# The Boronyl Ligand as a Member of the Isoelectronic Series $BO^- \rightarrow CO \rightarrow NO^+$: Viable Cobalt Carbonyl Boronyl Derivatives?

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## Supporting Information

**Tables S1-S24:** Theoretical harmonic vibrational frequencies for the 46 structures of $Co_2(BO)_2(CO)_n$ ($n$ = 8, 7, 6) and $Co(BO)(CO)_m$ ($m$ = 4, 3, 2, 1) using the BP86 and B3LYP method.

**Tables S25-S71:** Theoretical Cartesian coordinates for the 46 structures of $Co_2(BO)_2(CO)_n$ ($n$ = 8, 7, 6) and $Co(BO)(CO)_m$ ($m$ = 4, 3, 2, 1) using the BP86/DZP method.

**Tables S72-S75:** $\nu$(CO) and $\nu$(BO) frequencies ($cm^{-1}$) for the $Co_2(BO)_2(CO)_n$ ($n$ = 8, 7, 6) and $Co(BO)(CO)_m$ ($m$ = 4, 3, 2, 1) using the BP86/DZP method.

**Tables S76-S82.** Total energies ($E$, in hartree), relative energies ($\Delta E$, in kcal $mol^{-1}$), and numbers of imaginary vibrational frequencies ($N_{Imag}$) for the optimized $Co_2(BO)_2(CO)_n$ ($n$ = 8, 7, 6) and $Co(BO)(CO)_m$ ($m$ = 4, 3, 2, 1) structures.

Complete Gaussian 03 reference (Reference 52)

**Table S1.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co(BO)(CO)_4]$.

| **14S-1**($C_{3v}$) | | **14S-2**($C_{2v}$) | | **14S-3**($C_{4v}$) | |
|---|---|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 | B3LYP | BP86 |
| 54.7 (1.2) | 51.1 (1.0) | -29.1 (1.7) | -27.0 (1.7) | -175.9 (0.0) | -204.4(0.0) |
| 54.7 (1.2) | 51.1 (1.0) | 63.9 (0.0) | 65.3 (0.0) | 69.2(2.2) | 66.5(1.9) |
| 90.0 (1.0) | 84.0 (0.8) | 82.6 (0.0) | 77.8 (0.0) | 69.2(2.2) | 66.5(1.9) |
| 90.0 (1.0) | 84.0 (0.8) | 93.4 (1.0) | 88.9 (1.2) | 100.9(0.0) | 96.0(0.0) |
| 96.3 (1.4) | 91.6 (0.5) | 100.2(1.1) | 95.4 (0.6) | 105.9(1.1) | 101.6(0.6) |
| 96.3 (1.4) | 91.6 (0.5) | 101.1 (3.5) | 95.8 (1.7) | 105.9(1.1) | 101.6(0.6) |
| 108.5 (0.2) | 103.6 (0.3) | 112.8 (0.6) | 110.0 (0.8) | 108.0(1.1) | 103.8(1.1) |
| 343.5 (0.0) | 338.9 (0.0) | 319.6 (1.4) | 320.6 (0.0) | 187.9(0.0) | 172.2(0.0) |
| 351.7 (0.0) | 351.1 (0.3) | 339.8 (5.4) | 320.6 (0.3) | 321.4(1.6) | 320.9(1.9) |
| 351.7 (0.0) | 351.1 (0.3) | 343.5 (0.0) | 336.9 (3.1) | 321.4(1.6) | 320.9(1.9) |
| 372.5 (4.4) | 371.4 (0.3) | 344.7 (1.8) | 344.7 (0.0) | 367.7(0.0) | 373.9( 0.0) |
| 372.5 (4.4) | 371.4 (0.3) | 373.2 (5.5) | 377.4 (2.6) | 374.4(5.0) | 385.5(2.0) |
| 388.5 (7.1) | 401.0 (2.5) | 386.7 (0.5) | 387.5 (2.3) | 431.4(0.0) | 459.3(0.0) |
| 417.9 (0.0) | 432.4 (0.0) | 421.9 (1.9) | 437.4 (1.0) | 442.4(0.0) | 464.9(0.0) |
| 449.8 (0.0) | 467.8 (1.9) | 445.3 (8.8) | 469.8 (3.1) | 461.4(2.9) | 472.8(1.5) |
| 491.5 (0.6) | 491.8 (8.0) | 461.8 (3.0) | 472.9 (1.5) | 461.4(2.9) | 472.8(1.5) |
| 491.5 (0.6) | 491.8 (8.0) | 475.1 (2.9) | 489.4 (3.4) | 488.1(13.2) | 486.3(6.9) |
| 517.2 (17.2) | 509.6 (5.0) | 524.3 (6.2) | 510.5 (7.3) | 488.1(13.2) | 486.3(6.9) |
| 517.2 (17.1) | 509.6 (5.0) | 535.0 (0.0) | 529.0 (0.0) | 543.7(0.0) | 525.7(0.0) |
| 562.3 (90.9) | 563.9 (94.1) | 569.7 (81.3) | 566.9 (105.9) | 618.4(53.2) | 622.7(58.6) |
| 576.4 (85.6) | 580.4 (88.3) | 582.6 (99.9) | 581.1 (74.5) | 618.4(53.2) | 622.7(58.6) |
| 576.4 (85.6) | 580.4 (88.3) | 592.9 (86.7) | 585.6 (93.9) | 629.5(79.9) | 633.6(79.2) |
| 1940 (271.2) | 1869(235.3) | 1927(286.9) | 1854 (234.8) | 1930.7(204.0) | 1863.1(178.4) |
| 2111(1036.0) | 2026(893.3) | 2110(1291.7) | 2020 (1072) | 2112(1349.4) | 2025(1146.4) |
| 2111 (1036) | 2026(893.2) | 2115(983.4) | 2029 (857.0) | 2112(1349.4) | 2024.6(1146) |
| 2129(503.2) | 2039(470.9) | 2122(367.2) | 2033 (373.1) | 2118 (0.0) | 2034.7(0.0) |
| 2182 (131.0) | 2094.8(90.1) | 2178(72.5) | 2089 (63.9) | 2181.1(67.8) | 2101.3(63.4) |

**Table S2.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co(BO)(CO)_3]$

| **13S-1**($C_{2v}$/$C_s$) | | **13S-2** ($C_{3v}$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 27.2 (0.0) | 37.8 (0.9) | 57.2 (1.5) | 43.5 (0.9) |
| 57.1 (6.5) | 68.6 (3.9) | 57.7 (1.5) | 43.5 (0.9) |
| 84.6 (4.1) | 77.9 (2.6) | 82.0 (2.2) | 78.3 (0.8) |
| 94.2 (0.9) | 90.8 (0.5) | 82.2 (2.2) | 78.3 (0.8) |
| 96.9 (0.2) | 94.2 (0.4) | 96.8 (0.1) | 93.5 (0.1) |
| 307.1 (1.8) | 306.8 (3.9) | 276.6 (0.2) | 265.6 (1.3) |
| 341.3 (0.0) | 341.7 (0.9) | 276.7 (0.2) | 265.6 (1.3) |
| 345.8 (1.3) | 350.2 (0.1) | 333.4 (0.0) | 328.2 (0.0) |
| 375.7 (5.2) | 389.2 (1.9) | 343.9 (2.1) | 347.4 (0.1) |
| 410.8(10.7) | 399.8 (0.2) | 344.0 (2.1) | 347.4 (0.1) |
| 433.5 (3.3) | 430.1 (3.6) | 403.2 (4.6) | 428.2 (1.5) |
| 440.7 (1.0) | 457.1 (1.0) | 428.3 (0.6) | 441.6 (0.6) |
| 454.3 (4.4) | 477.3 (0.2) | 496.7 (0.1) | 503.5 (7.4) |
| 462.2 (0.6) | 495.9 (1.5) | 496.8 (0.1) | 503.5 (7.4) |
| 532.7(23.1) | 525.3 (5.8) | 508.2 (72.8) | 518.8 (61.0) |
| 596.6(108.9) | 582.0 (85.3) | 508.3 (72.8) | 518.8 (61.0) |
| 602.3(102.4) | 603.1 (84.4) | 541.4 (12.6) | 552.7 (14.2) |
| 1928.6(279.4) | 1853.5(228.1) | 1922.4(213.1) | 1845.5(176.3) |
| 2102.4(1568.2) | 2004.8(1291.6) | 2090.8(1126.6) | 1996.5(938.5) |
| 2115.8(698.1) | 2023.8(613.9) | 2090.9(1126.5) | 1996.5(938.3) |
| 2178.4(85.4) | 2081.1(121.5) | 2155.1(17.3) | 2059.5(10.4) |

**Table S3.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the triplet structures of $[Co(BO)(CO)_3]$.

| **13T-1** ($C_s$) | | **13T-2** ($C_s$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 50.6 (3.3) | 57.7 (1.3) | 55.5 (2.4) | 57.7 (1.7) |
| 59.6 (3.6) | 61.5 (1.9) | 67.4 (2.6) | 66.3 (2.1) |
| 70.7 (1.5) | 72.5 (1.5) | 76.2 (1.5) | 78.0 (0.5) |
| 71.1 (1.4) | 77.5 (0.9) | 77.0 (3.4) | 80.1 (1.8) |
| 81.0 (0.3) | 84.3 (0.9) | 84.1 (1.2) | 86.7 (1.0) |
| 264.1 (0.2) | 287.0 (0.1) | 280.1 (0.7) | 296.7 (0.4) |
| 270.2 (2.9) | 290.2 (1.9) | 292.5 (0.0) | 311.8 (0.1) |
| 274.2 (0.6) | 291.4 (0.1) | 297.2 (3.4) | 315.7 (0.2) |
| 300.4 (14.7) | 340.2 (13.0) | 320.1 (20.2) | 374.4 (10.0) |
| 364.8 (15.0) | 402.4 (0.7) | 362.7 (4.4) | 402.4 (1.4) |
| 367.8 (10.0) | 408.9 (5.8) | 380.4 (12.3) | 410.8 (0.8) |
| 374.5 (0.2) | 420.8 (0.5) | 391.6 (19.9) | 438.2 (0.2) |
| 393.1 (10.3) | 439.8 (1.1) | 435.1 (2.7) | 449.9 (3.4) |
| 409.2 (18.1) | 449.3 (14.9) | 442.6 (1.8) | 474.6 (3.7) |
| 437.2 (5.2) | 470.0 (29.8) | 455.8 (12.5) | 493.4 (22.7) |
| 441.5 (1.0) | 482.1 (21.4) | 468.4 (38.2) | 502.7 (19.7) |
| 456.2 (6.4) | 493.0 (6.9) | 474.9 (14.7) | 517.5 (41.7) |
| 1915.1(152.6) | 1824.0(90.1) | 1913.5(141.9) | 1832.7(97.1) |
| 2123.8(891.3) | 2014.7(731.8) | 2109.6(1511.4) | 2001.5(1290.2) |
| 2124.2(773.0) | 2016.2(816.1) | 2113.6(702.6) | 2009.4(631.4) |
| 2170.5(289.3) | 2058.7(294.0) | 2161.7(80.8) | 2053.8(65.9) |

**Table S4.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the triplet structures of $[Co(BO)(CO)_2]$.

| **12T-1** ($C_s$) | | **12T-2** ($C_{2v}$) | | **12T-3** ($C_s$) | |
|---|---|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 | B3LYP | BP86 |
| 51.4 (5.3) | 63.8 (3.5) | 66.7 (5.5) | 65.5 (3.8) | 49.1 (5.1) | 61.5 (3.8) |
| 65.9 (6.4) | 65.2 (5.8) | 74.9 (2.3) | 73.8 (2.0) | 53.2 (5.4) | 68.6 (1.5) |
| 70.0 (0.2) | 70.6 (0.2) | 77.8 (0.5) | 75.3 (0.2) | 69.3 (1.3) | 78.2 (3.1) |
| 240.0 (0.2) | 239.5 (0.3) | 262.1 (0.3) | 260.5 (1.6) | 260.8 (3.7) | 279.8 (4.0) |
| 267.6 (0.0) | 265.0 (0.2) | 292.2 (0.0) | 299.4 (0.0) | 266.7 (1.9) | 282.7 (0.2) |
| 270.8 (1.6) | 284.9 (1.2) | 292.6 (4.0) | 302.9 (0.6) | 267.9 (0.8) | 293.1 (1.2) |
| 318.5 (14.9) | 344.4 (13.4) | 346.2 (24.1) | 379.8 (7.9) | 303.6 (5.5) | 361.7 (5.8) |
| 366.2 (22.6) | 413.1 (2.3) | 376.2 (0.5) | 412.4 (3.5) | 367.0 (1.0) | 417.1 (1.1) |
| 376.5 (2.4) | 423.8 (0.0) | 422.3 (28.0) | 428.8 (1.8) | 378.6 (5.3) | 445.1 (1.8) |
| 396.5 (0.1) | 433.7 (4.3) | 441.6 (0.8) | 457.5 (0.1) | 380.2 (36.6) | 456.2 (0.9) |
| 416.1 (10.4) | 446.5 (30.1) | 460.6 (43.2) | 492.2 (51.5) | 404.5 (1.7) | 466.4 (29.3) |
| 454.5 (3.4) | 464.1 (7.7) | 498.1 (27.2) | 509.8 (25.0) | 441.4 (2.5) | 481.0 (8.5) |
| 1917(147) | 1835(107) | 1910(125) | 1835(106) | 1913(142) | 1821(93) |
| 2115(974) | 2009(864) | 2097(1727) | 1992(1488) | 2107(1060) | 1988(953) |
| 2163(389) | 2052(412) | 2151(82) | 2052(63) | 2155(378) | 2029(360) |

