	-2.125341
17	6	0	3.021907	1.073912	0.648026
18	1	0	2.984818	1.777316	-1.492289
19	6	0	3.117177	-0.243058	1.210632
20	1	0	3.304973	-2.239351	0.197109
21	1	0	2.935197	1.996957	1.206763
22	1	0	3.173791	-0.482245	2.264850
23	6	0	0.400472	1.634757	-0.143101
24	8	0	0.358383	2.813234	-0.228716
25	6	0	-1.904745	1.109565	1.441615
26	6	0	-2.142439	1.207380	-1.215507
27	8	0	-2.282327	1.751816	2.330706
28	8	0	-2.659018	1.918596	-1.971902

Table S34. Theoretical Cartesian coordinates (in Å) for the structure **3S-5** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.228249	2.042185	-1.002118
2	6	0	-0.146049	1.376604	-1.680454
3	6	0	1.124404	1.800217	-1.096460
4	6	0	0.759783	2.895865	-0.170662
5	6	0	-0.591916	3.018506	-0.097047
6	1	0	-2.182201	2.224111	-1.501132
7	1	0	-0.226434	0.938812	-2.669845
8	1	0	2.006657	1.867530	-1.729320
9	1	0	1.474967	3.459318	0.420756
10	1	0	-1.138953	3.684656	0.562368
11	6	0	3.178577	-0.622231	0.691079
12	6	0	2.218021	-1.578284	1.172370
13	6	0	2.836623	0.640239	1.228457
14	1	0	4.000093	-0.832190	0.017737
15	6	0	1.309605	-0.880487	2.035481
16	1	0	2.228181	-2.643504	0.979092
17	6	0	1.687407	0.495245	2.059992
18	1	0	3.350107	1.570841	1.019506
19	1	0	0.482544	-1.320120	2.577633
20	1	0	1.184490	1.282950	2.606052
21	75	0	-1.411187	-0.069924	-0.224583
22	75	0	0.974656	-0.189519	-0.103246
23	6	0	-2.183165	-1.823802	0.217867
24	6	0	-1.954928	0.509930	1.468804
25	8	0	-2.663151	-2.838772	0.497791
26	8	0	-2.106819	0.860859	2.577655
27	6	0	1.153193	-1.202151	-1.695425
28	8	0	1.342540	-1.872732	-2.636319

Table S35. Theoretical Cartesian coordinates (in Å) for the structure **3S-6** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.673569	-2.037157	-0.883256
2	6	0	-0.727168	-1.923036	-1.326792
3	6	0	-1.587488	-2.141549	-0.192229
4	6	0	-0.727311	-1.842264	0.939759
5	6	0	0.692205	-2.073948	0.537169
6	1	0	1.463541	-2.372301	-1.546080
7	1	0	-1.012488	-2.051615	-2.367174
8	1	0	-2.586958	-2.564908	-0.188689
9	1	0	-1.048092	-1.941263	1.971473
10	1	0	1.402517	-2.629029	1.140922
11	6	0	-0.727283	1.842268	0.939761
12	6	0	-1.587464	2.141552	-0.192223
13	6	0	0.692231	2.073956	0.537167
14	1	0	-1.048060	1.941266	1.971477
15	6	0	-0.727148	1.923040	-1.326790
16	1	0	-2.586930	2.564919	-0.188679
17	6	0	0.673591	2.037161	-0.883258
18	1	0	1.402547	2.629031	1.140919
19	1	0	-1.012470	2.051619	-2.367171
20	1	0	1.463561	2.372302	-1.546086
21	75	0	1.265488	0.000002	0.085369
22	75	0	-1.452460	0.000001	-0.260917
23	6	0	-3.029191	0.000008	0.801116
24	6	0	2.487009	-0.000010	1.536612
25	6	0	2.837727	-0.000013	-0.959497
26	8	0	3.207588	-0.000021	2.452568
27	8	0	3.781711	-0.000020	-1.650399
28	8	0	-3.998539	0.000005	1.445332

