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Metal Triangles versus Metal Chains and Terminal versus Bridging Hydrogen Atoms in Trinuclear Osmium Carbonyl Hydride Chemistry

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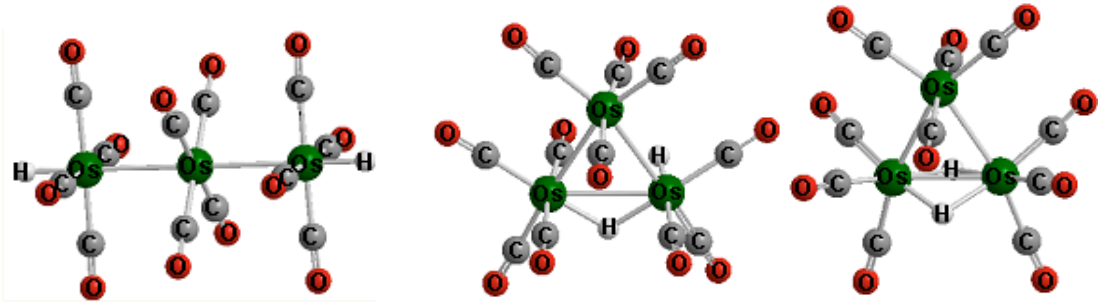
Supporting Information

Tables S1 to S5: Theoretical harmonic vibrational frequencies (in cm^{-1}) for the $H_2Os_3(CO)_n$ (n = 12, 11, 10, 9, 8) structures by the BP86/SDD method.

Tables S6 to S22. Theoretical Cartesian coordinates (in Å) for the $H_2Os_3(CO)_n$ (n = 12, 11, 10, 9, 8) structures using the MPW1PW91/SDD method.

Complete Gaussian 09 reference.



$H_2Os_3CO_{12}$ $H_2Os_3CO_{11}$ $H_2Os_3CO_{10}$

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Table S1. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the singlet structure of $H_2Os_3(CO)_n$ by the bP86/SDD method (infrared intensities in parentheses are in km/mol).

12-1(D_{4h})
23.7 (au, 0.0), 30.2 (eu, 0.0), 30.2 (eu, 0.0), 33.6 (ag, 0.0), 40.4 (bg, 0.0)
40.4 (bu, 0.0), 43.3 (bu, 0.0), 43.6 (eg, 0.0), 43.6(eg, 0.0), 49.1 (eu, 0.0)
49.1(eu, 0.0), 64.6(ag, 0.0), 72.1 (e, 0.2), 73.1(eg, 0.0), 73.1 (eg, 0.0)
84.6 (eu, 0.1), 84.6 (eu, 0.1), 85.6 (au, 0.4), 86.4 (eg, 0.0), 86.3 (eg, 0.0)
87.7 (eu, 0.0), 87.7 (eu, 0.0), 90.0 (au, 9.4), 92.0 (bg, 0.0), 92.9 (bg, 0.0)
93.1 (bu, 0.0), 104.7 (ag, 0.0), 143.2 (au, 1.3), 364.2 (ag, 0.0), 366.4 (au, 0.0)
368.0 (ag, 0.0), 394.4 (eg, 0.0), 394.4 (eg, 0.0), 396.8 (eu, 2.1),
396.8 (eu, 2.1) 409.5 (eu, 1.4), 409.5 (eu, 1.4), 411.7 (eg, 0.0),
411.7 (eg, 0.0), 414.0 (eu, 74.1) 414.0 (eu, 74.1), 455.4 (eg, 0.0),
455.4 (eg, 0.0), 465.7 (bu, 0.0), 478.2 (bu, 0.0), 478.2(bg, 0.0),
484.3 (bg, 0.0), 489.6 (au, 19.1), 490.4 (ag, 0.0),492.2 (ag, 0.0),
494.7(bg, 0.0), 495.6 (bu, 0.0), 500.8 (bg, 0.0), 505.6 (bu, 0.0),
505.6 (bg, 0.0), 584.0 (eu, 17.3) 584.0 (eu, 17.3), 584.5 (eg, 0.0),
584.5 (eg, 0.0), 590.7 (eu, 34.5), 590.7 (eu, 34.5), 611.8 (au, 684.3),
627.8 (au, 17.5), 628.1(ag, 0.0), 728.4 (eu, 124.6), 728.4 (eu, 124.6),
728.8 (eg, 0.0), 728.8 (eg, 0.0), 1963.7 (eu, 91.9), 1963.7(eu, 91.9),
1995.6 (eg, 0.0), 1995.6 (eg, 0.0), 2007.4 (bg, 0.0), 2008.0 (eu, 3114.6),
2008.0 (eu, 3114.6), 2030.3 (ag, 0.0), 2030.3 (bu, 0.0)), 2033.1 (bg, 0.0),
2055.05(au, 175.0), 2055.2(ag, 0.0), 2075.2 (au, 957.2), 2112.7 (ag, 0.0)

Table S2. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the three singlet structures of $H_2Os_3(CO)_{11}$ by the bP86/SDD method (infrared intensities in parentheses are in km/mol).