**Table S5.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co(BO)(CO)_2]$.

| **12S-1** ($C_s$) | | **12S-2** ($C_{2v}$) | | **12S-3** ($C_s$) | |
|---|---|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 | B3LYP | BP86 |
| 39.8(1.5) | 56.3(0.7) | -33.4(2.4) | -62.5(2.7) | 52.1(6.7) | 40.2(5.8) |
| 90.2(4.8) | 81.9(2.6) | 92.3 (0.0) | 95.1(2.8) | 81.1(5.0) | 80.7(3.3) |
| 94.4(1.0) | 95.3(1.6) | 92.7 (4.9) | 96.3(0.0) | 98.1(0.8) | 100.6(0.9) |
| 335.8(0.7) | 335.8(1.6) | 334.0(0.0) | 334.6(0.0) | 296.6(1.0) | 291.9(1.8) |
| 340.4(1.5) | 347.2(2.0) | 338.4(0.8) | 342.4(1.7) | 306.9(13.7) | 299.2(17.7) |
| 348.5(2.5) | 352.0(0.6) | 350.5(3.8) | 363.5(0.7) | 373.4(7.6) | 391.0(0.2) |
| 402.4(21.8) | 378.4(0.2) | 407.1(36.8) | 395.5(3.6) | 388.5(0.6) | 401.8(1.0) |
| 420.5(0.9) | 441.9(0.3) | 421.3(0.4) | 408.8(3.5) | 434.3(12.6) | 427.5(12.2) |
| 447.5(1.7) | 478.9(0.7) | 436.7(1.9) | 439.4(0.2) | 447.3(9.5) | 434.5(0.0) |
| 468.3(1.1) | 504.4(1.2) | 441.0(0.8) | 472.9(0.8) | 457.5(1.2) | 460.1(14.3) |
| 555.7(80.5) | 565.1(54.2) | 551.8(87.1) | 552.2(80.0) | 562.5(34.9) | 552.3(29.0) |
| 565.4(6.2) | 567.0(5.1) | 564.2(5.8) | 558.5(4.0) | 596.3(27.2) | 629.4(17.6) |
| 1910.5(213) | 1831.7(173) | 1908.2(219.5) | 1829(172.2) | 1920(225.7) | 1834(210.6) |
| 2075(1736.5) | 1975(1297) | 2080(1818.7) | 1981(1473) | 2080(865.8) | 1986(730.9) |
| 2149.6(50.3) | 2043.7(73) | 2160(3.8) | 2061(0.0) | 2140(604.2) | 2042(472.0) |

**Table S6.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the triplet and singlet structures of [Co(BO)(CO)].

| **11T-1** ($C_{\infty v}$) | | **11S-1** ($C_s$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 66.6 (6.9) | 62.8 (6.5) | 91.0 (4.7) | 96.5 (3.3) |
| 66.6 (6.9) | 62.8 (6.5) | 325.9 (0.2) | 333.4 (0.0) |
| 271.1 (0.2) | 270.3 (0.0) | 333.2 (4.2) | 350.9 (3.0) |
| 271.1 (0.2) | 270.3 (0.0) | 378.3 (2.7) | 392.6 (3.6) |
| 358.9 (9.0) | 358.1 (8.9) | 392.3 (0.8) | 430.3 (0.5) |
| 397.0 (0.5) | 453.6 (0.0) | 504.8 (4.7) | 512.1 (1.0) |
| 397.0 (0.5) | 453.6 (0.0) | 605.9 (7.0) | 639.7 (1.8) |
| 429.9 (7.0) | 462.5 (3.0) | 1901.2 (202.6) | 1806.3 (184.9) |
| 1928.1 (195.0) | 1847.3(125.0) | 2073.1 (663.8) | 1981.8 (438.5) |
| 2163.1 (565.5) | 2037.5(621.2) | | |

**Table S7.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_8]$.

| **28S-1**($C_1$) | | **28S-2**($C_s$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 16.3 (1.2) | 16.3 (0.6) | 16.1 (0.0) | 17.0 (0.0) |
| 38.7 (0.5) | 36.3 (0.6) | 38.4 (1.3) | 29.9 (1.1) |
| 42.7 (0.1) | 39.3 (0.0) | 42.6 (1.0) | 42.1 (0.8) |
| 55.5 (0.3) | 49.9 (0.1) | 47.9 (2.4) | 47.5 (0.2) |
| 57.0 (0.5) | 54.2 (0.2) | 55.2 (0.1) | 48.1 (0.5) |
| 63.0 (0.1) | 62.0 (0.1) | 60.4 (0.3) | 55.2 (0.0) |
| 67.9 (0.0) | 66.0 (0.1) | 63.4 (1.4) | 72.7 (0.6) |
| 79.0 (0.5) | 76.4 (0.1) | 76.5 (0.1) | 77.8 (0.3) |
| 81.6 (0.1) | 78.8 (1.4) | 80.4 (0.1) | 78.1 (0.2) |
| 84.4 (3.1) | 82.0 (0.1) | 84.6 (0.1) | 83.7 (0.3) |
| 90.7 (0.3) | 87.0 (0.4) | 90.0 (1.2) | 85.1 (0.1) |
| 92.1 (1.2) | 89.5 (0.5) | 91.0 (0.0) | 90.4 (0.9) |
| 95.1 (0.5) | 92.6 (0.1) | 97.6 (0.3) | 94.5 (0.2) |
| 99.1 (0.6) | 94.2 (0.5) | 97.6 (0.8) | 97.3 (1.2) |
| 103.0 (3.6) | 98.7 (1.4) | 101.7 (1.8) | 97.7 (3.0) |
| 105.6 (0.3) | 101.9 (0.4) | 103.6 (0.9) | 103.2 (1.9) |
| 108.2 (1.0) | 103.6 (0.3) | 103.8 (4.8) | 105.8 (0.9) |
| 116.7 (0.9) | 116.3 (0.2) | 109.9 (2.4) | 115.2 (0.9) |
| 140.9 (0.3) | 159.1 (1.4) | 129.5 (2.2) | 149.1 (0.3) |
| 220.8 (53.2) | 224.2 (37.7) | 229.6 (34.8) | 229.5 (31.4) |
| 283.9 (4.5) | 279.1 (5.9) | 273.9 (4.1) | 273.6 (5.7) |
| 312.7 (43.3) | 311.3 (3.9) | 305.5 (2.9) | 282.8 (15.2) |
| 323.5 (1.2) | 316.2 (33.2) | 323.3 (0.1) | 320.3 (0.0) |
| 329.5 (0.7) | 322.0 (1.1) | 347.4 (2.2) | 326.1 (2.7) |
| 344.1 (0.7) | 341.4 (5.8) | 348.9 (0.8) | 338.4 (2.2) |
| 349.2 (31.1) | 349.0 (23.6) | 352.4 (0.0) | 349.8 (0.2) |
| 359.2 (2.1) | 360.4 (3.3) | 358.5 (30.5) | 363.5 (1.9) |
| 360.8 (2.4) | 365.1 (7.7) | 364.8 (2.1) | 364.9 (20.2) |
| 367.8 (62.6) | 372.4 (8.6) | 372.3 (96.7) | 368.8 (1.0) |
| 376.6 (0.8) | 388.0 (52.8) | 379.1 (4.3) | 394.0 (108.1) |
| 385.4 (2.6) | 396.9 (2.1) | 391.2 (17.3) | 395.7 (0.2) |
| 394.1 (2.2) | 400.5 (7.7) | 401.6 (23.2) | 408.1 (12.5) |
| 401.5 (34.2) | 414.6 (10.0) | 409.5 (20.4) | 411.4 (12.4) |
| 409.6 (20.4) | 422.6 (20.5) | 417.3 (0.6) | 425.5 (74.1) |

| | | | |
|---|---|---|---|
| 420.8 (9.9) | 434.6 (50.3) | 428.1 (89.3) | 435.6 (1.8) |
| 434.0 (3.0) | 439.0 (3.2) | 435.7 (2.1) | 439.1 (11.7) |
| 441.1 (19.8) | 445.3 (33.2) | 456.9 (10.0) | 462.6 (1.2) |
| 459.1 (17.5) | 459.7 (17.6) | 468.2 (13.1) | 467.2 (10.8) |
| 467.7 (1.9) | 464.3 (3.1) | 471.9 (0.1) | 471.0 (1.8) |
| 473.9 (41.2) | 469.7 (3.5) | 477.1 (24.3) | 472.2 (37.3) |
| 480.8 (8.0) | 479.0 (19.3) | 491.4 (2.8) | 476.9 (2.2) |
| 486.0 (68.2) | 490.2 (44.7) | 508.8 (286.8) | 494.2 (208.2) |
| 516.6 (37.6) | 502.9 (31.1) | 517.3 (1.6) | 506.5 (0.6) |
| 523.6 (66.8) | 517.7 (64.9) | 526.5 (8.8) | 513.6 (5.4) |
| 529.1 (142.4) | 528.0 (34.2) | 533.9 (92.1) | 531.7 (3.2) |
| 537.7 (42.9) | 531.4 (149.8) | 536.5 (8.8) | 536.1 (149.4) |
| 544.5 (86.1) | 540.1 (43.9) | 555.3 (146.0) | 547.5 (63.4) |
| 545.7 (38.8) | 544.8 (53.6) | 570.0 (85.6) | 550.9 (73.9) |
| 566.5 (84.5) | 561.3 (94.5) | 571.4 (92.4) | 560.9 (106.1) |
| 590.5 (101.0) | 578.0 (70.3) | 611.1 (6.4) | 594.5 (8.1) |
| 1849.2 (278.4) | 1806.4 (172.2) | 1857.7 (257.0) | 1816.8 (155.4) |
| 1916.0 (178.1) | 1834.1 (147.6) | 1934.1 (193.0) | 1836.6 (224.6) |
| 1936.9 (328.0) | 1853.5 (236.2) | 1946.0 (356.8) | 1854.6 (217.4) |
| 2088.3 (512.0) | 2003.4 (508.1) | 2087.7 (306.8) | 2002.9(186.7) |
| 2118.8 (316.7) | 2023.6 (356.0) | 2102.2 (184.5) | 2016.5 (261.5) |
| 2126.8 (256.7) | 2029.8 (241.2) | 2126.3 (1544.7) | 2031.6 (402.5) |
| 2131.9 (1153.6) | 2034.5 (994.1) | 2128.3 (453.4) | 2032.0(1398.5) |
| 2135.8 (407.1) | 2039.9 (396.3) | 2136.4 (612.8) | 2038.3 (662.5) |
| 2158.1 (1543.5) | 2069.5 (980.8) | 2149.2 (927.8) | 2063.8 (416.0) |
| 2183.3 (122.5) | 2088.7 (135.0) | 2182.8 (189.1) | 2088.9 (205.1) |