Table S36. 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	6	0	1.785690	-2.617316	0.000000
2	6	0	1.001013	-2.918261	1.157441
3	6	0	-0.259396	-3.417098	0.720530
4	6	0	-0.259396	-3.417098	-0.720530
5	6	0	1.001013	-2.918261	-1.157441
6	1	0	2.792240	-2.217317	0.000000
7	1	0	1.302902	-2.770964	2.187208
8	1	0	-1.066857	-3.748783	1.360754
9	1	0	-1.066857	-3.748783	-1.360754
10	1	0	1.302902	-2.770964	-2.187208
11	75	0	-0.074984	-1.244752	0.000000
12	75	0	0.038736	1.324413	0.000000
13	6	0	-1.042483	3.376343	0.000000
14	6	0	-0.221969	3.292049	1.162636
15	6	0	-0.221969	3.292049	-1.162636
16	1	0	-2.124138	3.454341	0.000000
17	6	0	1.128849	3.106801	0.724126
18	1	0	-0.561662	3.322954	2.189956
19	6	0	1.128849	3.106801	-0.724126
20	1	0	-0.561662	3.322954	-2.189956
21	1	0	1.996784	3.025591	1.366739
22	1	0	1.996784	3.025591	-1.366739
23	6	0	0.258744	0.039957	1.604128
24	8	0	0.521283	0.010624	2.769967
25	6	0	0.258744	0.039957	-1.604128
26	8	0	0.521283	0.010624	-2.769967
27	6	0	-1.977224	-0.959547	0.000000
28	8	0	-3.139399	-0.884678	0.000000

Table S37. 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	-0.821359	3.089109	-1.092484
2	6	0	-2.164525	2.793846	-0.696864
3	6	0	-2.170064	2.627490	0.730035
4	6	0	-0.832868	2.804249	1.192406
5	6	0	0.000000	3.131339	0.070861
6	1	0	-0.486341	3.257814	-2.109555
7	1	0	-3.024212	2.737893	-1.352342
8	1	0	-3.030381	2.407407	1.348905
9	1	0	-0.509308	2.722607	2.222908
10	1	0	1.063752	3.332135	0.099411
11	75	0	-0.860818	0.973679	-0.174480
12	75	0	0.860818	-0.973679	-0.174480
13	6	0	0.832868	-2.804249	1.192406
14	6	0	0.000000	-3.131339	0.070861
15	6	0	2.170064	-2.627490	0.730035
16	1	0	0.509308	-2.722607	2.222908
17	6	0	0.821359	-3.089109	-1.092484
18	1	0	-1.063752	-3.332135	0.099411
19	6	0	2.164525	-2.793846	-0.696864
20	1	0	3.030381	-2.407407	1.348905
21	1	0	0.486341	-3.257814	-2.109555
22	1	0	3.024212	-2.737893	-1.352342
23	6	0	-2.282745	-0.295458	-0.226824
24	8	0	-3.211608	-1.003524	-0.236662
25	6	0	2.282745	0.295458	-0.226824
26	8	0	3.211608	1.003524	-0.236662
27	6	0	0.000000	0.000000	1.449918
28	8	0	0.000000	0.000000	2.639358

Table S38. 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	6	0	2.449789	-0.435224	1.604338
2	6	0	2.972196	-1.285012	0.564857
3	6	0	3.520958	-0.449217	-0.444720
4	6	0	3.349369	0.911632	-0.062932
5	6	0	2.689238	0.925171	1.210723
6	1	0	2.010469	-0.760215	2.537783
7	1	0	2.946005	-2.367384	0.549823
8	1	0	3.937414	-0.792088	-1.385333
9	1	0	3.655988	1.780830	-0.630467
10	1	0	2.430669	1.807158	1.782518
11	75	0	1.217419	0.003803	-0.183682
12	75	0	-1.155275	-0.014240	0.142932
13	6	0	-3.082632	0.244157	-1.023698
14	6	0	-3.129427	-1.013761	-0.342410
15	6	0	-3.010575	1.273251	-0.031832
16	1	0	-3.106024	0.393295	-2.095584
17	6	0	-3.072572	-0.771191	1.069297
18	1	0	-3.164955	-1.987933	-0.814051
19	6	0	-3.007183	0.651351	1.256419
20	1	0	-2.936416	2.335888	-0.229608
21	1	0	-3.116698	-1.522677	1.847090
22	1	0	-2.954783	1.165644	2.208858
23	6	0	-0.291989	-1.602841	-0.600909
24	8	0	-0.271022	-2.706146	-1.039245
25	6	0	0.229791	1.620273	-0.658987
26	8	0	0.012988	2.745987	-0.955219