11-1(C_1)	**11-2(C_s)**
13.7 (a, 0.0), 27.8 (a, 0.1) 39.3 (a, 0.2)	14.5 (a", 0.0), 31.5 (a", 0.0) 39.4 (a", 0.3)
49.7 (a, 0.1), 49.8 (a, 0.1), 54.0 (a, 0.0)	47.8 (a', 0.2), 48.5 (a", 0.1), 52.4 (a', 0.1)
60.9 (a, 0.3), 72.2 (a, 0.1) 75.3 (a, 0.2)	53.0 (a", 0.1), 72.6 (a', 0.2), 73.7 (a', 0.1)
75.9 (a, 0.1), 78.1 (a, 0.2), 82.0 (a, 0.1)	74.2 (a", 0.1), 78.4 (a", 0.1), 80.2 (a', 0.0)
88.0 (a, 0.1), 88.5 (a, 0.2) 90.1 (a, 0.3)	87.5 (a', 0.7), 88.5 (a", 0.1), 90.4 (a', 0.5)
91.8 (a, 1.0), 93.4 (a, 0.4), 95.4 (a, 0.1)	92.0 (a', 0.7), 92.8 (a", 0.0), 95.8 (a", 0.0)
96.2 (a, 0.3), 97.2 (a, 0.3) 109.6 (a, 0.4)	100.2(a', 0.5), 106.3(a', 1.3), 116.3(a", 0.0)
114.1 (a, 0.9), 132.7 (a, 0.2), 135.5 (a, 0.1)	120.3(a', 0.2), 128.6(a', 0.1), 132.8 (a", 0.0)
138.4 (a, 0.0), 320.3 (a, 0.9) 386.3 (a, 0.9)	135.7(a", 0.2), 334.0(a", 0.9), 385.1(a', 1.4)
391.0 (a, 0.2), 395.4 (a, 8.2), 399.9 (a, 5.5)	386.4(a", 0.0) 392.0(a", 0.1), 397.1(a", 1.7)
401.5 (a, 5.8), 404.8 (a, 3.3), 408.4 (a, 3.3)	400.2(a", 7.0), 409.1(a", 8.5), 410.3(a", 2.6)
410.4(a, 17.7), 430.2(a, 28.1), 435.2(a, 4.1)	416.6(a", 18.7), 426.2(a', 4.5), 433.8(a", 1.7)
441.1 (a, 2.2), 454.1 (a, 1.2), 455.3(a, 4.2)	436.3(a", 52.7), 452.4(a', 12.6), 452.7(a',2.4)
464.1(a, 12.0), 467.2(a, 0.5), 476.6(a, 21.4)	462.3(a', 3.0), 471.3(a', 0.5), 479.9(a', 28.9)
481.4(a, 8.2), 488.3 (a, 0.2), 496.6(a, 19.5)	483.5(a', 17.4), 485.1(a', 0.3) 493.9(a',12.3),
502.9(a, 9.0), 505.2 (a, 4.1), 508.3 (a, 1.4)	97.2(a',15.6), 508.2(a',12.0), 514.2(a", 1.7)
520.6(a, 0.6), 525.9 (a, 5.4), 533.2(a, 19.8)	516.8(a", 0.1), 532.1(a',11.0), 540.6(a",23.9)
543.5(a, 21.3), 546.6(a, 76.4), 560.2(a, 68.6)	549.2 (a", 0.0), 551.6(a',17.5), 567.1(a', 73.3)
569.8(a, 33.5),575.9(a,78.8.), 583.4(a,195.1)	573.4(a',56.5),585.0(a',153.8),597.2(a',139.8)
592.2(a, 84.9), 626.5 (a, 54.9)	603.6 (a', 1.0), 617.0 (a", 59.8),
800.9(a, 71.7), 809.2 (a, 22.6)	700.5 (a', 175.6), 768.3 (a", 31.9)
1251.2(a, 16.3) ,1498.1(a, 62.7)	1152.5 (a', 26.1), 1418.4 (a', 17.1)
1941.7(a, 130.6), 1976.9 (a, 296.4)	1964.7 (a', 114.1), 1979.2 (a', 550.2)
1983.8 (a, 317.2), 1989.3 (a, 238.9)	1986.3 (a", 442.8), 1988.0 (a', 132.5)
2000.8(a, 468.1), 2010.1 (a, 483.8)	1999.9 (a', 456.8), 2008.6 (a', 436.9)
2024.7 (a, 778.2), 2032.7 (a, 1655.4)	2026.6 (a', 273.7), 2027.2 (a", 2141.6)
2032.9 (a, 335.8), 2052.8 (a, 1137.7)	2039.2 (a', 1440.9), 2058.4 (a', 943.5)
2068.0 (a, 1005.4), 2106.0 (a, 92.8)	2102.2 (a', 80.5), 2109.8(a', 2.4)
11-3(C_1)	**11-4(C_1)**
28.1 (a, 0.0), 41.4 (a, 0.0) 43.2 (a, 0.0)	11.6 (a, 0.1), 29.9 (a, 0.2), 34.8 (a, 0.0)
45.9 (a, 0.1) 52.4 (a, 0.0), 63.9 (a, 0.1)	47.2 (a, 0.3), 55.7 (a, 0.1), 56.5 (a, 0.0)
65.8 (a, 0.2), 70.6 (a, 0.6) 73.5 (a, 0.1)	63.2 (a, 0.1), 72.5 (a, 0.1), 73.9 (a, 0.0)
74.8 (a, 0.3) 76.6 (a, 0.2), 78.8 (a, 0.1)	78.6 (a, 0.1), 79.9 (a, 0.1), 83.2 (a, 0.8)
84.3 (a, 0.0), 85.0 (a, 0.1) 86.6 (a, 0.1)	84.8 (a, 0.4), 88.9 (a, 0.0), 90.0 (a', 0.1)
88.0 (a, 0.3) 91.2 (a, 0.2), 93.5 (a, 0.4)	93.1 (a, 1.3), 95.1 (a, 0.0), 96.7 (a, 0.6)
94.5 (a, 0.7), 97.1 (a, 0.3), 106.0 (a, 0.1)	97.2 (a, 0.0), 104.4 (a, 0.1), 111.3 (a, 0.9)
111.8 (a, 0.2), 121.7 (a, 1.3), 149.8 (a, 0.0)	113.0 (a, 0.4), 130.8 (a, 0.0), 131.1 (a, 0.1)
208.9 (a, 8.9), 320.9 (a, 0.9), 344.8(a, 1.1)	134.9 (a, 0.2), 362.6 (a, 0.3), 382.7 (a, 4.6)
355.2 (a, 14.4), 374.6 (a, 4.4), 391.0 (a, 0.5)	384.9 (a, 0.0) 394.2 (a, 5.2), 396.7 (a, 1.4)

402.6(a, 13.5), 408.5(a, 12.3), 409.8(a, 0.7)	397.9 (a, 1.0), 406.3 (a, 8.5), 412.0 (a, 3.0)
415.7 (a, 23.2), 421.8(a, 13.9),428.7(a, 35.5)	415.5 (a, 28.1), 422.3(a, 16.6), 433.1(a, 31.6)
447.6(a, 9.2), 449.7(a, 13.7), 459.3(a, 36.1)	434.6 (a, 6.6), 451.1(a, 12.7), 459.5(a, 0.3)
463.5 (a, 48.7), 469.6(a, 40.4), 475.9(a, 4.2)	462.0 (a, 9.3), 472.5(a, 4.1), 478.7(a, 23.9)
477.9 (a, 1.5), 481.0 (a, 4.4), 483.2(a, 7.2)	483.4 (a, 10.9), 486.3 (a, 12.0), 495.6(a,17.4)
493.3 (a, 24.7), 500.4 (a, 6.9), 504.0 (a, 2.6)	498.6 (a,10.5), 510.5 (a,2.6), 510.7 (a, 0.2)
507.7(a, 12.1), 514.9(a, 74.3) 528.4 (a, 11.8)	520.5 (a, 0.0), 537.9 (a,39.1), 540.4 (a,4.5)
550.6(a, 19.9),555.0(a, 39.5),562.6(a, 208.7)	558.4 (a, 48.3), 572.4 (a, 2.5), 574.3 (a, 64.2)
572.5(a, 14.7),583.5(a, 114.1),584.9(a, 30.9)	586.8(a,53.2), 591.6(a,134.1), 593.1(a,139.5)
612.4 (a, 118.1), 630.3 (a, 43.4)	597.8(a, 10.1), 663.9(19.8)
704.2 (a, 49.8), 1158.9 (a, 18.3)	719.0 (a, 112.5), 750.8 (a, 63.0)
1275.7 (a, 77.1), 1366.5 (a, 10.2)	1246.4 (a, 11.5), 1390.0 (a, 86.7)
1591.3 (a, 14.3), 1786.7 (a, 443.5)	1965.7 (a, 17.4), 1976.8 (a, 227.0)
1976.4 (a, 321.1), 1984.2 (a, 470.6)	1982.4 (a, 602.4), 1985.4 (a, 156.9)
1986.6 (a, 289.9), 2002.9 (a, 512.1)	2001.8 (a, 842.2), 2008.9 (a, 392.0)
2011.8 (a, 408.8), 2026.1 (a, 1284.2)	2025.6 (a, 228.3), 2027.6 (a, 2084.1)
2030.8 (a, 934.3), 2039.7 (a, 1462.1)	2033.4 (a, 1281.8), 2060.4 (a, 384.7)
2061.9 (a, 965.9), 2101.7 (a, 175.5)	2063.8 (a, 764.7), 2105.8(a, 51.2)

Table S3. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the two singlet structures of $H_2Os_3(CO)_{10}$ by the bP86/SDD method (infrared intensities in parentheses are in km/mol).