**Table S8.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_8]$

| **28S-3**($C_s$) | | **28S-4**($C_s$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 22.2 (0.3) | 15.7 (0.2) | 7.7 (0.3) | -10.3 (0.1) |
| 39.8 (8.0) | 36.9 (0.0) | 36.0 (1.2) | 23.0 (0.8) |
| 44.6 (0.0) | 42.7 (0.0) | 41.2 (0.0) | 38.9 (0.0) |
| 50.5 (40.8) | 52.1 (0.7) | 45.4 (0.0) | 41.6 (0.1) |
| 57.1 (0.6) | 54.4 (1.3) | 55.7 (0.4) | 53.3 (4.0) |
| 57.5 (3.0) | 64.1 (6.4) | 57.9 (4.9) | 55.2 (0.2) |
| 65.4 (1.9) | 64.1 (1.3) | 65.6 (1.7) | 62.7 (2.3) |
| 72.6 (1.1) | 74.7 (0.0) | 67.6 (0.1) | 64.8 (0.1) |
| 75.7 (0.6) | 77.1 (1.1) | 75.7 (20.7) | 77.5 (0.0) |
| 82.9 (2.1) | 82.4 (0.0) | 82.8 (3.0) | 79.2 (2.2) |
| 87.5 (0.0) | 83.6 (1.5) | 83.6 (0.0) | 81.6 (2.9) |
| 87.7 (1.9) | 85.5 (0.1) | 93.8 (1.2) | 89.1 (0.0) |
| 90.2 (4.9) | 92.4 (6.5) | 93.9 (0.1) | 91.0 (1.4) |
| 96.0 (3.6) | 93.6 (1.3) | 95.7 (2.7) | 92.5 (1.4) |
| 99.6 (0.9) | 96.4 (1.5) | 100.4 (5.7) | 99.2 (5.7) |
| 103.3 (0.9) | 98.8 (1.0) | 104.8 (0.3) | 100.5 (0.2) |
| 106.8 (0.0) | 99.7 (0.1) | 111.7 (2.5) | 106.4 (2.2) |
| 107.2 (5.0) | 104.4 (2.4) | 113.6 (0.2) | 113.0 (0.6) |
| 119.8 (4.3) | 118.6 (4.3) | 120.3 (0.8) | 116.1 (0.4) |
| 180.4 (52.3) | 198.4 (44.5) | 197.2 (69.7) | 205.9 (60.0) |
| 291.2 (15.8) | 291.9 (0.3) | 292.6 (5.0) | 287.5 (6.4) |
| 317.6 (0.0) | 317.2 (0.0) | 322.1 (0.4) | 321.3 (0.2) |
| 342.5 (0.3) | 335.8 (0.0) | 330.2 (0.0) | 325.4 (0.0) |
| 343.0 (26.0) | 339.0 (9.7) | 339.6 (0.1) | 331.9 (0.2) |
| 345.9 (0.0) | 349.1 (0.1) | 347.2 (16.4) | 351.7 (0.0) |
| 355.1 (7.9) | 356.9 (13.2) | 351.5 (0.2) | 352.5 (18.0) |
| 357.2 (31.9) | 364.5 (11.9) | 353.8 (3.5) | 359.7 (7.3) |
| 364.9 (28.4) | 368.1 (0.0) | 364.9 (0.1) | 363.2 (3.8) |
| 365.4 (18.8) | 372.4 (3.1) | 370.6 (35.8) | 373.1 (11.8) |
| 374.8 (2.7) | 384.5 (7.3) | 373.5 (0.8) | 386.8 (2.1) |
| 377.9 (22.2) | 394.0 (63.1) | 388.5 (1.7) | 396.2 (33.0) |
| 395.7 (0.8) | 400.3 (9.6) | 391.2 (17.2) | 409.0 (9.1) |
| 406.1 (90.1) | 414.7 (81.1) | 404.5 (65.2) | 416.3 (55.3) |
| 418.0 (15.3) | 433.3 (51.4) | 413.7 (1.7) | 423.3 (7.9) |

| | | | |
|---|---|---|---|
| 430.5 (6.3) | 440.6 (1.7) | 422.3 (16.1) | 436.1 (31.7) |
| 437.3 (22.0) | 445.7 (12.7) | 435.1 (6.8) | 444.4 (17.1) |
| 449.4 (0.5) | 457.9 (20.0) | 439.6 (12.5) | 449.0 (5.0) |
| 456.3 (0.2) | 466.2 (70.9) | 454.3 (3.1) | 450.5 (0.0) |
| 467.2 (244.3) | 472.2 (0.6) | 460.5 (4.4) | 459.2 (20.4) |
| 482.0 (88.0) | 481.6 (44.3) | 467.9 (1.2) | 475.5 (0.8) |
| 490.3 (43.9) | 489.3 (126.8) | 496.7 (223.1) | 489.0 (121.4) |
| 503.8 (1.1) | 493.4 (0.2) | 519.1 (0.4) | 498.3 (0.5) |
| 519.2 (5.8) | 506.7 (1.3) | 519.8 (0.3) | 512.8 (0.3) |
| 523.6 (5.8) | 516.8 (5.7) | 520.4 (14.8) | 514.9 (27.5) |
| 532.2 (39.9) | 539.4 (123.5) | 530.6 (84.6) | 538.2 (95.3) |
| 545.3 (117.7) | 542.3 (13.5) | 544.8 (19.4) | 540.0 (20.4) |
| 546.6 (12.5) | 547.3 (86.7) | 552.9 (98.2) | 554.5 (113.9) |
| 570.6 (88.5) | 574.5 (93.5) | 573.8 (199.6) | 574.1 (150.7) |
| 584.6 (23.5) | 575.6 (81.8) | 601.1 (92.8) | 592.0 (14.1) |
| 590.0 (69.7) | 585.8 (11.3) | 601.5 (8.3) | 593.8 (100.5) |
| 1913.0 (242.7) | 1837.2 (191.7) | 1851.4 (326.1) | 1803.6 (189.3) |
| 1932.9 (207.5) | 1848.9 (154.1) | 1930.8 (309.5) | 1861.7(248.6) |
| 1947.0 (240.9) | 1873.1 (129.3) | 1943.1 (21.3) | 1874.7 (15.4) |
| 2091.5 (591.8) | 2014.6 (22.5) | 2117.0 (896.1) | 2020.6(795.6) |
| 2114.7 (173.5) | 2029.7 (635.3) | 2117.7 (331.1) | 2023.8 (383.9) |
| 2131.8 (839.7) | 2034.0 (371.5) | 2128.1 (89.7) | 2030.8 (382.1) |
| 2138.1 (1181.1) | 2036.7(1528.1) | 2132.5 (994.9) | 2041.2 (612.1) |
| 2139.7 (115.1) | 2043.2 (161.3) | 2150.3 (667.9) | 2054.6 (604.8) |
| 2149.7 (1203.9) | 2070.4 (766.7) | 2167.0 (1306.6) | 2080.5 (798.3) |
| 2190.1 (249.2) | 2095.1 (112.5) | 2190.1 (14.6) | 2100.0 (51.1) |

**Table S9.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_8]$

| **28S-5**($C_{2h}$) | | **28S-6**($C_{2v}$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 27.2 (1.6) | 22.8 (1.4) | 7.6 (0.0) | -11.2 (0.0) |
| 54.3 (0.0) | 48.4 (0.0) | 51.9 (0.0) | 45.7 (0.0) |
| 54.8 (0.5) | 50.3 (0.6) | 54.3 (0.6) | 49.5 (0.7) |
| 62.5 (3.7) | 55.5 (0.0) | 57.9 (4.6) | 51.5 (3.5) |
| 66.4 (0.0) | 59.8 (2.3) | 63.2 (1.9) | 58.4 (1.3) |
| 69.2 (1.5) | 64.6 (1.3) | 65.7 (0.5) | 63.2 (0.2) |
| 73.5 (0.0) | 70.0 (0.0) | 72.6 (0.9) | 64.9 (0.5) |
| 75.2 (0.0) | 73.3 (2.2) | 74.8 (0.0) | 72.2 (0.0) |
| 78.2 (1.7) | 73.3 (0.0) | 78.6 (0.0) | 73.3 (0.0) |
| 86.7 (4.4) | 81.6 (2.0) | 84.1 (2.5) | 79.3 (2.6) |
| 88.4 (0.0) | 84.1 (0.0) | 89.1 (0.1) | 84.9 (0.8) |
| 92.0 (1.4) | 89.0 (1.2) | 90.1 (2.2) | 86.0 (0.1) |
| 105.0 (0.0) | 98.5 (0.0) | 100.2 (0.0) | 94.6 (0.0) |
| 109.3 (0.0) | 104.3 (0.0) | 106.1 (0.0) | 96.2 (0.0) |
| 112.0 (0.7) | 107.6 (0.3) | 108.2 (0.1) | 104.0 (0.0) |
| 126.1 (2.9) | 119.8 (2.5) | 112.3 (0.1) | 107.1 (0.0) |
| 128.6 (0.0) | 122.7 (0.0) | 112.4 (0.3) | 108.0 (0.4) |
| 202.1 (0.0) | 191.2 (0.0) | 203.4 (0.1) | 193.2 (0.1) |
| 230.5 (0.0) | 231.0 (0.0) | 217.1 (0.0) | 225.5 (0.0) |
| 243.7 (0.7) | 238.4 (0.6) | 245.6 (0.2) | 240.6 (0.5) |
| 268.8 (0.0) | 283.6 (1.9) | 265.5 (0.0) | 281.9 (2.4) |
| 284.2 (5.4) | 294.5 (0.0) | 282.7 (6.0) | 285.4 (0.0) |
| 334.7 (30.4) | 331.0 (0.2) | 332.1 (0.3) | 329.3 (0.2) |
| 335.7 (0.0) | 337.5 (0.0) | 332.8 (0.0) | 330.2 (0.9) |
| 336.7 (0.0) | 344.0 (6.6) | 333.6 (0.0) | 331.2 (0.0) |
| 342.3 (0.0) | 353.0 (0.0) | 338.5 (13.7) | 334.8 (5.0) |
| 352.9 (22.7) | 356.3 (0.0) | 344.7 (26.5) | 354.3 (0.0) |
| 353.8 (0.0) | 362.9 (0.0) | 350.4 (1.0) | 369.5 (0.0) |
| 360.5 (0.0) | 364.0 (14.2) | 371.2 (0.1) | 372.1 (1.5) |
| 362.3 (2.6) | 368.1 (0.0) | 371.3 (1.6) | 374.0 (0.4) |
| 374.5 (7.2) | 383.5 (3.9) | 373.4 (6.2) | 376.6 (3.2) |
| 377.5 (0.0) | 395.3 (2.2) | 376.2 (0.1) | 392.0 (3.6) |
| 379.6 (0.0) | 404.2 (0.0) | 378.4 (0.0) | 393.0 (4.1) |
| 400.9 (1.0) | 413.0 (11.6) | 407.9 (0.1) | 417.2 (0.6) |

| | | | |
|---|---|---|---|
| 415.3 (0.1) | 423.3 (0.4) | 410.5 (6.3) | 425.8 (35.3) |
| 433.2 (19.1) | 426.4 (42.1) | 428.5 (18.3) | 428.0 (6.0) |
| 448.3 (0.0) | 450.5 (0.0) | 447.3 (0.0) | 451.1 (0.2) |
| 449.1 (0.0) | 452.7 (0.0) | 461.3 (25.1) | 453.0 (1.0) |
| 465.3 (0.0) | 458.7 (0.0) | 463.9 (0.1) | 455.0 (0.0) |
| 469.6 (0.0) | 467.1 (2.0) | 464.9 (1.9) | 469.2 (23.8) |
| 474.6 (0.3) | 471.8 (0.0) | 478.3 (0.0) | 471.9 (0.0) |
| 485.1 (104.1) | 481.0 (33.5) | 486.8 (39.7) | 489.1 (3.4) |
| 500.2 (0.0) | 498.3 (0.0) | 492.2 (8.8) | 489.4 (3.4) |
| 503.1 (65.6) | 499.6 (0.0) | 505.9 (12.9) | 492.9 (12.4) |
| 509.2 (0.0) | 501.8 (104.7) | 510.6 (116.4) | 507.1 (135.0) |
| 516.6 (0.0) | 515.5 (0.0) | 534.2 (14.8) | 529.3 (15.4) |
| 527.7 (80.6) | 529.7 (90.0) | 535.2 (66.6) | 535.5 (77.7) |
| 605.0 (78.0) | 588.8 (98.6) | 603.8 (76.6) | 588.4 (0.0) |
| 609.9 (0.0) | 591.2 (0.0) | 606.2 (0.0) | 589.6 (90.7) |
| 683.4 (440.1) | 640.0 (425.2) | 681.0 (446.9) | 640.0 (424.7) |
| 1826.6 (677.2) | 1789.1(506.0) | 1827.5(675.4) | 1789.4(502.9) |
| 1839.9 (0.0) | 1799.6 (0.0) | 1840.8 (6.8) | 1800.0 (5.4) |
| 1929.6 (0.0) | 1858.1 (0.0) | 1939.3 (14.6) | 1864.5(5.7) |
| 1930.1 (350.0) | 1859.1(287.8) | 1947.5(368.3) | 1871.2(297.0) |
| 2146.3 (0.0) | 2039.9 (0.0) | 2115.8 (43.3) | 2022.1 (0.0) |
| 2153.3 (1145.1) | 2047.6(1105.7) | 2142.1(858.0) | 2043.1 (0.0) |
| 2155.5 (0.0) | 2051.1(824.0) | 2150.3 (0.0) | 2043.2(771.7) |
| 2155.6 (851.2) | 2051.2 (0.0) | 2157.7(1117.8) | 2051.2(1087.3) |
| 2169.0 (1739.6) | 2073.9(1443.7) | 2168.0(1590.1) | 2071.0(1354.2) |
| 2193.6 (0.0) | 2093.8 (0.0) | 2191.7(110.8) | 2092.6(126.1) |