Table S39. 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	1.054632	-3.072228	0.000000
2	6	0	0.214157	-3.063510	1.157211
3	6	0	-1.148971	-3.056400	0.717004
4	6	0	-1.148971	-3.056400	-0.717004
5	6	0	0.214157	-3.063510	-1.157211
6	1	0	2.137436	-3.071181	0.000000
7	1	0	0.551656	-3.041856	2.186137
8	1	0	-2.022339	-3.058652	1.357844
9	1	0	-2.022339	-3.058652	-1.357844
10	1	0	0.551656	-3.041856	-2.186137
11	75	0	-0.158436	-1.147627	0.000000
12	75	0	0.160329	1.207422	0.000000
13	6	0	-1.426745	2.614398	-0.715427
14	6	0	-1.426745	2.614398	0.715427
15	6	0	-0.178893	3.172695	-1.159061
16	1	0	-2.230264	2.263369	-1.349752
17	6	0	-0.178893	3.172695	1.159061
18	1	0	-2.230264	2.263369	1.349752
19	6	0	0.570276	3.522336	0.000000
20	1	0	0.129458	3.309746	-2.187531
21	1	0	0.129458	3.309746	2.187531
22	1	0	1.579198	3.919531	0.000000
23	6	0	0.631729	-0.042545	1.574416
24	8	0	1.027471	-0.154659	2.690341
25	6	0	0.631729	-0.042545	-1.574416
26	8	0	1.027471	-0.154659	-2.690341

Table S40. Theoretical Cartesian coordinates (in Å) for the structure **2S-3** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.877577	1.179386	-0.921964
2	6	0	1.893967	0.719031	-2.271834
3	6	0	1.893967	-0.719031	-2.271834
4	6	0	1.877577	-1.179386	-0.921964
5	6	0	1.824836	0.000000	-0.075123
6	1	0	1.923971	2.203058	-0.575535
7	1	0	1.917284	1.348512	-3.152827
8	1	0	1.917284	-1.348512	-3.152827
9	1	0	1.923971	-2.203058	-0.575535
10	1	0	2.003648	0.000000	1.066335
11	6	0	-1.877577	-1.179386	-0.921964
12	6	0	-1.893967	-0.719031	-2.271834
13	6	0	-1.824836	0.000000	-0.075123
14	1	0	-1.923971	-2.203058	-0.575535
15	6	0	-1.893967	0.719031	-2.271834
16	1	0	-1.917284	-1.348512	-3.152827
17	6	0	-1.877577	1.179386	-0.921964
18	1	0	-2.003648	0.000000	1.066335
19	1	0	-1.917284	1.348512	-3.152827
20	1	0	-1.923971	2.203058	-0.575535
21	75	0	0.000000	0.000000	1.314103
22	75	0	0.000000	0.000000	-1.269079
23	6	0	0.000000	1.326583	2.669392
24	6	0	0.000000	-1.326583	2.669392
25	8	0	0.000000	2.213078	3.432743
26	8	0	0.000000	-2.213078	3.432743

Table S41. Theoretical Cartesian coordinates (in Å) for the structure **2S-4** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.584762	3.265365	-1.176337
2	6	0	0.076188	3.619581	0.016020
3	6	0	1.325846	2.924817	0.065161
4	6	0	1.477729	2.209160	-1.172807
5	6	0	0.273982	2.389511	-1.926133
6	1	0	-1.574252	3.588786	-1.476893
7	1	0	-0.332935	4.234802	0.808886
8	1	0	2.070829	3.009516	0.845940
9	1	0	2.355895	1.656770	-1.479053
10	1	0	0.071250	2.001219	-2.916262
11	75	0	-0.152328	1.157480	-0.046927
12	75	0	0.152328	-1.157480	-0.046927
13	6	0	-0.273982	-2.389511	-1.926133
14	6	0	0.584762	-3.265365	-1.176337
15	6	0	-1.477729	-2.209160	-1.172807
16	1	0	-0.071250	-2.001219	-2.916262
17	6	0	-0.076188	-3.619581	0.016020
18	1	0	1.574252	-3.588786	-1.476893
19	6	0	-1.325846	-2.924817	0.065161
20	1	0	-2.355895	-1.656770	-1.479053
21	1	0	0.332935	-4.234802	0.808886
22	1	0	-2.070829	-3.009516	0.845940
23	6	0	-0.888238	1.072459	1.734777
24	8	0	-1.325846	1.114739	2.811605
25	6	0	0.888238	-1.072459	1.734777
26	8	0	1.325846	-1.114739	2.811605