10-1S(C_{2v})	**10-2S(C_1)**
32.0 (b1, 0.0), 33.1 (a2, 0.0), 35.9 (b2, 0.0)	26.8 (a, 0.2), 31.5 (a, 0.0), 43.6 (a, 0.0)
49.8 (a2, 0.0), 55.8 (a1, 0.4), 58.2 (b1, 0.1)	47.6 (a, 0.1), 58.9 (a, 0.1), 66.4 (a, 0.1)
71.3 (b1, 0.1), 72.8 (a1, 0.0), 72.8(b2, 0.7)	69.5 (a, 0.5), 72.5 (a, 0.0), 75.8 (a, 0.1)
76.4 (a2, 0.0), 84.5 (a1, 0.1), 84.6 (b2, 0.1)	78.9 (a, 0.5), 81.4 (a, 0.1), 83.8 (a, 0.0)
86.8 (b1, 0.0), 88.7 (a1, 0.2), 89.4 (a2, 0.0)	87.1 (a, 0.1), 89.2 (a, 0.1), 90.7 (a, 0.2)
90.9 (b2, 1.0), 91.8 (b1, 0.0), 95.3 (a1, 0.3)	92.5 (a, 0.0), 94.8 (a, 1.6), 96.8 (a, 0.7)
96.8 (a2, 0.0), 97.2 (b2, 0.1), 125.5(b2, 0.5)	98.0 (a, 0.4), 106.9 (a, 0.1), 118.1 (a, 0.4)
129.2 (a1, 1.1), 169.0 (a1, 0.0)	126.7 (a, 0.4), 171.3 (a, 0.3)
391.1(a2, 0.0), 395.2 (b1, 2.8)	361.2 (a, 5.0), 387.8 (a, 4.3)
402.1 (b2, 3.2), 412.9 (a1, 1.8)	393.5 (a, 1.2), 398.1 (a, 0.8)
414.3 (b1, 0.0), 431.1 (a2, 0.0)	403.7 (a, 13.0), 412.4 (a, 12.1)
432.5 (b1, 22.8), 439.6 (b2, 0.5)	418.5 (a, 15.7), 427.1 (a, 7.8)
444.1 (b1, 11.7), 448.5 (b2, 0.3)	439.2 (a, 3.6), 443.2 (a, 3.2)
456.2 (a1, 0.7), 458.5 (b2, 0.0)	449.1 (a, 8.1), 457.6 (a, 12.8)
463.6 (a2, 0.0), 471.1 (a1, 13.5)	459.0 (a, 5.1), 465.1 (a, 3.9)
472.5 (a2, 0.0), 476.7 (a1, 17.0)	471.6 (a, 10.9), 479.3 (a, 3.3)
487.6 (b2, 1.2), 487.8 (a1, 8.9)	480.4 (a, 5.1), 489.2 (a, 19.4)
489.9 (b1, 3.4), 499.5 (a2, 0.0)	494.7 (a, 4.1), 502.6 (a, 7.3)
506.4 (a1, 0.0), 512.4 (b1, 91.9)	504.8 (a, 11.0), 519.6 (a, 47.6)
519.4 (a2, 0.0), 529.2 (b1, 2.7)	528.9 (a, 39.2), 537.7 (a, 44.9)
546.4 (b2, 169.5), 562.5 (a1, 81.7)	540.7 (a, 17.7), 555.3 (a, 77.9)
574.3 (a1, 181.3), 576.2 (b2, 1.9)	560.1 (a, 160.8), 568.7 (a, 61.4)
590.8 (a1, 2.6), 592.9 (b2, 80.8)	575.7 (a, 58.9), 581.4 (a, 51.6)
629.7 (b1, 0.7), 706.7 (a1, 54.1)	673.4 (a, 55.6), 676.2 (a, 29.9)
1249.4(a2, 0.0), 1257.8(b2, 197.7)	1221.5 (a, 72.8), 1275.8 (a, 16.7)
1417.6 (b1, 2.9), 1461.4 (a1, 2.7)	1440.9 (a, 90.6), 1451.6(a, 18.0)
1976.3 (b1, 104.3), 1976.7 (b2, 279.3)	1966.0 (a, 155.3), 1974.7 (a, 304.3)
1989.7 (b2, 157.0), 1993.8 (a1, 1291.8)	1983.4 (a, 195.1), 1994.4 (a, 575.7)
2000.2 (a1, 8.5), 2001.7 (a2, 0.0)	2003.5 (a, 365.3), 2011.5 (a, 1769.1)
2011.2 (b1, 2198.1), 2038.9 (a1, 1108.6)	2020.6 (a, 385.5), 2032.2 (a, 1678.5)
2055.7 (b2, 1546.3), 2084.2 (a1, 17.9)	2051.5 (a, 1242.3), 2088.3 (a, 149.5)

Table S4. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the six singlet structures of $H_2Os_3(CO)_9$ by the bP86/SDD method (infrared intensities in parentheses are in km/mol).

9-1S(C_s)	**9-2 (C_1)**
15.0 (a, 0.0), 36.4 (a, 0.0), 40.7 (a, 1.2)	23.7 (a, 0.1), 31.3 (a, 0.2) 41.0 (a, 0.3)
42.7 (a, 0.0), 51.9 (a, 0.3), 56.9 (a, 0.0)	44.2 (a, 0.3), 55.6 (a, 0.3), 64.3 (a, 0.1)
62.9 (a, 0.2), 66.9 (a, 1.7), 73.0 (a, 0.0)	66.8 (a, 0.2), 75.5 (a, 0.6), 77.7 (a, 0.6)
81.6 (a, 0.6), 82.5 (a, 0.1), 83.3 (a, 0.1)	80.6 (a, 0.0), 83.9 (a, 0.3), 85.8 (a, 0.0)
84.9 (a, 0.2), 91.2 (a, 0.1) 93.1 (a, 0.0)	89.5 (a, 0.2), 91.2 (a, 0.6), 92.6 (a, 0.3)
94.0 (a, 0.2), 94.8 (a, 0.0), 97.8 (a, 0.2)	96.1 (a, 0.3), 100.7 (a, 0.0), 113.8 (a, 1.0)
130.7 (a, 1.4), 134.4 (a, 0.3), 174.7 (a, 0.3)	132.4(a, 0.4), 161.2(a, 1.2), 194.7(a, 3.6)
360.2(a, 7.6), 374.9(a, 13.6), 385.8 (a, 4.3)	337.6(a, 34.5), 356.9(a, 2.5), 376.5(a,3.3)
395.1 (a, 0.2), 410.8 (a, 3.3), 417.2(a, 12.2)	387.6(a, 0.9), 389.9(a, 3.1), 420.5(a,12.4)
431.2 (a, 4.6), 432.3(a, 15.4), 441.0 (a, 5.1)	429.9(a, 7.2), 436.5 (a, 4.4), 450.2(a, 6.2)
441.6(a, 4.3), 449.9(a, 0.7), 465.9(a, 21.5)	461.8(a, 4.1), 464.5(a, 27.1) 469.6(a, 4.7)
468.0(a, 100.3), 472.5(a, 4.0), 484.6(a, 3.9)	473.2 (a, 7.0), 482.2(a, 7.5), 490.1(a, 2.7)
499.8(a, 9.1), 504.6 (a, 0.1), 505.3 (a, 1.1)	497.1(a,52.7), 502.6(a,20.8), 505.8(a,7.3)
512.1(a, 27.4), 514.9(a, 40.1), 531.2(a, 54.8)	514.9(a, 1.8) 517.8(a,39.2), 529.8(a,26.1)
537.8(a, 50.9), 555.6 (a, 2.9), 564.0 (a, 6.4)	544.0(a,31.6),554.8(a,56.8),559.6(a,135.7)
566.0 (a, 38.8), 584.0 (a, 5.5), 591.1 (a, 79.4)	571.9(a,1.1), 591.8(a,10.2), 592.9(a, 25.2.)
591.7(a, 31.4), 640.7(a, 114.4), 1235.4(a,0.3)	622.8(a,87.4),638.3(a,34.1),1279.1(a,48.1)
1251.1 (a, 106.8), 1407.0 (a, 2.5)	1330.8 (a, 25.9), 1465.3 (a, 3.7)
1456.8 (a, 6.1), 1957.5(a, 382.3)	1565.3 (a, 80.0), 1838.9 (a, 429.5)
1959.1 (a, 278.5), 1990.3 (a, 66.0)	1976.1 (a, 267.8), 1984.8 (a, 318.0)
1997.8 (a, 671.6), 1998.2 (a, 1.3)	1987.8 (a, 441.4), 1996.7 (a, 1184.9)
2002.5 (a, 1840.2), 2019.4 (a, 1671.3)	2003.3 (a, 318.9), 2027.8 (a, 2116.7)
2049.1 (a, 1648.9), 2070.8 (a, 12.6)	2042.1 (a, 1518.6), 2070.5 (a, 189.5)