**Table S10.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_8]$

| **28S-7**($C_{2v}$) | |
|---|---|
| B3LYP | BP86 |
| 31.6 (0.0) | 29.2 (0.0) |
| 42.9 (0.1) | 34.4 (0.2) |
| 48.5 (1.5) | 44.5 (1.4) |
| 50.9 (0.3) | 48.3 (0.4) |
| 63.0 (1.4) | 58.6 (1.6) |
| 66.6 (1.9) | 63.2 (1.5) |
| 70.7 (3.9) | 65.0 (3.1) |
| 75.4 (0.0) | 73.7 (0.0) |
| 79.7 (0.0) | 75.7 (0.0) |
| 89.3 (0.6) | 85.8 (0.5) |
| 93.9 (0.0) | 90.1 (0.0) |
| 95.7 (0.1) | 92.3 (0.0) |
| 97.4 (0.0) | 92.6 (0.1) |
| 98.0 (3.9) | 94.0 (2.4) |
| 102.1 (4.7) | 102.8 (0.0) |
| 105.3 (0.0) | 103.1 (2.8) |
| 107.4 (2.2) | 105.6 (1.3) |
| 183.3 (1.7) | 176.6 (0.9) |
| 212.1 (2.2) | 216.6 (1.0) |
| 231.2 (0.0) | 226.6 (0.4) |
| 288.6 (0.9) | 287.3 (0.1) |
| 305.3 (6.6) | 327.3 (0.2) |
| 333.4 (0.0) | 328.4 (0.1) |
| 335.5 (1.1) | 328.7 (0.7) |
| 341.9 (3.3) | 335.6 (0.0) |
| 343.9 (0.0) | 342.3 (14.8) |
| 350.1 (0.5) | 350.3 (0.8) |
| 356.9 (4.7) | 356.4 (3.0) |
| 359.3 (2.7) | 359.7 (2.0) |
| 365.9 (5.2) | 375.9 (5.7) |
| 370.3 (8.0) | 376.0 (0.0) |
| 376.3 (0.0) | 377.5 (1.5) |
| 402.9 (55.5) | 418.7 (29.1) |
| 411.2 (0.7) | 419.0 (0.3) |

| | |
|---|---|
| 422.5 (8.1) | 423.2 (2.0) |
| 431.0 (1.6) | 443.0 (0.1) |
| 440.2 (0.3) | 454.9 (2.2) |
| 466.3 (5.3) | 456.7 (0.0) |
| 466.7 (9.3) | 462.0 (7.7) |
| 477.5 (0.0) | 463.1 (9.4) |
| 506.0 (0.0) | 500.4 (4.1) |
| 511.0 (0.0) | 505.3 (0.0) |
| 517.9 (10.9) | 518.7 (5.6) |
| 527.5 (6.9) | 522.1 (0.0) |
| 529.2 (378.8) | 523.5 (371.0) |
| 558.9 (108.2) | 552.7 (104.8) |
| 576.2 (1.0) | 565.1 (0.9) |
| 604.0 (63.3) | 595.3 (81.0) |
| 619.6 (15.2) | 602.6 (75.6) |
| 646.7 (284.0) | 616.4 (206.5) |
| 1849.0 (444.5) | 1811.5 (354.2) |
| 1908.0 (221.3) | 1856.5 (77.2) |
| 1940.2 (261.0) | 1864.9 (187.7) |
| 1944.3 (212.2) | 1870.1 (261.6) |
| 2104.6 (0.0) | 2011.4 (0.0) |
| 2122.2 (191.3) | 2033.1 (12.0) |
| 2130.5 (1979.9) | 2033.5 (1765.6) |
| 2147.7 (389.5) | 2048.5 (454.5) |
| 2156.5 (1084.8) | 2059.0 (1019.5) |
| 2186.8 (211.6) | 2089.7 (138.2) |

**Table S11.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_7]$

| **27S-1**($C_{2v}$) | | **27S-2**($C_s$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 49.4 (0.6) | 45.3 (0.5) | 9.6 (0.4) | 14.0 (0.1) |
| 49.5 (1.5) | 45.6 (0.0) | 37.8 (0.0) | 35.9 (0.9) |
| 50.8 (0.0) | 46.6 (1.4) | 43.5 (1.2) | 38.2 (0.2) |
| 75.5 (0.0) | 69.7 (0.9) | 46.5 (0.6) | 44.2 (0.7) |
| 76.2 (0.9) | 73.6 (0.0) | 58.9 (0.4) | 61.3 (2.6) |
| 76.4 (0.0) | 74.6 (0.0) | 70.6 (2.4) | 64.8 (0.2) |
| 79.6 (0.4) | 76.6 (0.4) | 77.6 (1.3) | 68.2 (1.7) |
| 84.9 (0.1) | 82.4 (0.1) | 82.1 (1.8) | 80.9 (0.3) |
| 89.4 (0.6) | 87.1 (0.6) | 86.7 (0.5) | 84.5 (0.0) |
| 90.6 (0.0) | 91.5 (0.0) | 89.0 (0.1) | 86.1 (1.2) |
| 92.0 (0.8) | 92.0 (2.4) | 95.3 (0.1) | 89.9 (0.1) |
| 96.4 (3.7) | 101.2 (0.0) | 95.9 (0.0) | 90.8 (0.1) |
| 100.2 (1.6) | 101.7 (0.1) | 101.6 (3.4) | 99.5 (1.8) |
| 106.4 (0.5) | 103.2 (1.2) | 108.3 (0.1) | 104.5 (0.4) |
| 154.0 (0.0) | 164.1 (0.0) | 111.9 (0.0) | 112.8 (0.1) |
| 165.3 (0.2) | 172.2 (0.1) | 123.6 (10.0) | 122.1 (9.7) |
| 214.1 (4.8) | 215.9 (1.3) | 139.0 (0.5) | 148.6 (0.4) |
| 230.8 (0.4) | 227.3 (0.2) | 163.7 (1.0) | 175.7 (0.2) |
| 244.8 (0.0) | 249.6 (0.0) | 319.7 (21.2) | 322.8 (6.1) |
| 281.6 (7.5) | 289.0 (6.6) | 328.0 (0.5) | 323.8 (0.0) |
| 341.6 (6.8) | 340.8 (0.1) | 340.6 (0.3) | 330.3 (0.8) |
| 342.3 (4.0) | 341.9 (1.6) | 341.3 (0.9) | 342.4 (0.1) |
| 346.7 (0.2) | 342.2 (3.0) | 349.2 (3.8) | 347.2 (14.0) |
| 378.4 (2.1) | 373.4 (0.0) | 357.1 (0.1) | 348.3 (0.5) |
| 379.2 (0.0) | 373.6 (0.4) | 370.8 (2.5) | 358.8 (7.0) |
| 391.6 (0.8) | 386.1 (1.0) | 382.7 (7.7) | 373.7 (5.5) |
| 395.7 (11.2) | 393.5 (0.2) | 399.1 (89.9) | 392.8 (0.1) |
| 401.5 (54.3) | 398.3 (0.6) | 410.4 (0.4) | 420.2 (60.6) |
| 403.4 (13.0) | 409.8 (0.0) | 412.2 (0.9) | 433.6 (3.7) |
| 405.4 (8.9) | 413.3 (2.9) | 423.3 (6.4) | 441.5 (18.8) |
| 407.4 (0.0) | 419.4 (18.3) | 431.1 (3.0) | 444.0 (2.7) |
| 412.1 (0.0) | 428.4 (25.2) | 445.9 (11.8) | 450.7 (1.1) |
| 434.0 (0.0) | 445.9 (20.5) | 452.6 (3.1) | 459.3 (8.2) |
| 435.8 (20.2) | 452.7 (0.0) | 467.6 (45.0) | 467.0 (8.3) |

| | | | |
|---|---|---|---|
| 443.4 (0.0) | 460.3 (0.0) | 476.4 (3.9) | 467.6 (10.8) |
| 458.4 (15.1) | 465.0 (5.5) | 482.1 (11.1) | 488.3 (17.3) |
| 497.7 (0.6) | 491.7 (0.0) | 497.6 (2.1) | 498.3 (16.1) |
| 517.0 (18.6) | 509.9 (13.5) | 528.3 (0.5) | 517.0 (0.4) |
| 522.3 (212.5) | 518.8 (67.3) | 535.9 (1.5) | 525.7 (1.0) |
| 528.8 (0.8) | 521.6 (0.0) | 542.8 (128.6) | 535.0 (351.6) |
| 529.8 (0.0) | 525.1 (161.8) | 546.8 (306.6) | 547.8 (3.8) |
| 533.3 (98.6) | 533.7 (113.6) | 555.6 (70.5) | 551.4 (83.6) |
| 543.8 (8.8) | 545.7 (1.7) | 563.0 (42.0) | 552.3 (50.0) |
| 587.8 (66.2) | 572.9 (84.7) | 575.7 (5.0) | 569.4 (26.7) |
| 640.6 (435.9) | 612.9 (388.4) | 576.7 (46.4) | 570.0 (50.9) |
| 1838.8 (390.4) | 1771.2 (286.1) | 1911.6 (151.4) | 1828.9 (108.2) |
| 1849.3 (195.4) | 1779.4 (121.8) | 1934.8 (332.2) | 1851.6 (222.9) |
| 1945.6 (489.0) | 1894.9 (401.6) | 2084.8 (179.0) | 2001.6 (139.6) |
| 2135.8 (0.0) | 2043.1 (0.0) | 2094.1 (393.5) | 2003.7 (338.1) |
| 2137.1 (1335.1) | 2044.9 (1180.8) | 2107.7 (214.6) | 2026.6 (265.1) |
| 2141.7 (180.2) | 2048.0 (94.3) | 2115.1 (1714.7) | 2027.3 (1416.5) |
| 2146.8 (1144.6) | 2052.8 (1023.3) | 2130.9 (411.4) | 2036.5 (327.1) |
| 2165.9 (1253.6) | 2076.0 (1067.5) | 2142.5 (1376.5) | 2053.4 (1045.7) |
| 2195.4 (4.5) | 2101.2 (1.9) | 2184.3 (132.4) | 2092.3 (125.8) |