Table S42. Theoretical Cartesian coordinates (in Å) for the structure **2S-5** using the MPW1PW91/SDD method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.239926	1.681012	0.864244
2	6	0	-0.164845	1.675765	1.342015
3	6	0	-0.963054	2.150990	0.241130
4	6	0	-0.175117	1.989652	-0.960902
5	6	0	1.255788	1.986437	-0.546028
6	1	0	2.062473	1.906510	1.537153
7	1	0	-0.425599	1.817311	2.384753
8	1	0	-1.896190	2.698713	0.307847
9	1	0	-0.504493	2.328332	-1.936311
10	1	0	2.017851	2.574213	-1.064812
11	6	0	-2.040312	-1.930284	-0.639748
12	6	0	-1.811408	-2.044957	0.778719
13	6	0	-0.803060	-1.700101	-1.295300
14	1	0	-3.004966	-2.005906	-1.125855
15	6	0	-0.431042	-1.860444	1.025886
16	1	0	-2.576172	-2.200212	1.529195
17	6	0	0.265238	-1.674841	-0.271546
18	1	0	-0.646962	-1.675074	-2.365492
19	1	0	0.064277	-1.896366	1.987294
20	1	0	1.346257	-2.076665	-0.514252
21	75	0	1.600678	-0.071481	-0.448007
22	75	0	-1.150002	0.018626	0.063481
23	6	0	-2.992282	0.576720	0.196774
24	6	0	2.674273	-0.553717	0.988233
25	8	0	3.295549	-0.793370	1.957969
26	8	0	-4.115780	0.882859	0.261909

Table S43. 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	0.000000	3.390390	-1.036048
2	6	0	-1.157396	3.208177	-0.221975
3	6	0	-0.716495	2.916266	1.111439
4	6	0	0.716495	2.916266	1.111439
5	6	0	1.157396	3.208177	-0.221975
6	1	0	0.000000	3.593446	-2.100684
7	1	0	-2.187708	3.268442	-0.549464
8	1	0	-1.359676	2.728493	1.961983
9	1	0	1.359676	2.728493	1.961983
10	1	0	2.187708	3.268442	-0.549464
11	75	0	0.000000	1.233229	-0.195133
12	75	0	0.000000	-1.233229	-0.195133
13	6	0	0.716495	-2.916266	1.111439
14	6	0	-0.716495	-2.916266	1.111439
15	6	0	1.157396	-3.208177	-0.221975
16	1	0	1.359676	-2.728493	1.961983
17	6	0	-1.157396	-3.208177	-0.221975
18	1	0	-1.359676	-2.728493	1.961983
19	6	0	0.000000	-3.390390	-1.036048
20	1	0	2.187708	-3.268442	-0.549464
21	1	0	-2.187708	-3.268442	-0.549464
22	1	0	0.000000	-3.593446	-2.100684
23	6	0	-1.538611	0.000000	0.402499
24	8	0	-2.632043	0.000000	0.879796
25	6	0	1.538611	0.000000	0.402499
26	8	0	2.632043	0.000000	0.879796