9-3 (C_1)	**9-4 (C_1)**
32.1 (a, 0.0), 41.7 (a, 0.0) 45.5 (a, 0.1)	20.4 (a, 0.1), 28.2 (a, 0.1), 36.8 (a, 0.3)
49.8 (a, 0.2), 55.0 (a, 0.0), 60.6 (a, 0.2)	44.1 (a, 0.1), 51.3 (a, 0.1), 61.0 (a, 0.1)
64.9 (a, 0.2), 70.9 (a, 0.1), 73.8 (a, 0.1)	65.9 (a, 0.3), 66.9 (a, 0.1), 72.4 (a, 0.5)
75.9 (a, 0.1), 78.5 (a, 0.1), 83.9 (a, 0.1)	77.6 (a, 0.1), 83.1 (a, 0.3), 84.0 (a, 0.3)
87.2 (a, 0.3), 91.2 (a, 0.0), 92.5 (a, 0.2)	88.0 (a, 0.3), 89.8 (a, 0.2), 91.2 (a, 0.3)
94.4 (a, 0.2), 95.9 (a, 0.4), 105.7 (a, 0.0)	92.2 (a, 0.1), 94.8 (a, 0.0), 104.2 (a, 0.4)
123.5 (a, 1.2), 158.6 (a, 0.8), 205.6 (a, 2.2)	111.6 (a, 0.2), 168.9(a, 1.2), 207.3(a, 1.1)
341.4 (a, 1.3), 365.5 (a, 4.2), 370.3(a, 15.0)	351.3 (a, 0.5), 370.3(a, 6.8), 378.1(a, 8.2)
391.9(a, 17.9), 399.9(a,25.0), 410.0(a, 7.2)	385.2(a, 4.3), 402.6(a, 12.0), 413.5(a,5.5)
424.2 (a, 3.8), 443.9 (a, 4.4), 448.8 (a, 9.8)	421.0(a,12.9),425.4(a,12.6),432.0(a,10.9)
459.3 (a, 3.9), 460.7 (a, 2.6), 472.0 (a, 3.8)	452.1(a, 4.9), 456.1(a, 4.5), 458.7 (a, 9.7)
476.0 (a, 2.1), 491.8 (a, 8.7), 499.2(a, 29.0)	464.3(a,18.8), 478.2(a, 1.1), 487.0(a, 5.0)
501.6(a, 12.0), 508.0(a, 4.9), 509.6(a, 11.1)	500.7(a, 30.6), 502.6(a, 6.0), 510.0(a,5.3)
529.8(a, 20.2), 531.6 (a, 50.3), 556.9(a, 9.7)	519.7(a,18.6),527.3(a,19.5),532.0(a,45.5)

560.2 (a, 23.4), 568.0(a, 19.2), 573.2(a, 76.7)	542.8(a,14.2),552.7(a,43.5),557.3(a,100.1)
588.6 (a, 17.6), 596.3(a, 13.9)	587.8 (a, 1.5), 596.0(a, 52.2)
606.9(a, 53.8), 635.3 (a, 39.9)	603.1(a, 45.1), 694.7 (a, 20.2)
737.3 (a, 26.3), 1115.6 (a, 40.3)	772.5 (a, 46.4), 779.4 (a, 21.5)
1226.7 (a, 3.2), 1537.5 (a, 1.0)	1167.2 (a, 7.7), 1520.3 (a, 10.7)
1585.1 (a, 40.7), 1812.3(a, 344.7)	1834.3 (a, 453.8), 1961.9 (a, 582.5)
1955.7 (a, 379.0), 1987.3 (a, 620.6)	1978.4 (a, 247.5), 1993.3 (a, 915.3)
1997.3 (a, 352.7), 2007.6 (a, 1502.8)	1994.8 (a, 1101.6), 2003.9 (a, 1243.1)
2012.5 (a, 950.0), 2020.0 (a, 1213.1)	2011.9 (a, 1316.2), 2045.2 (a, 1031.1),
2068.8 (a, 1110.3), 2088.0 (a, 58.5)	2075.9 (a, 154.9), 2245.0 (a, 8.3)

Table S5. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the six singlet structures of $H_2Os_3(CO)_8$ by the bP86/SDD method (infrared intensities in parentheses are in km/mol).