**Table S12.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_7]$

| **27S-3**($C_1$) | | **27S-4**($C_1$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 17.2 (1.3) | 45.3 (0.5) | 16.2 (0.8) | 16.1 (0.9) |
| 24.8 (0.6) | 45.6 (0.0) | 38.9 (1.7) | 35.4 (0.3) |
| 39.1 (0.1) | 46.6 (1.4) | 45.6 (0.4) | 40.0 (0.7) |
| 47.5 (0.4) | 69.7 (0.9) | 55.4 (0.6) | 49.2 (1.4) |
| 50.4 (2.2) | 73.6 (0.0) | 62.8 (0.7) | 65.6 (0.2) |
| 54.2 (0.9) | 74.6 (0.0) | 70.2 (0.6) | 70.0 (0.8) |
| 59.2 (2.3) | 76.6 (0.4) | 80.2 (0.4) | 77.7 (0.1) |
| 72.5 (2.6) | 82.4 (0.1) | 87.0 (0.7) | 79.3 (0.1) |
| 83.9 (1.0) | 87.1 (0.6) | 89.8 (0.9) | 84.2 (0.9) |
| 86.5 (2.5) | 91.5 (0.0) | 91.3 (0.6) | 89.7 (0.9) |
| 88.7 (4.0) | 92.0 (2.4) | 94.4 (2.5) | 93.0 (1.2) |
| 93.0 (0.5) | 101.2 (0.0) | 98.8 (1.3) | 95.7 (1.7) |
| 94.3 (0.8) | 101.7 (0.1) | 104.0 (0.4) | 99.7 (0.1) |
| 97.8 (1.4) | 103.2 (1.2) | 105.9 (3.1) | 104.4 (0.3) |
| 99.9 (0.7) | 164.1 (0.0) | 109.1 (0.4) | 108.6 (0.7) |
| 104.8 (0.7) | 172.2 (0.1) | 116.2 (0.5) | 111.0 (1.2) |
| 110.9 (0.0) | 215.9 (1.3) | 168.1 (0.8) | 185.6 (1.4) |
| 121.1 (0.1) | 227.3 ( 0.2) | 233.8 (9.0) | 231.5 (1.6) |
| 324.6 (2.3) | 249.6 (0.0) | 334.4 (6.5) | 292.1 (4.7) |
| 331.1 (0.9) | 289.0 (6.6) | 344.5 (4.6) | 343.3 (0.3) |
| 348.1 (7.0) | 340.8 (0.1) | 348.5 (5.7) | 349.1 (1.9) |
| 351.6 (0.4) | 341.9 (1.6) | 357.8 (2.3) | 350.1 (4.3) |
| 354.9 (0.6) | 342.2 (3.0) | 363.0 (8.2) | 357.7 (13.1) |
| 356.7 (8.0) | 373.4 (0.0) | 367.6 (1.8) | 362.0 (1.9) |
| 375.3 (0.5) | 373.6 (0.4) | 375.4 (34.6) | 377.7 (8.4) |
| 377.4 (11.5) | 386.1 (1.0) | 378.9 (12.5) | 389.0 (1.0) |
| 386.6 (6.4) | 393.5 (0.2) | 383.6 (9.8) | 392.2 (2.4) |
| 389.6 (2.4) | 398.3 (0.6) | 394.3 (16.5) | 401.1 (13.8) |
| 412.1 (3.6) | 409.8 (0.0) | 399.2 (3.8) | 405.6 (3.7) |
| 412.9 (1.9) | 413.3 (2.9) | 407.9 (13.3) | 415.3 (4.3) |
| 423.8 (4.8) | 419.4 (18.3) | 425.7 (5.1) | 433.9 (2.4) |
| 435.4 (0.4) | 428.4 (25.2) | 431.6 (2.4) | 437.9 (0.8) |
| 442.1 (2.9) | 445.9 (20.5) | 447.0 (4.6) | 458.0 (0.8) |
| 455.1 (0.2) | 452.7 (0.0) | 456.8 (3.7) | 464.5 (13.8) |

| | | | |
|---|---|---|---|
| 478.9 (9.9) | 460.3 (0.0) | 466.0 (61.3) | 473.7 (11.4) |
| 502.1 (15.9) | 465.0 (5.6) | 494.3 (113.6) | 495.0 (26.5) |
| 505.6 (21.7) | 491.7 (0.0) | 510.3 (11.4) | 500.5 (63.5) |
| 519.0 (1.8) | 509.9 (13.5) | 518.0 (36.3) | 508.5 (62.1) |
| 536.0 (31.0) | 518.8 (67.3) | 523.8 (21.5) | 514.0 (20.8) |
| 538.4 (5.6) | 521.6 (0.0) | 531.4 (17.5) | 529.4 (27.9) |
| 559.5 (73.7) | 525.1 (161.7) | 559.3 (114.9) | 547.3 (195.8) |
| 560.5 (44.9) | 533.7 (113.6) | 563.6 (82.6) | 560.1 (91.1) |
| 563.9 (104.3) | 545.7 (1.7) | 570.6 (98.4) | 561.8 (44.6) |
| 579.4 (79.0) | 572.9 (84.7) | 574.1 (41.5) | 567.8 (72.3) |
| 590.9 (73.9) | 612.9 (388.4) | 599.1 (50.6) | 599.6 (105.7) |
| 1918.6 (198.0) | 1771.2 (286.1) | 1926.7 (203.1) | 1822.4 (175.3) |
| 1940.1 (184.8) | 1779.4 (121.8) | 1935.5 (222.4) | 1863.5 (177.0) |
| 2075.4 (334.2) | 1894.9 (401.6) | 1968.1 (535.7) | 1894.7 (442.4) |
| 2103.6 (1336.4) | 2043.1 (0.0) | 2103.1 (324.2) | 2019.9 (169.2) |
| 2111.8 (313.9) | 2044.9 (1180.8) | 2112.2 (257.8) | 2024.3 (432.8) |
| 2128.8 (723.5) | 2048.0 (94.3) | 2129.1 (1029.5) | 2037.2 (995.5) |
| 2149.4 (584.5) | 2052.8 (1023.2) | 2138.0 (982.9) | 2050.2 (683.3) |
| 2162.8 (708.1) | 2076.0 (1067.5) | 2153.2 (1061.1) | 2061.8 (969.0) |
| 2195.5 (198.3) | 2101.2 (1.9) | 2185.1 (37.2) | 2093.7 (30.4) |

**Table S13.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_7]$

| **27S-5**($C_1$) | | **27S-6**($C_{2v}$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 28.6 (0.9) | 27.0 (0.8) | 14.7 (0.0) | 10.4 (0.0) |
| 39.4 (0.2) | 39.8 (0.2) | 39.6 (4.4) | 36.5 (3.8) |
| 46.1 (0.7) | 42.4 (0.6) | 43.6 (0.8) | 37.7 (1.0) |
| 64.4 (0.1) | 58.4 (0.1) | 46.0 (2.3) | 38.4 (1.5) |
| 67.6 (0.4) | 65.7 (0.3) | 54.3 (0.0) | 55.8 (0.1) |
| 76.6 (0.2) | 74.4 (0.1) | 75.4 (0.2) | 77.1 (0.0) |
| 79.0 (0.4) | 76.4 (0.4) | 81.4 (0.0) | 80.0 (0.6) |
| 84.1 (0.0) | 80.8 (0.0) | 87.8 (0.1) | 84.0 (0.1) |
| 87.6 (0.7) | 86.5 (0.3) | 90.2 (0.5) | 91.6 (0.1) |
| 90.8 (0.4) | 92.4 (0.5) | 95.6 (0.0) | 93.9 (0.0) |
| 96.7 (0.5) | 92.8 (1.0) | 98.5 (0.7) | 95.1 (0.4) |
| 101.1 (3.9) | 98.9 (1.3) | 100.7 (3.6) | 97.2 (4.3) |
| 109.1 (0.6) | 105.2 (0.3) | 103.0 (3.4) | 99.5 (0.2) |
| 112.8 (0.3) | 110.2 (0.1) | 104.6 (0.3) | 100.6 (0.0) |
| 136.8 (0.6) | 154.6 (0.9) | 104.9 (0.0) | 101.4 (0.2) |
| 181.2 (0.5) | 202.7 (0.1) | 114.3 (0.8) | 112.6 (1.5) |
| 215.2 (0.2) | 216.4 (0.5) | 171.5 (0.0) | 176.3 (0.1) |
| 233.6 (2.6) | 233.9 (1.3) | 235.5 (7.4) | 239.6 (2.0) |
| 300.5 (35.9) | 300.1 (43.7) | 343.5 (3.9) | 341.3 (0.4) |
| 312.8 (10.0) | 312.2 (5.6) | 343.9 (1.8) | 342.1 (0.1) |
| 333.8 (0.5) | 320.2 (1.8) | 346.7 (2.9) | 342.3 (0.0) |
| 342.7 (0.3) | 341.0 (0.6) | 348.6 (0.0) | 345.6 (4.0) |
| 352.7 (0.6) | 346.8 (1.6) | 363.0 (0.1) | 351.6 (3.2) |
| 355.0 (26.3) | 359.6 (15.7) | 370.9 (4.6) | 364.2 (0.0) |
| 368.0 (4.8) | 368.0 (0.8) | 373.4 (0.0) | 379.6 (0.5) |
| 379.5 (6.7) | 373.5 (1.7) | 377.5 (24.8) | 389.6 (0.1) |
| 392.8 (7.7) | 393.6 (2.7) | 387.9 (14.9) | 402.0 (6.4) |
| 400.5 (12.7) | 402.6 (2.3) | 398.7 (3.0) | 406.8 (0.2) |
| 404.4 (4.5) | 405.2 (1.9) | 410.8 (0.8) | 416.7 (0.0) |
| 408.6 (10.5) | 423.2 (7.0) | 419.6 (78.4) | 418.0 (0.1) |
| 418.6 (1.7) | 429.2 (8.5) | 429.0 (1.8) | 439.0 (69.2) |
| 425.0 (5.1) | 431.8 (5.0) | 436.9 (1.6) | 448.6 (0.0) |
| 431.8 (2.7) | 435.1 (2.7) | 447.8 (56.0) | 450.5 (3.6) |
| 436.6 (18.1) | 450.4 (2.3) | 454.6 (1.2) | 466.1 (126.9) |

| | | | |
|---|---|---|---|
| 450.5 (1.7) | 462.1 (9.2) | 464.0 (130.7) | 478.6 (0.3) |
| 462.0 (3.9) | 471.2 (4.9) | 467.1 (0.0) | 484.1 (66.4) |
| 497.1 (34.9) | 490.9 (28.4) | 516.6 (1.5) | 499.1 (0.0) |
| 506.9 (58.4) | 494.9 (22.7) | 523.4 (0.0) | 514.8 (0.0) |
| 516.8 (17.0) | 515.8 (7.6) | 530.7 (45.3) | 524.9 (26.8) |
| 525.5 (65.1) | 522.7 (108.7) | 535.4 (0.0) | 543.9 (0.0) |
| 541.9 (41.9) | 536.8 (41.8) | 568.7 (68.6) | 563.2 (212.2) |
| 551.9 (79.4) | 550.0 (62.3) | 577.3 (199.5) | 567.5 (94.2) |
| 572.1 (6.9) | 562.8 (6.2) | 580.6 (103.7) | 568.4 (80.6) |
| 585.2 (76.6) | 574.9 (80.0) | 587.6 (5.6) | 574.2 (18.3) |
| 643.2 (431.3) | 628.0 (444.4) | 607.5 (36.2) | 604.3 (49.0) |
| 1904.8 (173.3) | 1819.0 (130.1) | 1935.6 (406.7) | 1860.4 (327.2) |
| 1934.7 (344.1) | 1851.5 (224.5) | 1936.9 (48.2) | 1861.3 (30.1) |
| 1951.8 (798.5) | 1890.7 (597.9) | 1973.7 (581.6) | 1896.0 (462.3) |
| 1974.4 (177.8) | 1905.5 (174.3) | 2105.5 (0.0) | 2012.4 (0.0) |
| 2121.9 (695.3) | 2031.9 (563.4) | 2107.3 (108.6) | 2018.6 (55.3) |
| 2137.4 (507.5) | 2042.1 (404.6) | 2125.4 (2036.8) | 2029.1 (1731.6) |
| 2142.8 (750.2) | 2046.6 (768.6) | 2131.8 (921.4) | 2042.5 (845.5) |
| 2156.8 (1424.4) | 2065.0 (1187.6) | 2134.9 (406.9) | 2047.6 (415.8) |
| 2185.9 (69.5) | 2091.0 (77.7) | 2181.5 (89.9) | 2088.8 (78.8) |