Table S44. 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	6	0	0.724868	2.894458	1.225097
2	6	0	0.673671	3.474975	-0.088660
3	6	0	-0.673671	3.477277	-0.519665
4	6	0	-1.476388	2.890106	0.505746
5	6	0	-0.619296	2.557127	1.607826
6	1	0	1.610661	2.797550	1.839902
7	1	0	1.526865	3.819601	-0.659602
8	1	0	-1.029298	3.807093	-1.488772
9	1	0	-2.549321	2.745824	0.466171
10	1	0	-0.932608	2.154115	2.562203
11	75	0	-0.005350	1.208364	-0.072186
12	75	0	0.005350	-1.208364	-0.072186
13	6	0	-0.724868	-2.894458	1.225097
14	6	0	-0.673671	-3.474975	-0.088660
15	6	0	0.619296	-2.557127	1.607826
16	1	0	-1.610661	-2.797550	1.839902
17	6	0	0.673671	-3.477277	-0.519665
18	1	0	-1.526865	-3.819601	-0.659602
19	6	0	1.476388	-2.890106	0.505746
20	1	0	0.932608	-2.154115	2.562203
21	1	0	1.029298	-3.807093	-1.488772
22	1	0	2.549321	-2.745824	0.466171
23	6	0	1.649718	0.513639	-0.753635
24	8	0	2.746453	0.331776	-1.145777
25	6	0	-1.649718	-0.513639	-0.753635
26	8	0	-2.746453	-0.331776	-1.145777

Table S45. 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	0.399747	-2.059519	0.430384
2	6	0	1.742394	-1.890938	0.937116
3	6	0	2.597856	-1.656436	-0.185904
4	6	0	1.805309	-1.569095	-1.375434
5	6	0	0.438620	-1.859077	-1.009620
6	1	0	-0.424683	-2.471072	1.007845
7	1	0	2.049851	-2.042047	1.963735
8	1	0	3.668327	-1.496437	-0.134418
9	1	0	2.169083	-1.431241	-2.385390
10	1	0	-0.352005	-2.086154	-1.719701
11	6	0	0.567860	2.188050	-0.507895
12	6	0	1.933650	1.964716	-0.854968
13	6	0	0.427336	2.000485	0.909526
14	1	0	-0.217180	2.488363	-1.189834
15	6	0	2.639645	1.660682	0.358020
16	1	0	2.363494	2.064413	-1.843225
17	6	0	1.709173	1.663638	1.450673
18	1	0	-0.479835	2.150953	1.482946
19	1	0	3.698866	1.446192	0.432998
20	1	0	1.941145	1.513521	2.496858
21	75	0	-1.410659	-0.219968	-0.048866
22	75	0	1.178199	0.035770	0.010379
23	6	0	-2.613927	-0.113770	1.430140
24	6	0	-2.560097	0.544519	-1.367148
25	8	0	-3.264151	-0.016019	2.396685
26	8	0	-3.174346	1.070874	-2.211007

Table S46. 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	1.408487	1.832469	0.745676
2	6	0	0.022830	1.720419	1.272468
3	6	0	-0.874415	2.102175	0.212413
4	6	0	-0.121775	1.905227	-1.021579
5	6	0	1.315334	2.027169	-0.690120
6	1	0	2.235721	2.157255	1.368904
7	1	0	-0.202470	1.834504	2.326546
8	1	0	-1.749432	2.733501	0.311105
9	1	0	-0.505197	2.171656	-1.999874
10	1	0	2.033134	2.527947	-1.335528
11	6	0	-2.193321	-1.899247	-0.687729
12	6	0	-1.996667	-2.032997	0.732452
13	6	0	-0.930699	-1.723331	-1.317138
14	1	0	-3.151192	-1.907125	-1.192346
15	6	0	-0.606352	-1.937905	1.008121
16	1	0	-2.779802	-2.160980	1.468809
17	6	0	0.095118	-1.761188	-0.268866
18	1	0	-0.745164	-1.662636	-2.380901
19	1	0	-0.131710	-2.044416	1.974228
20	1	0	1.185431	-2.033957	-0.456443
21	75	0	1.546039	-0.024695	-0.270081
22	75	0	-1.196108	-0.012858	0.061299
23	6	0	-2.980754	0.711875	0.223100
24	6	0	3.134900	-0.683070	0.536820
25	8	0	4.076258	-1.123597	1.081251
26	8	0	-4.085045	1.077488	0.306300

Complete Gaussian 03 reference (Reference 34)

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A. Gaussian 03, Revision C.02; Gaussian, Inc., Wallingford CT, **2004**.