8-1 (C_1)	**8-2 (C_1)**	**8-3 (C_1)**
12.4 (a, 0.0), 28.5 (a, 0.2)	16.6 (a, 0.1), 33.9 (a, 0.1)	15.7 (a, 0.4), 28.7 (a, 0.3)
40.8 (a, 0.0), 54.1 (a, 0.2)	42.9 (a, 0.2), 52.7 (a, 0.2)	39.5 (a, 0.2), 46.1 (a, 0.6)
57.3 (a, 0.1), 59.2 (a, 0.5)	62.1 (a, 0.1), 66.6 (a, 0.2)	54.2 (a, 0.2), 63.1 (a, 0.2)
66.2 (a, 0.0), 76.5 (a, 0.1)	70.6 (a, 0.1), 76.3 (a, 0.3),	70.5 (a, 0.1), 76.7 (a, 0.3)
77.9 (a, 0.7), 84.1 (a, 0.4)	80.4 (a, 0.0), 82.6 (a, 0.4)	80.2 (a, 0.6), 82.7 (a, 0.3)
86.5 (a, 0.1), 87.3 (a, 0.1)	87.3 (a, 0.7), 89.2 (a, 0.1)	88.4 (a, 0.6), 88.8 (a, 0.1)
91.9 (a, 0.4), 92.4 (a, 0.1)	94.1 (a, 0.5), 95.3 (a, 0.0)	89.9 (a, 0.3), 91.5 (a, 0.2)
95.8 (a, 0.0), 98.5 (a, 0.6)	97.1 (a, 0.0), 100.1 (a, 0.3)	97.6 (a, 0.1), 122.5 (a, 0.3)
116.2 (a, 0.7), 160.8 (a, 2.9)	122.6 (a, 0.7), 149.6 (a, 2.1)	132.2 (a, 0.1), 166.7 (a, 2.0)
189.3 (a, 1.4), 365.8 (a, 2.6)	184.5 (a, 0.6), 363.1(a, 2.5)	260.3 (a, 0.4), 336.5(a, 19.9)
394.4 (a, 1.6), 400.9(a, 16.6)	400.1 (a, 12.0), 407.1(a, 4.4)	376.3 (a, 4.2), 401.0 (a, 4.4)
407.3 (a, 1.0), 428.5 (a, 4.5)	415.3 (a, 13.5), 432.7(a, 7.0)	414.3(a, 19.6), 423.2(a, 8.1)
431.3 (a, 7.6), 437.4(a, 14.5)	442.0(a, 0.3), 446.7 (a, 7.4)	425.2(a, 2.9), 429.1 (a, 5.2)
442.0 (a, 4.6), 449.7 (a, 2.6)	449.1 (a, 3.6), 456.1(a, 0.9)	438.2 (a, 13.1), 453.5(a, 0.8)
465.2 (a, 8.8), 473.6 (a, 3.8)	462.1 (a, 29.1) 467.0 (a, 5.6)	461.4 (a, 20.5), 467.3(a, 3.3)
475.8(a, 3.6), 484.6(a, 1.0)	473.9 (a, 3.2), 483.6 (a, 8.5)	475.4 (a, 6.3), 480.0 (a, 3.1)
504.4 (a, 4.0), 509.0 (a, 2.7)	496.0(a, 27.8), 504.0 (a, 0.3)	495.3 (a, 10.9), 503.3(a, 3.5)
518.2(a, 46.8), 520.3(a, 5.3)	508.5(a,10.2), 521.7(a, 38.8)	508.8(a, 23.0), 521.4(a,28.0)
523.8(a, 1.9), 531.8 (a, 41.4)	535.0(a,38.2), 543.0(a,37.9)	534.3 (a, 58.9), 556.0(a, 5.0)
535.4(a, 93.4), 548.5(a,35.6)	545.1(a, 22.6), 553.7(a,51.3)	568.7 (a, 6.6), 580.4(a, 29.7)
582.4(a,28.8), 591.8(a, 10.7)	558.1(a,15.9), 576.6(a, 55.5)	586.4(a, 35.9), 598.1(a,22.2)
595.7 (a, 19.4)	610.1 (a, 15.0)	603.6 (a, 38.6)
611.2 (a, 13.0)	664.3 (a, 37.4)	630.2 (a, 98.1)
678.1 (a, 68.8)	684.1 (a, 22.9.)	709.3 (a, 4.0)
1205.0 (a, 8.4)	1205.2 (a, 4.9)	1046.3 (a, 26.2)
1214.1 (a, 21.8)	1306.7 (a, 13.3)	1252.1 (a, 2.4)
1451.6 (a, 1.2)	1484.3 (a, 15.9)	1332.1 (a, 5.6)
1497.4 (a, 14.3)	1522.9 (a, 1.5)	1498.6 (a, 4.2)
1965.3 (a, 59.4)	1944.1 (a, 414.7)	1807.8 (a, 323.7)
1970.2 (a, 718.9)	1977.5 (a, 115.9)	1964.6 (a, 291.5)
1973.9 (a, 275.5)	1990.4 (a, 580.0)	1987.3 (a, 364.3)
1993.2 (a, 385.9)	1995.4 (a, 70.3)	1992.2 (a, 1158.3)
2002.7 (a, 1353.5)	2000.8 (a, 1798.9)	1994.5 (a, 783.5)
2015.6 (a, 1563.7)	2006.8 (a, 1402.8)	2008.5 (a, 1790.0)
2035.1 (a, 1450.8)	2047.1 (a, 1573.4)	2032.1 (a, 1848.5)
2066.6 (a, 235.6)	2070.9 (a, 183.7)	2057.2 (a, 78.7)

8-4S(C_1)	**8-5S(C_s)**	**8-6S(C_1)**

28.5 (a, 0.1), 44.3 (a, 0.1)	7.5 (a, 0.2), 29.9 (a, 0.0)	20.7 (a, 0.0), 29.3 (a, 0.1)
45.5 (a, 0.2), 52.4 (a, 0.0)	38.0 (a, 0.0), 54.0 (a, 0.7)	37.0 (a, 0.3), 48.0 (a, 0.1)
59.0 (a, 0.0), 64.9 (a, 0.4)	60.0 (a, 0.6), 64.9 (a, 0.2)	63.4 (a, 0.1), 67.2 (a, 0.5)
66.3 (a, 0.2), 69.8 (a, 0.1)	66.5 (a, 0.1), 73.5 (a, 0.4),	69.4 (a, 0.2), 75.3 (a, 0.3)
76.7 (a, 0.2), 84.8 (a, 0.3)	81.9 (a, 0.1), 85.1 (a, 0.1)	78.4 (a, 0.7), 80.6 (a, 0.3)
87.3 (a, 0.3), 89.5 (a, 0.2)	85.6 (a, 0.1), 90.0 (a, 0.0)	84.6 (a, 0.2), 87.4 (a, 0.1)
90.3 (a, 0.2), 92.2 (a, 0.2)	92.6 (a, 0.4), 95.1 (a, 0.1)	91.7 (a, 0.7), 94.3 (a, 0.5)
93.4 (a, 0.3), 106.1 (a, 0.0)	100.8 (a, 0.1), 112.1 (a, 0.0)	99.0 (a, 0.3), 110.0 (a, 0.0)
130.5 (a, 1.2), 168.1 (a, 0.9)	128.7 (a, 0.7), 134.2 (a, 2.1)	117.6 (a, 1.6), 134.0 (a, 1.0)
251.3 (a, 0.4), 342.0 (a, 2.1)	178.1 (a, 1.4), 383.1(a, 0.5)	176.4 (a, 0.3), 333.6 (a, 9.9)
369.4 (a, 8.8), 398.0(a, 39.8)	394.2 (a, 3.1), 412.8(a, 19.1)	387.7 (a, 7.3), 399.6(a, 13.1)
423.7 (a, 3.4), 432.8 (a, 9.6)	412.8 (a, 0.6), 423.6(a, 1.5)	404.1 (a, 3.0), 425.1 (a, 2.6)
440.8 (a, 1.2), 456.4(a, 13.1)	430.8(a, 3.7), 431.7 (a, 0.2)	433.3 (a, 4.0), 441.9 (a, 8.7)
461.8 (a, 1.5), 471.4 (a, 2.9)	440.3 (a, 8.9), 447.0(a, 34.9)	449.9 (a, 6.0), 452.2 (a, 4.0)
474.0 (a, 0.3), 482.5(a, 15.8)	462.3 (a, 4.0) 462.7 (a, 9.7)	460.3 (a, 4.6), 462.3(a, 10.5)
485.8(a, 23.8), 493.3(a, 8.6)	475.8 (a, 20.6), 479.8(a, 0.7)	476.9 (a, 14.8), 488.9(a, 4.0)
499.9 (a, 12.8), 507.5(a, 4.8)	493.0(a, 16.1), 503.8 (a, 9.6)	492.6 (a, 6.6), 502.7 (a, 8.6)
512.1(a, 2.9), 537.8(a, 14.5)	503.9 (a, 0.5), 519.2(a,12.7)	504.4 (a, 9.2), 515.5(a, 31.2)
545.0(a, 2.9), 567.1 (a, 13.0)	527.1(a, 18.6), 532.9(a,18.6)	524.1(a, 76.4), 538.7(a,53.3)
580.6 (a, 17.1), 582.7(a, 3.1)	541.2(a,111.6), 559.3(a, 4.8)	552.0(a, 20.2), 560.7(a,15.1)
588.1(a, 7.2), 595.7 (a, 11.0)	584.3 (a, 34.7), 584.7(a, 8.8)	565.2(a, 33.6), 569.9(a,75.2)
617.2 (a, 99.7)	591.4 (a, 3.3)	604.2 (a, 9.2)
639.4 (a, 55.1)	668.0(a, 45.8)	631.6 (a, 52.2)
747.7 (a, 16.7)	707.5 (a, 9.5)	646.4 (a, 27.6)
1259.7 (a, 6.9)	1237.2 (a, 10.6)	1238.7 (a, 31.1)
1298.7 (a, 3.3)	1244.2 (a, 13.9)	1366.1 (a, 41.1)
1448.7 (a, 1.6)	1465.1 (a, 0.1)	1405.5 (a, 9.9)
1567.4 (a, 38.9)	1479.5 (a, 0.6)	1572.8 (a, 116.4)
1816.4 (a, 285.9)	1963.7 (a, 30.4)	1951.6 (a, 386.1)
1962.3 (a, 225.4)	1971.7 (a, 0.3)	1972.3 (a, 165.1)
1981.3 (a, 177.3)	1981.3 (a, 92.9)	1988.5 (a, 83.6)
1993.7 (a, 1936.7)	1982.4 (a, 884.9)	1992.6 (a, 201.4)
1998.6 (a, 509.1)	1998.7 (a, 1343.7)	1993.9 (a, 1609.7)
2013.9 (a, 2019.5)	2019.1 (a, 1838.2)	2009.5 (a, 1614.1)
2037.2 (a, 903.4)	2033.5 (a, 1394.6)	2041.9 (a, 1686.2)
2082.2 (a, 158.3)	2066.6 (a, 276.6)	2066.9 (a, 253.5)