**Table S14.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_7]$

| **27S-7**($C_1$) | | **27S-8**($C_s$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 5.7 (0.2) | 33.4 (0.0) | 8.1 (0.8) | 12.6 (0.5) |
| 21.3 (1.1) | 40.5 (0.6) | 31.5 (3.5) | 30.6 (3.1) |
| 36.5 (1.0) | 44.9 (0.8) | 38.0 (2.0) | 31.8 (2.3) |
| 50.1 (1.4) | 59.6 (1.4) | 51.7 (1.1) | 46.7 (1.1) |
| 59.1 (1.3) | 63.2 (1.6) | 60.8 (0.3) | 60.6 (0.0) |
| 65.0 (0.7) | 74.3 (0.4) | 67.4 (0.0) | 68.2 (0.1) |
| 66.3 (0.3) | 76.9 (0.5) | 81.1 (0.8) | 76.2 (1.0) |
| 79.9 (1.0) | 81.1 (1.2) | 86.4 (0.5) | 80.9 (0.2) |
| 86.8 (0.7) | 82.9 (0.3) | 91.7 (0.3) | 86.9 (0.0) |
| 89.7 (0.5) | 87.8 (1.2) | 94.2 (3.2) | 90.1 (1.8) |
| 93.0 (1.0) | 90.3 (1.0) | 98.5 (0.1) | 95.1 (0.0) |
| 95.5 (4.2) | 96.2 (0.8) | 100.0 (0.8) | 96.2 (0.5) |
| 102.0 (0.1) | 99.0 (0.3) | 104.1 (0.0) | 98.4 (0.0) |
| 106.8 (0.4) | 105.5 (0.0) | 109.1 (3.3) | 106.9 (1.9) |
| 109.7 (0.8) | 115.6 (2.2) | 109.9 (0.6) | 108.3 (1.0) |
| 118.5 (1.2) | 143.0 (0.8) | 114.5 (0.8) | 111.3 (0.5) |
| 130.5 (7.4) | 205.2 (0.3) | 169.5 (0.6) | 180.2 (0.5) |
| 155.8 (0.4) | 210.3 (0.5) | 229.2 (10.4) | 233.8 (5.6) |
| 277.1 (31.5) | 270.1 (12.3) | 338.3 (12.8) | 331.5 (0.1) |
| 334.1 (3.9) | 336.0 (3.5) | 343.1 (0.0) | 339.6 (1.7) |
| 345.0 (2.1) | 342.1 (3.5) | 346.4 (0.3) | 341.6 (0.1) |
| 349.8 (24.2) | 344.0 (1.8) | 347.4 (1.8) | 343.4 (0.3) |
| 353.3 (2.9) | 348.4 (1.0) | 349.2 (9.6) | 352.5 (1.6) |
| 361.7 (2.9) | 358.8 (1.5) | 363.8 (0.1) | 360.4 (0.7) |
| 367.0 (17.3) | 366.4 (8.1) | 368.1 (0.0) | 360.9 (8.4) |
| 377.1 (5.1) | 378.4 (0.8) | 369.3 (12.2) | 372.9 (5.2) |
| 405.5 (11.9) | 383.3 (2.2) | 379.8 (57.6) | 400.8 (3.3) |
| 410.2 (15.9) | 396.1 (1.8) | 393.9 (13.2) | 409.6 (27.0) |
| 417.7 (11.7) | 406.2 (0.2) | 403.8 (15.3) | 410.0 (0.1) |
| 419.1 (1.9) | 423.0 (5.3) | 419.3 (6.5) | 416.6 (36.1) |
| 430.2 (9.4) | 428.7 (7.9) | 420.9 (0.8) | 433.1 (7.9) |
| 433.5 (6.7) | 442.1 (15.2) | 434.8 (5.5) | 439.2 (0.3) |
| 448.8 (1.6) | 447.1 (7.0) | 449.2 (10.0) | 454.1 (1.8) |

| | | | |
|---|---|---|---|
| 460.7 (11.9) | 453.5 (2.8) | 458.6 (11.9) | 473.8 (28.0) |
| 471.0 (6.7) | 465.3 (2.8) | 460.1 (0.5) | 480.4 (9.0) |
| 497.4 (0.2) | 482.0 (3.9) | 495.4 (113.0) | 497.3 (0.1) |
| 525.7 (5.6) | 499.8 (33.9) | 513.5 (0.0) | 498.8 (87.9) |
| 532.3 (6.6) | 511.8 (28.3) | 521.0 (23.0) | 513.2 (14.4) |
| 533.3 (5.0) | 522.1 (5.0) | 534.0 (0.0) | 523.7 (0.2) |
| 540.5 (58.0) | 524.6 (90.7) | 543.6 (0.2) | 544.3 (8.8) |
| 559.3 (126.2) | 534.1 (69.2) | 559.9 (93.6) | 554.5 (235.5) |
| 570.4 (172.0) | 553.5 (155.5) | 569.8 (194.6) | 557.6 (112.2) |
| 582.0 (74.6) | 559.3 (94.4) | 575.3 (119.1) | 565.8 (2.5) |
| 591.0 (86.7) | 564.9 (25.4) | 582.2 (2.5) | 566.2 (83.6) |
| 595.5 (42.1) | 597.2 (285.9) | 595.9 (57.7) | 591.3 (83.0) |
| 1884.8 (201.7) | 1778.7 (184.6) | 1929.1 (308.4) | 1857.6 (206.3) |
| 1943.6 (253.9) | 1870.6 (254.6) | 1935.4 (252.5) | 1859.7 (250.8) |
| 2064.5 (411.5) | 1898.3 (333.7) | 1970.4 (411.7) | 1895.4 (323.7) |
| 2102.9 (633.7) | 2001.4 (284.3) | 2095.8 (137.7) | 2004.1 (52.4) |
| 2114.7 (348.4) | 2031.9 (632.1) | 2118.3 (125.9) | 2026.4 (1631.1) |
| 2131.8 (1148.5) | 2038.7 (751.9) | 2122.8 (1883.0) | 2029.4 (144.8) |
| 2136.2 (613.1) | 2049.0 (552.7) | 2136.4 (261.6) | 2039.8 (349.2) |
| 2141.5 (1355.1) | 2063.8 (1142.5) | 2145.8 (1206.0) | 2056.2 (947.7) |
| 2186.9 (51.0) | 2092.8 (44.1) | 2181.3 (10.2) | 2087.8 (13.7) |

**Table S15.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_7]$

| **27S-9**($C_s$) | | **27S-10**($C_2$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 41.6 (0.3) | 37.7 (0.1) | 21.9 (0.4) | 26.1 (0.5) |
| 44.7 (1.5) | 41.3 (1.6) | 33.8 (0.1) | 33.2 (1.4) |
| 50.6 (0.5) | 49.3 (1.0) | 37.8 (0.1) | 35.7 (0.0) |
| 67.8 (2.8) | 63.2 (0.8) | 41.8 (5.7) | 41.5 (3.4) |
| 71.9 (0.0) | 66.8 (0.9) | 64.3 (0.1) | 66.1 (0.1) |
| 73.6 (2.8) | 68.7 (1.6) | 75.1 (0.3) | 74.5 (1.7) |
| 77.0 (0.1) | 76.6 (0.1) | 79.9 (0.0) | 76.4 (0.0) |
| 82.9 (1.5) | 79.1 (1.1) | 85.6 (3.4) | 77.7 (1.6) |
| 84.4 (0.3) | 79.5 (0.4) | 86.8 (0.5) | 84.2 (0.9) |
| 93.6 (0.1) | 88.3 (0.6) | 92.5 (2.1) | 88.9 (1.1) |
| 97.9 (1.7) | 94.1 (0.4) | 98.3 (0.0) | 95.6 (0.0) |
| 100.0 (2.3) | 94.7 (1.6) | 101.8 (2.1) | 96.3 (0.1) |
| 103.4 (1.1) | 99.5 (0.7) | 105.1 (1.1) | 98.3 (1.1) |
| 104.9 (1.0) | 112.2 (0.3) | 105.8 (1.0) | 101.8 (0.8) |
| 122.1 (0.3) | 114.9 (0.2) | 111.1 (0.2) | 108.2 (0.2) |
| 194.8 (0.6) | 184.9 (0.5) | 117.2 (1.2) | 116.2 (1.7) |
| 220.5 (1.9) | 211.0 (2.4) | 169.9 (1.9) | 185.2 (1.1) |
| 237.9 (0.2) | 235.2 (0.9) | 223.7 (9.5) | 227.2 (3.8) |
| 300.0 (3.6) | 269.1 (5.4) | 325.9 (27.8) | 332.7 (0.9) |
| 317.3 (1.4) | 317.0 (0.8) | 341.2 (0.6) | 334.5 (0.0) |
| 342.5 (0.2) | 338.8 (0.1) | 343.7 (0.4) | 335.5 (2.9) |
| 352.7 (8.1) | 345.9 (2.5) | 344.8 (0.4) | 339.1 (2.1) |
| 354.0 (0.3) | 354.7 (0.3) | 346.2 (2.2) | 342.4 (0.2) |
| 362.2 (10.0) | 360.1 (4.1) | 348.0 (1.5) | 356.1 (10.9) |
| 371.2 (2.0) | 373.9 (0.1) | 361.0 (9.0) | 356.9 (0.0) |
| 375.5 (8.0) | 380.2 (0.4) | 362.1 (0.0) | 363.1 (1.1) |
| 384.2 (3.5) | 382.2 (16.8) | 391.7 (1.6) | 398.7 (2.3) |
| 393.6 (8.5) | 402.0 (3.4) | 396.9 (0.6) | 400.7 (1.9) |
| 394.6 (4.7) | 406.9 (7.4) | 407.4 (2.7) | 407.4 (0.2) |
| 401.0 (5.0) | 416.4 (4.1) | 412.7 (0.6) | 424.6 (0.3) |
| 425.0 (33.1) | 425.0 (8.6) | 424.6 (6.9) | 434.5 (2.1) |
| 428.3 (10.0) | 426.6 (3.0) | 443.3 (5.0) | 443.8 (10.8) |
| 433.7 (0.8) | 446.7 (18.6) | 449.8 (24.6) | 456.9 (4.3) |
| 449.4 (0.0) | 451.0 (0.7) | 453.5 (1.1) | 467.8 (11.4) |

| | | | |
|---|---|---|---|
| 470.1 (12.4) | 465.7 (1.8) | 459.7 (2.9) | 474.7 (0.1) |
| 474.1 (12.5) | 475.4 (1.5) | 507.6 (14.0) | 495.7 (60.5) |
| 495.7 (26.0) | 483.0 (13.0) | 522.7 (68.1) | 514.8 (22.4) |
| 509.5 (24.9) | 502.5 (12.8) | 527.1 (12.9) | 517.0 (9.1) |
| 515.5 (83.3) | 518.8 (77.7) | 532.8 (1.6) | 522.0 (0.7) |
| 529.9 (5.9) | 521.4 (38.7) | 540.1 (2.8) | 537.1 (334.7) |
| 547.4 (34.8) | 539.3 (36.7) | 547.4 (209.0) | 538.8 (5.9) |
| 549.3 (39.5) | 550.9 (12.1) | 559.5 (251.1) | 550.7 (67.4) |
| 567.1 (37.6) | 563.3 (53.3) | 566.7 (63.5) | 556.6 (93.9) |
| 598.5 (71.0) | 591.8 (79.8) | 571.1 (44.0) | 565.6 (25.1) |
| 659.0 (468.1) | 638.3 (484.9) | 582.4 (43.4) | 581.7 (147.9) |
| 1911.5(268.7) | 1812.3 (202.8) | 1934.8 (172.6) | 1861.6 (368.9) |
| 1943.9 (111.6) | 1871.3 (133.4) | 1934.8 (529.9) | 1862.6 (161.0) |
| 1951.7 (802.9) | 1899.2 (585.3) | 1970.1 (188.9) | 1898.3 (194.6) |
| 1969.9 (255.8) | 1909.9 (234.6) | 2098.2 (335.3) | 2004.9 (379.6) |
| 2131.9 (775.6) | 2040.4 (658.1) | 2108.7 (533.7) | 2010.5 (517.5) |
| 2144.7 (346.9) | 2048.2 (304.5) | 2123.0 (1347.9) | 2032.2 (1056.5) |
| 2151.2 (798.4) | 2055.7 (725.3) | 2131.0 (365.8) | 2038.8 (313.8) |
| 2164.4 (1286.4) | 2073.3 (1073.9) | 2144.2 (1178.6) | 2055.5 (969.9) |
| 2190.1 (66.8) | 2096.7 (62.2) | 2178.5 (96.2) | 2085.4 (89.1) |

**Table S16.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_7]$

| **27S-11**($C_s$) | |
|---|---|
| B3LYP | BP86 |
| 31.4 (0.0) | 32.4 (0.0) |
| 35.8 (0.3) | 34.7 (0.3) |
| 42.5 (1.1) | 41.5 (0.7) |
| 63.7 (2.5) | 56.6 (2.2) |
| 66.6 (0.9) | 65.0 (1.0) |
| 73.6 (0.2) | 71.9 (0.2) |
| 82.5 (0.4) | 79.1 (0.4) |
| 84.7 (0.1) | 81.3 (1.1) |
| 86.6 (0.7) | 85.5 (0.0) |
| 90.0 (0.0) | 87.2 (2.6) |
| 93.5 (4.4) | 91.7 (0.0) |
| 105.4 (0.9) | 99.2 (0.2) |
| 107.6 (0.2) | 102.8 (0.7) |
| 107.7 (0.6) | 106.1 (0.0) |
| 116.0 (2.6) | 112.2 (1.6) |
| 183.6 (0.8) | 194.4 (0.2) |
| 208.0 (1.4) | 212.5 (0.6) |
| 235.3 (2.8) | 232.2 (3.2) |
| 309.5 (1.6) | 314.1 (0.3) |
| 339.3 (0.1) | 338.3 (0.0) |
| 350.8 (10.9) | 348.5 (0.1) |
| 359.0 (0.0) | 350.8 (7.4) |
| 360.8 (1.5) | 356.2 (1.0) |
| 367.3 (0.9) | 362.8 (2.1) |
| 374.0 (1.4) | 375.4 (0.8) |
| 383.1 (19.3) | 380.1 (12.2) |
| 390.7 (7.1) | 390.1 (1.7) |
| 405.8 (13.5) | 404.4 (1.4) |
| 408.3 (0.4) | 405.4 (0.5) |
| 409.1 (27.0) | 418.4 (0.0) |
| 414.7 (0.0) | 424.7 (12.0) |
| 426.0 (8.4) | 433.4 (8.7) |
| 431.8 (15.6) | 443.3 (7.4) |
| 451.3 (0.9) | 459.7 (10.1) |

| | |
|---|---|
| 458.0 (3.8) | 469.7 (0.2) |
| 485.5 (1.4) | 476.7 (0.7) |
| 508.7 (32.2) | 499.7 (22.9) |
| 513.1 (20.9) | 506.7 (6.9) |
| 529.5 (68.3) | 527.1 (92.0) |
| 535.9 (10.1) | 529.2 (17.2) |
| 560.6 (37.9) | 550.3 (57.1) |
| 570.3 (78.6) | 562.3 (32.8) |
| 577.6 (77.9) | 572.7 (111.6) |
| 597.5 (49.6) | 585.3 (44.6) |
| 623.6 (418.5) | 608.7 (425.6) |
| 1944.8 (660.2) | 1871.2 (302.3) |
| 1952.4 (212.6) | 1877.9 (162.4) |
| 1956.6 (444.0) | 1895.1 (532.6) |
| 1986.7 (218.4) | 1915.7 (177.9) |
| 2116.2 (253.2) | 2024.9 (36.6) |
| 2120.8 (623.7) | 2029.4 (542.3) |
| 2130.7 (1246.2) | 2035.3 (1338.1) |
| 2150.9 (1193.3) | 2060.7 (980.7) |
| 2183.4 (48.5) | 2090.1 (31.3) |