Table S6. Theoretical Cartesian coordinates (in Å) for the structure 12-**1** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	0.000000	0.000000	2.956588
76	0.000000	0.000000	0.000000
76	0.000000	0.000000	-2.956588
1	0.000000	0.000000	4.592867
6	0.000006	1.956518	2.977075
8	0.000000	3.104494	3.018741
6	-1.956518	0.000006	2.977075
8	-3.104494	0.000000	3.018741
6	-0.000006	-1.956518	2.977075
8	0.000000	-3.104494	3.018741
6	1.956518	-0.000006	2.977075
8	3.104494	0.000000	3.018741
6	-1.379731	1.379779	0.000000
6	-1.379779	-1.379731	0.000000
6	1.379731	-1.379779	0.000000
6	1.379779	1.379731	0.000000
8	-2.194842	2.194896	0.000000
8	-2.194896	-2.194842	0.000000
8	2.194842	-2.194896	0.000000
8	2.194896	2.194842	0.000000
1	0.000000	0.000000	-4.592867
6	0.000006	1.956518	-2.977075
6	-1.956518	0.000006	-2.977075
6	-0.000006	-1.956518	-2.977075
6	1.956518	-0.000006	-2.977075
8	0.000000	3.104494	-3.018741
8	-3.104494	0.000000	-3.018741
8	0.000000	-3.104494	-3.018741
8	3.104494	0.000000	-3.018741

Table S7. Theoretical Cartesian coordinates (in Å) for the structure 11-**1** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	-1.688237	-0.507786	-0.027851
76	1.249302	-1.236331	-0.103463
76	0.440527	1.546811	-0.012024
1	0.976688	-1.066789	-1.734673
1	-0.483110	-1.841870	0.025581
6	0.596230	1.386300	-1.960717
6	-0.612435	3.162014	-0.064509
6	0.452931	1.420816	1.937011
6	-2.908800	0.990505	-0.054188
6	-1.542593	-0.528127	-1.993295
6	3.033004	-0.726187	-0.498179
6	1.517841	-1.403429	1.842280
6	1.521554	-3.071670	-0.530271
6	-1.632104	-0.551732	1.934508
8	0.739466	1.388461	-3.101441
8	-1.197351	4.155191	-0.094433
8	-1.539233	-0.597931	-3.135564
8	-3.661522	1.858972	-0.065760
8	4.112400	-0.428961	-0.777082
8	1.699699	-4.175586	-0.815323
8	1.729403	-1.567049	2.963240
8	-1.648896	-0.652195	3.075145
8	0.513617	1.422598	3.086332
6	-2.977536	-1.941378	-0.068097
6	2.185191	2.320171	0.046907
8	-3.777920	-2.766313	-0.093653
8	3.228558	2.807843	0.090290

Table S8. Theoretical Cartesian coordinates (in Å) for the structure 11-**2** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	1.671486	-0.395583	0.000000
76	-0.531100	1.741977	0.000000
76	-1.204752	-1.107071	0.000000
6	-1.160747	-1.090615	1.955084
8	-1.203366	-1.161243	3.102651
1	1.312224	1.358265	0.000000
1	-2.080793	2.240014	0.000000
6	-0.790095	1.798141	-1.926423
6	-1.160747	-1.090615	-1.955084
6	1.613994	-0.287679	-1.959794
6	3.518263	0.141197	0.000000
6	1.882777	-2.325373	0.000000
6	1.613994	-0.287679	1.959794
6	-0.790095	1.798141	1.926423
6	-1.306413	-3.030814	0.000000
8	-1.436191	-4.177097	0.000000
8	-1.203366	-1.161243	-3.102651
8	1.662218	-0.180873	-3.099433
8	2.048387	-3.463023	0.000000
8	4.634244	0.420083	0.000000
8	-1.038232	1.936413	-3.042192
8	-1.038232	1.936413	3.042192
8	1.662218	-0.180873	3.099433
6	-3.038715	-0.565969	0.000000
8	-4.152203	-0.270400	0.000000
6	0.068447	3.535961	0.000000
8	0.434076	4.632476	0.000000

Table S9. Theoretical Cartesian coordinates (in Å) for the structure 11-**3** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	1.439365	-1.004167	-0.049963
76	0.115942	1.598126	0.094112
76	-1.642502	-0.687734	0.055300
1	-0.965262	0.591853	1.189011
1	-0.145921	-1.778058	-0.210138
6	-1.023468	0.738864	-1.444574
6	-3.338453	0.166177	0.157534
6	-1.934091	-1.744886	1.700761
6	1.422697	-0.740134	-2.004201
6	2.101503	-2.824164	-0.151649
6	1.316527	2.456475	-1.123953
6	-1.058996	3.097308	0.163865
6	1.039083	2.045925	1.775454
6	1.229497	-1.013786	1.901271
8	-1.289438	0.922327	-2.589796
8	-4.361097	0.690244	0.220440
8	2.530626	-3.888521	-0.210064
8	1.444125	-0.616758	-3.141020
8	2.035661	2.970210	-1.864229
8	1.597017	2.391654	2.722469
8	-1.774015	4.000378	0.206517
8	1.119878	-1.039068	3.041545
8	-2.217730	-2.407800	2.597134
6	3.116717	-0.048344	0.092476
6	-2.290420	-1.915238	-1.273415
8	4.122153	0.501685	0.176197
8	-2.675373	-2.648857	-2.071499