**Table S17.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_6]$

| **26S-1**($C_{2h}$) | | **26S-2**($C_s$/$C_1$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 21.9 (0.2) | 26.0 (0.1) | 21.5 (0.0) | 33.6 (0.8) |
| 32.5 (0.1) | 30.9 (0.0) | 32.8 (1.9) | 45.0 (1.4) |
| 46.8 (0.5) | 49.3 (0.4) | 52.8 (0.0) | 50.8 (0.1) |
| 48.4 (0.0) | 53.8 (0.0) | 53.9 (0.5) | 59.6 (0.7) |
| 72.0 (0.0) | 62.9 (0.0) | 77.8 (0.3) | 75.1 (0.4) |
| 73.8 (0.0) | 73.0 (0.0) | 79.5 (0.1) | 77.6 (0.8) |
| 74.7 (0.7) | 75.7 (0.7) | 80.7 (0.3) | 81.8 (0.1) |
| 79.7 (0.0) | 80.1 (0.0) | 86.6 (3.4) | 82.6 (2.0) |
| 91.4 (0.0) | 86.7 (0.1) | 87.5 (0.2) | 88.3 (0.0) |
| 94.9 (0.0) | 95.6 (0.1) | 95.4 (1.0) | 89.9 (0.6) |
| 98.9 (0.1) | 100.0 (0.0) | 104.5 (0.5) | 98.6 (0.4) |
| 101.3(0.0) | 103.0 (0.0) | 107.9 (0.6) | 103.3 (0.1) |
| 125.2 (0.8) | 131.0 (0.4) | 121.5 (2.1) | 162.5 (3.8) |
| 143.7 (0.0) | 175.1 (0.0) | 141.4 (2.7) | 180.1 (0.9) |
| 210.5 (0.0) | 275.1 (4.2) | 156.4 (7.3) | 196.1 (0.6) |
| 244.8 (16.7) | 284.1 (0.0) | 174.3 (1.1) | 221.5 (1.1) |
| 328.9 (0.0) | 333.0 (0.1) | 231.8 (2.7) | 236.7 (1.7) |
| 341.8 (0.6) | 340.6 (0.0) | 327.5 (22.7) | 279.7 (2.5) |
| 349.6 (0.0) | 345.0 (0.2) | 345.1 (0.0) | 325.3 (1.6) |
| 353.6 (1.6) | 346.1 (0.0) | 358.2 (12.2) | 353.5 (1.1) |
| 358.9 (0.0) | 357.1 (17.3) | 361.1 (2.1) | 359.2 (2.0) |
| 365.6 (19.5) | 359.0 (0.0) | 362.1 (9.6) | 369.5 (2.1) |
| 397.7 (54.2) | 389.5 (0.0) | 371.2 (3.0) | 379.5 (2.1) |
| 399.7 (0.0) | 399.9 (0.9) | 385.6 (1.0) | 382.1 (3.6) |
| 412.5 (2.5) | 414.9 (0.0) | 390.2 (10.8) | 396.9 (10.8) |
| 416.1 (0.0) | 428.5 (1.6) | 397.6 (0.4) | 408.9 (3.4) |
| 417.2 (0.0) | 433.4 (0.0) | 415.5 (16.6) | 417.2 (2.3) |
| 429.6 (17.0) | 446.9 (58.1) | 423.4 (0.5) | 423.5 (1.3) |
| 431.7 (14.0) | 456.0 (0.0) | 426.4 (0.2) | 442.7 (5.2) |
| 433.8 (0.0) | 456.8 (85.8) | 451.0 (21.0) | 450.1 (29.7) |
| 476.2 (30.2) | 496.0 (51.7) | 464.1 (39.9) | 466.5 (0.4) |
| 485.9 (0.0) | 503.3 (0.0) | 494.2 (2.7) | 471.5 (4.5) |
| 523.8 (0.0) | 505.4 (0.0) | 494.4 (39.0) | 480.0 (10.4) |
| 533.6 (9.9) | 515.1 (1.9) | 509.3 (0.6) | 507.5 (43.0) |

| | | | |
|---|---|---|---|
| 544.8 (0.0) | 537.7 (92.0) | 515.0 (26.2) | 512.7 (30.4) |
| 547.2 (99.4) | 541.6 (0.0) | 544.2 (68.3) | 527.9 (95.3) |
| 566.9 (152.5) | 563.1 (221.0) | 544.9 (209.5) | 535.7 (116.9) |
| 569.7 (0.0) | 568.7 (0.0) | 568.4 (80.1) | 550.9 (12.4) |
| 583.4 (0.0) | 579.5 (0.0) | 574.6 (12.5) | 558.3 (57.8) |
| 586.7 (127.2) | 583.0 (102.5) | 590.1 (77.4) | 593.8 (158.0) |
| 1776.5 (0.0) | 1663.6 (0.0) | 1863.7(276.5) | 1766.9 (190.4) |
| 1791.3 (396.3) | 1670.6 (254.5) | 1867.9 (95.5) | 1777.3 (103.7) |
| 2072.1 (0.0) | 1994.2 (0.0) | 2074.0 (328.8) | 1896.0 (458.6) |
| 2081.7 (2412.0) | 2001.6 (1843.7) | 2121.2 (616.3) | 2032.8 (599.3) |
| 2106.0 (694.1) | 2018.9 (717.7) | 2122.0 (751.9) | 2045.4 (596.0) |
| 2111.9 (0.0) | 2022.8 (0.0) | 2126.0 (1593.6) | 2046.9 (610.5) |
| 2156.0 (1498.5) | 2062.6 (1418.3) | 2154.7 (1049.6) | 2057.4 (1342.9) |
| 2171.1 (0.0) | 2078.7 (0.0) | 2186.5 (19.8) | 2092.7 (97.2) |

**Table S18.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_6]$

| **26S-3**($C_{2h}$) | | **26S-4**($C_s$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 16.2 (1.1) | -26.7 (1.5) | 31.1 (0.0) | 29.1 (0.0) |
| 20.8 (1.2) | 20.0 (1.5) | 38.0 (4.7) | 37.9 (2.9) |
| 44.6 (0.0) | 52.6 (0.0) | 46.9 (0.1) | 45.4 (0.0) |
| 51.1 (0.2) | 54.0 (0.4) | 50.3 (0.1) | 51.0 (0.1) |
| 57.7 (0.0) | 54.4 (0.0) | 69.6 (5.8) | 69.9 (0.2) |
| 63.0 (0.0) | 71.1 (2.8) | 73.6 (0.1) | 70.5 (5.9) |
| 75.2 (1.8) | 78.1 (0.0) | 80.1 (0.5) | 79.1 (0.2) |
| 87.1 (0.0) | 80.8 (3.4) | 89.5 (0.2) | 87.1 (1.0) |
| 87.6 (5.1) | 84.7 (0.0) | 93.4 (0.0) | 88.4 (0.9) |
| 89.3 (0.0) | 92.4 (0.0) | 97.1 (3.8) | 89.9 (2.8) |
| 97.0 (0.0) | 93.7 (0.2) | 97.9 (2.8) | 95.1 (0.5) |
| 97.1 (0.3) | 94.4 (1.2) | 101.3 (0.8) | 98.0 (0.8) |
| 98.8 (1.7) | 96.7 (0.0) | 107.0 (0.6) | 103.4 (0.1) |
| 109.2 (0.0) | 111.9 (0.0) | 118.5 (3.4) | 116.8 (4.9) |
| 116.2 (15.0) | 114.9 (9.9) | 169.8 (0.4) | 183.8 (0.2) |
| 160.0 (0.0) | 200.4 (0.0) | 225.9 (5.8) | 241.7 (4.8) |
| 252.9 (12.1) | 246.3 (0.0) | 295.8 (9.8) | 311.7 (3.8) |
| 289.6 (0.0) | 249.4 (7.2) | 342.2 (0.7) | 336.6 (5.1) |
| 342.6 (0.4) | 330.9 (0.0) | 348.6 (0.0) | 340.3 (0.0) |
| 346.9 (0.0) | 342.8 (0.0) | 360.3 (0.6) | 354.7 (0.3) |
| 358.7 (0.0) | 352.7 (0.0) | 368.1 (0.9) | 357.2 (0.0) |
| 360.1 (23.4) | 358.1 (13.2) | 377.8 (6.3) | 377.2 (0.4) |
| 376.0 (0.0) | 369.1 (0.0) | 382.6 (3.9) | 386.8 (7.5) |
| 385.1 (0.0) | 381.3 (0.0) | 404.3 (2.7) | 401.8 (0.9) |
| 406.8 (26.6) | 397.1 (0.0) | 408.9 (11.3) | 410.7 (6.7) |
| 407.2 (6.0) | 400.7 (0.2) | 411.7 (0.6) | 414.5 (7.7) |
| 412.0 (0.0) | 402.0 (32.6) | 412.3 (2.0) | 415.3 (1.0) |
| 415.0 (0.0) | 413.7 (0.0) | 424.2 (1.9) | 423.3 (0.0) |
| 429.4 (16.8) | 457.6 (10.2) | 427.6 (2.5) | 457.2 (0.7) |
| 433.5 (0.0) | 462.1 (0.0) | 452.4 (15.5) | 470.6 (60.7) |
| 444.7 (22.1) | 464.0 (27.2) | 460.5 (32.2) | 473.8 (15.2) |
| 457.2 (0.0) | 475.1 (0.0) | 490.5 (71.0) | 480.6 (1.2) |
| 516.3 (0.0) | 506.1 (0.0) | 501.9 (0.3) | 481.2 (23.7) |
| 519.9 (0.0) | 519.9 (0.0) | 517.1 (14.8) | 508.5 (6.2) |

| | | | |
|---|---|---|---|
| 523.0 (12.1) | 519.9 (4.6) | 536.3 (37.0) | 539.1 (28.7) |
| 530.9 (16.7) | 529.7 (23.9) | 542.2 (42.6) | 541.0 (52.5) |
| 578.5 (0.0) | 563.1 (0.0) | 567.9 (82.9) | 560.9 (100.2) |
| 580.1 (0.0) | 575.0 (100.1) | 578.8 (50.9) | 571.5 (52.5) |
| 586.6 (121.6) | 575.1 (0.0) | 584.5 (70.6) | 581.7 (71.5) |
| 587.5 (122.2) | 587.6 (94.5) | 585.3 (17.8) | 584.0 (13.4) |
| 1864.5(0.0) | 1766.3 (0.0) | 1846.5 (116.5) | 1766.7 (106.6) |
| 1864.7 (250.3) | 1767.5 (194.5) | 1930.7 (325.0) | 1853.5 (232.9) |
| 2085.7 (0.0) | 1996.9 (0.0) | 1983.6 (413.4) | 1897.7 (332.2) |
| 2108.6 (2281.6) | 2020.8 (1827.3) | 2094.8 (565.4) | 2009.9 (117.3) |
| 2120.9 (444.8) | 2029.4 (488.8) | 2116.8 (362.7) | 2024.3 (1680.7) |
| 2130.9 (0.0) | 2037.0 (0.0) | 2125.5 (1545.3) | 2028.6 (352.5) |
| 2151.0 (1825.9) | 2056.1 (1700.8) | 2148.7 (970.5) | 2057.5 (811.0) |
| 2182.4 (0.0) | 2089.1 (0.0) | 2179.7 (73.8) | 2086.0 (116.0) |