Table S9. Theoretical Cartesian coordinates (in Å) for the structure 11-**4** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	-1.714978	-0.454701	-0.000009
76	1.205251	-1.377070	0.000028
76	0.524533	1.475640	-0.000011
1	-0.572340	-1.861578	0.000036
6	0.554233	1.362362	-1.951235
6	-0.287268	3.219229	-0.000116
6	0.553981	1.362476	1.951222
6	-2.785123	1.158025	-0.000036
6	-1.661514	-0.483347	-1.964207
6	3.094655	-1.355535	0.000029
6	1.243910	-1.568037	1.937483
6	-1.661630	-0.483372	1.964194
8	0.617031	1.374642	-3.101146
8	-0.703938	4.295551	-0.000184
8	-1.711343	-0.554718	-3.106191
8	-3.454663	2.092367	-0.000051
8	4.250055	-1.367241	0.000033
8	1.317101	-1.787365	3.064801
8	-1.711506	-0.554800	3.106172
8	0.616621	1.374817	3.101141
6	-3.092555	-1.801537	-0.000050
6	2.386504	1.893994	0.000091
8	-3.948381	-2.569819	-0.000083
8	3.505210	2.174011	0.000159
1	1.165858	-3.007903	0.000077
6	1.243922	-1.568161	-1.937414
8	1.317130	-1.787590	-3.064711

Table S10. Theoretical Cartesian coordinates (in Å) for the structure 10-**1** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	1.357670	-0.921705	0.000000
76	-0.000054	1.580883	0.000001
76	-1.357601	-0.921797	-0.000001
1	0.000048	-1.329177	-1.181427
1	0.000049	-1.329177	1.181425
6	-2.582767	-0.349826	-1.346884
6	-1.884310	-2.780664	-0.000002
6	-2.582765	-0.349831	1.346886
6	1.884496	-2.780540	-0.000001
6	2.582797	-0.349656	-1.346884
6	-0.000042	1.355383	-1.940531
6	-0.000033	1.355382	1.940532
6	1.481272	2.816263	-0.000002
6	2.582798	-0.349655	1.346883
8	-3.296232	-0.008589	-2.183712
8	-2.233775	-3.877146	0.000001
8	3.296239	-0.008374	-2.183715
8	2.234025	-3.877001	-0.000003
8	-0.000032	1.226186	-3.084745
8	2.360100	3.562966	-0.000003
8	-0.000021	1.226181	3.084746
8	3.296240	-0.008372	2.183712
8	-3.296226	-0.008598	2.183720
6	-1.481511	2.816104	0.000003
8	-2.360422	3.562707	0.000004

Table S11. Theoretical Cartesian coordinates (in Å) for the structure 10-**2** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	-1.575177	-1.768192	-0.383845
76	1.414339	0.387675	-1.343513
76	0.300281	-0.668777	-0.002174
1	-0.203798	-1.768192	-0.383845
1	1.050286	0.387675	-1.343513
6	2.052016	-2.149736	-1.447875
6	-0.483609	2.350318	1.452420
6	-1.580527	-0.425644	-1.951874
6	-2.591292	-2.323610	0.021181
6	-3.047831	0.556175	0.242622
6	-1.145961	-0.640128	1.914020
6	1.873025	2.579219	-0.000420
6	1.615558	-2.217296	1.290331
6	3.066370	-0.084501	0.355887
8	-0.670116	2.595125	-1.274937
8	-1.223351	3.232652	-2.062039
8	-0.940316	2.845380	2.390273
8	-1.566622	-0.295310	-3.091302
8	-3.931412	1.278939	0.380799
8	-3.215234	-3.289573	0.033352
8	2.486881	-2.805578	-2.289571
8	4.099827	0.347640	0.629531
8	1.703890	-2.983611	2.147427
6	-0.943033	-0.638457	3.044162
8	2.783136	3.287264	0.028452

Table S12. Theoretical Cartesian coordinates (in Å) for the structure 9-**1** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	1.356263	-0.869345	0.002079
76	0.000002	1.520358	-0.059003
76	-1.356267	-0.869341	0.002081
1	-0.000006	-1.400731	-1.137004
1	0.000002	-1.083308	1.244271
6	-2.584288	-0.514796	-1.412063
6	-1.861884	-2.740832	0.225083
6	-2.556420	-0.089220	1.261058
6	1.861888	-2.740834	0.225069
6	2.584289	-0.514796	-1.412060
6	-1.531515	2.468057	-0.704681
6	0.000007	2.595195	1.460499
6	1.531520	2.468054	-0.704679
6	2.556406	-0.089227	1.261068
8	-3.293496	-0.306848	-2.296053
8	-2.187092	-3.832293	0.383193
8	3.293497	-0.306845	-2.296050
8	2.187104	-3.832295	0.383170
8	-2.407215	3.048469	-1.184808
8	2.407226	3.048456	-1.184809
8	0.000022	3.170114	2.464942
8	3.258448	0.382325	2.044284
8	-3.258472	0.382338	2.044262

Table S13. Theoretical Cartesian coordinates (in Å) for the structure 9-**2** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	0.010455	1.486655	-0.026575
76	-1.403205	-0.866781	-0.064299
76	1.542099	-0.840877	-0.272519
1	0.030000	-1.838101	-0.447545
1	0.878912	0.579934	-1.303212
6	2.204500	-2.496374	0.364637
6	1.258535	0.218636	1.354757
6	-1.097907	2.297449	-1.373899
6	-2.882583	0.328745	0.304035
6	-1.841637	-2.233855	1.164380
6	1.445490	2.790669	-0.089862
8	2.595091	-3.502492	0.779358
8	-1.748097	2.796497	-2.184310
8	-2.068644	-2.997953	1.996040
8	-3.811413	0.970816	0.524945
8	2.305506	3.551003	-0.146933
8	1.539967	0.258131	2.498821
6	-0.906041	2.328335	1.440481
6	3.335108	-0.286607	-0.569772
6	-2.271142	-1.905509	-1.381824
8	-1.432269	2.822416	2.336911
8	-2.768863	-2.457765	-2.262423
8	4.423058	0.035035	-0.781025

Table S13. Theoretical Cartesian coordinates (in Å) for the structure 9-**3** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	1.676310	-0.330220	0.028062
76	-0.619949	1.308454	-0.303834
76	-1.247997	-1.332762	0.034561
1	-1.413477	-1.673771	0.322520
1	-1.531615	0.440703	-1.290539
6	2.204500	-2.496374	0.364637
8	1.258535	0.218636	1.354757
6	-1.097907	2.297449	-1.373899
6	-2.882583	0.328745	0.304035
6	-1.841637	-2.233855	1.164380
6	1.445490	2.790669	-0.089862
6	2.595091	-3.502492	0.779358
6	-1.748097	2.796497	-2.184310
6	-2.068644	-2.997953	1.996040
6	-3.811413	0.970816	0.524945
8	2.305506	3.551003	-0.146933
8	1.539967	0.258131	2.498821
8	-0.906041	2.328335	1.440481
8	3.335108	-0.286607	-0.569772
8	-2.271142	-1.905509	-1.381824
8	-1.432269	2.822416	2.336911
8	-2.768863	-2.457765	-2.262423
8	4.423058	0.035035	-0.781025

Table S14. Theoretical Cartesian coordinates (in Å) for the structure 9-**4** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	-0.539529	1.396898	-0.057891
76	-1.146547	-1.206523	-0.204705
76	1.742963	-0.348387	-0.028936
1	-1.141671	0.325247	-1.349745
1	1.643554	-1.921933	0.094963
6	1.596840	-0.301919	1.920130
8	1.499907	-0.352927	3.062147
6	-1.097907	2.297449	-1.373899
6	-2.882583	0.328745	0.304035
6	-1.841637	-2.233855	1.164380
6	1.445490	2.790669	-0.089862
6	2.595091	-3.502492	0.779358
6	-1.748097	2.796497	-2.184310
6	-2.068644	-2.997953	1.996040
6	-3.811413	0.970816	0.524945
8	2.305506	3.551003	-0.146933
8	1.539967	0.258131	2.498821
8	-0.906041	2.328335	1.440481
8	3.335108	-0.286607	-0.569772
8	-2.271142	-1.905509	-1.381824
8	-1.432269	2.822416	2.336911
8	-2.768863	-2.457765	-2.262423
8	4.423058	0.035035	-0.781025

Table S17. Theoretical Cartesian coordinates (in Å) for the structure 8-**1** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
6	-2.417856	0.696814	-1.397677
8	-2.885137	1.285112	-2.270996
1	-0.628755	-1.279848	1.208764
1	-0.656133	-1.345859	-1.166092
76	0.776294	1.127088	-0.017949
76	0.806272	-1.458386	0.006898
76	-1.605216	-0.323468	0.004535
6	2.157527	-1.680441	1.294995
6	-2.958205	-1.727251	0.070916
6	0.461383	2.367046	1.350051
6	2.691897	1.469092	-0.118397
6	0.233451	2.466844	-1.222910
6	2.129516	-1.730561	-1.299695
6	-2.364714	0.814896	1.344393
8	-2.801442	1.483206	2.175054
8	-3.783122	-2.527466	0.118858
8	0.272307	3.054970	2.259267
8	-0.094000	3.224979	-2.030831
8	3.816890	1.694644	-0.194079
8	2.973183	-1.794848	2.108106
8	2.927361	-1.879426	-2.125065

Table S18. Theoretical Cartesian coordinates (in Å) for the structure 8-**2** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	-0.712165	1.202307	0.083778
76	-0.799393	-1.413204	-0.083020
76	1.636763	-0.208240	0.074523
1	0.766276	-1.482178	0.943549
1	0.767732	0.904916	1.196984
6	2.273599	-1.516419	-1.179809
6	2.501118	1.261339	-0.840957
6	3.061765	-0.479617	1.359108
6	-0.005654	2.966259	-0.231840
6	-2.160505	1.437185	-1.131633
6	-1.832209	-2.048516	1.313623
6	-2.308379	-1.606444	-1.176109
6	-1.812885	1.761566	1.528619
8	2.639434	-2.302038	-1.939173
8	3.022708	2.122977	-1.397339
8	-3.008763	1.592348	-1.893739
8	0.411706	4.019158	-0.441452
8	-3.215261	-1.759790	-1.882724
8	-2.459512	-2.347732	2.243882
8	-2.443317	2.040119	2.451363
8	3.884163	-0.642605	2.145695

Table S19. Theoretical Cartesian coordinates (in Å) for the structure 8-**3** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	0.192948	1.517970	-0.091112
76	-1.511232	-0.560018	-0.068391
76	1.134330	-1.182651	-0.025848
1	-0.386245	-1.478688	0.989175
1	0.002157	-0.260499	-1.243384
6	2.143338	-2.232436	1.183381
6	1.741544	0.592780	0.785077
6	-2.714478	0.551098	-1.084448
6	-2.463873	-0.151161	1.508980
6	1.329437	2.604725	-1.153792
8	2.741425	-2.867298	1.935884
8	-3.010160	0.087828	2.497036
8	-3.436313	1.202395	-1.702942
8	1.981401	3.229054	-1.874354
8	2.621673	0.898563	1.517407
6	0.072045	2.926189	1.123511
6	2.600481	-1.242569	-1.223893
6	-2.314109	-2.273917	-0.613325
8	-0.012026	3.762486	1.917391
8	-2.850270	-3.248370	-0.904469
8	3.464058	-1.293654	-1.987458

Table S20. Theoretical Cartesian coordinates (in Å) for the structure 8-**4** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
6	-1.346494	-1.100146	1.835331
8	-1.333363	-1.066720	2.980491
1	0.242853	-1.887653	-0.040015
1	0.777404	0.467857	-1.366399
76	1.598750	-0.668213	-0.201491
76	-0.308141	1.355213	-0.164235
76	-1.385705	-1.160749	-0.123124
6	0.565345	2.982871	-0.547314
6	-1.322442	-1.136204	-2.079085
6	3.236541	0.189721	-0.618719
6	2.494533	-1.868402	0.978985
6	1.113250	0.787995	1.133937
6	-1.496962	2.235510	1.021474
6	-3.200155	-0.574742	-0.132573
8	-4.296059	-0.213301	-0.131854
8	-1.293996	-1.124112	-3.226723
8	3.030043	-2.563180	1.727941
8	4.239257	0.681253	-0.907201
8	1.100175	3.974057	-0.810513
8	-2.193408	2.762508	1.778086
8	1.490515	1.090132	2.215615

Table S21. Theoretical Cartesian coordinates (in Å) for the structure 8-**5** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	-1.375873	-0.576828	0.001834
76	1.375879	-0.576817	0.001834
76	-0.000008	1.677414	-0.440074
1	1.216912	0.652935	-1.356383
1	-1.216920	0.652926	-1.356384
6	1.340801	2.670458	0.446819
6	-1.730932	-1.973679	-1.194826
6	-3.225559	0.031136	0.139888
6	1.479119	-1.811002	1.458272
6	3.225564	0.031156	0.139872
8	2.170670	3.245357	1.010009
8	-4.334632	0.326052	0.220177
8	-1.912629	-2.800345	-1.980538
8	4.334638	0.326074	0.220143
8	1.578169	-2.528288	2.355250
6	-1.479086	-1.811012	1.458274
6	-1.340825	2.670453	0.446813
6	1.730923	-1.973665	-1.194832
8	-1.578121	-2.528297	2.355255
8	1.912611	-2.800329	-1.980547
8	-2.170698	3.245348	1.009999

Table S22. Theoretical Cartesian coordinates (in Å) for the structure 8-**6** using the MPW1PW91/SDD method.

Atomic Number	X	Y	Z
76	-0.675248	1.169843	-0.007961
76	-0.955864	-1.452307	-0.301415
76	1.650923	-0.220420	-0.118832
1	0.829673	-1.744915	-0.475769
1	0.600819	0.735481	-1.304268
6	2.917849	-0.758054	-1.466042
6	2.494029	-1.264129	1.238826
6	-2.003666	1.750546	-1.250215
6	0.056335	2.927715	0.257089
6	-2.821209	-1.471785	-0.580691
6	-1.191800	-1.863891	1.451802
8	3.668464	-1.005966	-2.303878
8	2.962005	-1.900678	2.076976
8	0.455847	3.997241	0.415802
8	-2.752668	2.101393	-2.053887
8	-1.332479	-2.096681	2.580902
8	-3.967494	-1.462052	-0.743172
6	-1.890246	1.336678	1.445636
6	2.534888	1.396934	0.459254
8	-2.607547	1.413266	2.344181
8	3.134717	2.316550	0.806813

Complete Gaussian 03 reference

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