**Table S19.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_6]$

| **26S-5**($C_1$) | | **26S-6**($C_1$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 33.3 (0.4) | 23.1 (0.8) | 22.9 (0.7) | 22.2 (0.8) |
| 41.1 (0.8) | 42.7 (0.5) | 28.9 (2.5) | 34.9 (0.6) |
| 52.3 (0.0) | 48.3 (0.2) | 39.5 (0.7) | 42.2 (0.1) |
| 62.3 (1.2) | 59.0 (0.4) | 51.9 (0.9) | 49.4 (0.3) |
| 70.4 (0.7) | 68.5 (1.2) | 68.5 (3.8) | 73.0 (0.1) |
| 72.6 (1.4) | 69.9 (0.2) | 73.1 (0.7) | 74.1 (0.3) |
| 77.6 (2.4) | 72.3 (0.9) | 78.5 (0.4) | 75.7 (1.3) |
| 89.3 (0.3) | 84.1 (0.6) | 82.9 (2.0) | 83.5 (0.6) |
| 89.4 (1.3) | 87.2 (0.1) | 88.3 (2.1) | 88.1 (1.0) |
| 93.9 (1.0) | 93.6 (0.3) | 97.1 (0.5) | 92.4 (1.1) |
| 101.7 (0.8) | 94.7 (1.1) | 99.2 (0.2) | 93.7 (0.2) |
| 108.1 (1.1) | 99.5 (0.8) | 101.2 (1.2) | 98.4 (0.5) |
| 125.3 (2.8) | 113.3 (1.1) | 112.0 (0.4) | 100.7(0.5) |
| 170.3 (6.9) | 168.0 (2.8) | 115.6 (4.7) | 120.6 (8.3) |
| 200.6 (9.2) | 208.7 (3.2) | 120.0 (0.9) | 146.4 (1.2) |
| 225.0 (9.9) | 219.2 (10.4) | 165.2 (12.7) | 179.1 (10.0) |
| 324.3 (15.3) | 314.1 (2.2) | 320.6 (11.8) | 297.2 (16.0) |
| 332.8 (18.4) | 338.7 (13.5) | 341.1 (5.2) | 326.5 (7.5) |
| 353.9 (0.9) | 339.6 (3.6) | 344.2 (0.1) | 339.6 (2.1) |
| 362.4 (5.0) | 357.2 (2.3) | 353.1 (3.7) | 344.9 (0.1) |
| 364.8 (9.9) | 367.2 (1.5) | 360.3 (3.3) | 355.6 (3.9) |
| 371.9 (7.8) | 376.1 (6.5) | 370.3 (8.0) | 362.9 (10.7) |
| 385.4 (8.1) | 387.7 (4.7) | 380.1 (0.6) | 378.9 (0.3) |
| 390.0 (2.2) | 397.2 (5.1) | 392.4 (18.9) | 391.3 (8.3) |
| 404.8 (6.3) | 400.4 (0.4) | 395.2 (3.9) | 403.6 (1.9) |
| 415.6 (4.6) | 418.6 (3.9) | 410.0 (11.0) | 422.5 (2.2) |
| 424.9 (1.2) | 431.3 (1.1) | 435.6 (4.6) | 438.0 (2.0) |
| 444.1 (5.6) | 452.7 (15.6) | 441.7 (17.8) | 454.5 (56.8) |
| 451.7 (28.3) | 464.3 (19.2) | 444.4 (5.8) | 464.2 (4.5) |
| 457.9 (0.4) | 468.0 (5.8) | 463.5 (9.0) | 472.9 (15.2) |
| 463.7 (9.2) | 469.9 (2.7) | 472.0 (20.7) | 487.9 (1.3) |
| 477.4 (35.1) | 479.8 (25.7) | 477.5 (10.9) | 488.9 (8.5) |
| 496.9 (3.0) | 495.5 (2.2) | 487.2 (3.0) | 495.6 (13.9) |
| 504.8 (51.0) | 501.5 (46.1) | 503.8 (9.0) | 506.7 (8.6) |

| | | | |
|---|---|---|---|
| 520.8 (5.0) | 518.1 (9.9) | 516.3 (31.6) | 508.4 (5.6) |
| 538.4 (203.6) | 537.4 (179.0) | 548.9 (76.1) | 544.1 (62.6) |
| 547.8 (3.3) | 544.6 (18.1) | 564.7 (159.5) | 556.0 (99.9) |
| 555.2 (49.2) | 557.4 (47.9) | 568.5 (85.7) | 563.0 (71.2) |
| 571.8 (74.0) | 573.1 (71.5) | 572.3 (39.9) | 573.0 (31.1) |
| 584.9 (78.3) | 590.3 (114.3) | 581.1 (14.4) | 585.6 (49.1) |
| 1790.7 (135.3) | 1724.0 (119.7) | 1834.4 (184.6) | 1737.0 (144.9) |
| 1929.4 (186.6) | 1851.3 (147.7) | 1920.4 (229.7) | 1836.7 (169.9) |
| 1960.0 (501.7) | 1879.9 (414.6) | 2084.3 (471.4) | 1988.2 (549.2) |
| 2099.9 (406.5) | 2016.8 (122.1) | 2108.1 (173.5) | 2010.5 (183.9) |
| 2122.5 (817.8) | 2031.8 (993.0) | 2121.8 (1180.3) | 2031.8 (819.3) |
| 2130.2 (990.9) | 2037.5 (757.0) | 2126.1 (423.1) | 2036.4 (386.4) |
| 2149.2 (1308.4) | 2057.0 (1140.4) | 2143.9 (1795.2) | 2057.2 (1316.3) |
| 2175.9 (62.3) | 2083.9 (90.9) | 2177.0 (113.0) | 2083.6 (138.9) |

**Table S20.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_6]$

| **26S-7**($C_1$) | | **26S-8**($C_s$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 23.8 (0.5) | 24.2 (0.3) | 24.2 (0.6) | 19.2 (0.7) |
| 38.5 (0.8) | 44.3 (0.8) | 37.9 (0.1) | 32.3 (0.1) |
| 45.9 (1.0) | 48.6 (0.5) | 39.7 (1.1) | 45.3 (1.8) |
| 51.2 (0.6) | 54.5 (0.8) | 47.4 (0.0) | 47.1 (0.3) |
| 62.0 (0.6) | 70.0 (1.7) | 70.2 (3.7) | 61.6 (2.8) |
| 67.3 (1.3) | 72.8 (1.5) | 74.5 (0.9) | 62.5 (1.1) |
| 71.8 (0.5) | 78.6 (1.6) | 86.7 (3.1) | 84.1 (0.9) |
| 83.9 (1.9) | 83.1 (1.3) | 89.4 (1.1) | 87.5 (1.3) |
| 91.0 (0.4) | 86.0 (1.1) | 93.4 (0.1) | 87.9 (1.2) |
| 92.0 (0.4) | 92.2 (0.4) | 95.9 (0.3) | 93.2 (0.3) |
| 93.9 (1.7) | 96.2 (0.7) | 99.6 (0.5) | 95.6 (0.0) |
| 101.5 (0.6) | 98.3 (0.2) | 102.2 (0.4) | 95.9 (0.6) |
| 103.9 (0.8) | 109.5 (0.3) | 104.3 (0.1) | 100.2 (0.2) |
| 117.4 (0.4) | 119.1 (4.3) | 111.3 (4.7) | 130.5 (3.9) |
| 134.8 (0.5) | 184.8 (2.0) | 131.3 (5.0) | 139.2 (6.3) |
| 220.1 (8.1) | 233.2 (8.7) | 176.8 (4.6) | 194.2 (1.5) |
| 328.8 (1.6) | 307.8 (4.4) | 281.4 (11.6) | 249.0 (5.5) |
| 344.9 (0.3) | 326.4 (3.5) | 344.2 (19.0) | 338.2 (0.0) |
| 353.0 (2.6) | 340.2 (2.0) | 347.9 (0.2) | 340.5 (37.1) |
| 363.1 (1.1) | 347.8 (5.8) | 353.2 (1.4) | 353.0 (1.3) |
| 368.5 (8.0) | 356.9 (0.4) | 362.1 (0.3) | 354.4 (0.0) |
| 369.6 (18.1) | 374.4 (11.4) | 377.9 (0.8) | 368.5 (1.6) |
| 378.6 (3.9) | 383.8 (3.7) | 379.7 (0.0) | 370.7 (22.0) |
| 391.9 (5.9) | 391.5 (2.7) | 389.2 (0.6) | 383.2 (0.6) |
| 406.2 (12.7) | 405.8 (3.9) | 390.5 (7.7) | 389.4 (1.9) |
| 414.1 (1.7) | 413.4 (1.6) | 401.3 (19.7) | 390.2 (14.8) |
| 420.7 (5.5) | 418.9 (5.8) | 418.8 (21.8) | 426.3 (1.0) |
| 429.9 (8.5) | 431.1 (1.8) | 438.2 (29.8) | 436.5 (0.7) |
| 440.5 (19.0) | 434.9 (3.9) | 446.3 (0.9) | 450.3 (0.2) |
| 448.1 (2.2) | 468.2 (50.2) | 460.6 (9.1) | 451.5 (1.7) |
| 472.2 (9.7) | 474.2 (1.4) | 460.6 (0.6) | 474.9 (0.1) |
| 481.8 (11.4) | 484.6 (13.7) | 489.6 (18.5) | 481.9 (4.6) |
| 523.5 (32.2) | 488.8 (17.1) | 504.0 (5.1) | 497.3 (2.4) |
| 531.5 (9.8) | 505.3 (4.7) | 509.2 (13.4) | 508.5 (16.3) |

| | | | |
|---|---|---|---|
| 534.6 (37.3) | 533.3 (59.0) | 514.3 (4.6) | 509.0 (5.1) |
| 537.0 (26.9) | 537.5 (24.5) | 542.5 (77.7) | 542.1 (86.4) |
| 551.3 (33.1) | 560.7 (86.5) | 551.2 (93.5) | 543.4 (65.8) |
| 568.7 (59.7) | 572.8 (78.0) | 570.8 (112.3) | 560.1 (96.5) |
| 585.0 (78.3) | 578.3 (63.8) | 581.5 (28.5) | 570.8 (31.5) |
| 592.4 (73.4) | 589.1 (28.6) | 595.1 (64.4) | 594.2 (63.0) |
| 1777.6 (77.0) | 1755.4 (105.8) | 1869.4 (182.1) | 1787.7 (111.1) |
| 1933.8 (174.3) | 1854.1 (148.4) | 1939.5 (255.3) | 1865.7 (195.0) |
| 2064.4 (338.3) | 1897.5 (318.5) | 2062.3 (653.0) | 1955.8 (496.2) |
| 2085.6 (960.6) | 2013.4 (480.7) | 2097.1 (398.0) | 2010.2 (132.4) |
| 2117.2 (686.8) | 2027.4 (894.4) | 2126.5 (1142.7) | 2036.0 (1564.9) |
| 2131.4 (1003.6) | 2034.7 (453.6) | 2130.9 (104.9) | 2036.4 (818.8) |
| 2148.2 (1176.3) | 2055.5 (1267.6) | 2136.2 (1581.9) | 2043.6 (370.5) |
| 2176.9 (174.3) | 2084.0 (160.9) | 2191.4 (126.7) | 2099.7 (117.4) |

**Table S21.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the singlet structures of $[Co_2(BO)_2(CO)_6]$

| **26S-9**($C_s$) | |
|---|---|
| B3LYP | BP86 |
| 16.1 (0.6) | -27.9 (0.2) |
| 30.2 (0.4) | 28.9 (0.0) |
| 41.4 (0.4) | 37.8 (0.8) |
| 51.2 (0.6) | 45.8 (0.5) |
| 60.2 (0.4) | 60.9 (2.0) |
| 73.3 (1.0) | 65.5 (0.1) |
| 75.6 (1.2) | 76.1 (1.4) |
| 82.4 (2.2) | 79.9 (0.6) |
| 85.3 (0.8) | 80.6 (1.6) |
| 94.2 (0.1) | 88.0 (0.3) |
| 98.5 (3.8) | 94.5 (2.2) |
| 100.5 (0.3) | 98.4 (0.1) |
| 108.8 (0.1) | 105.3 (2.9) |
| 113.8 (4.6) | 107.9 (2.9) |
| 146.3 (1.4) | 155.3 (0.8) |
| 175.1 (1.2) | 187.4 (0.2) |
| 325.8 (21.5) | 311.8 (0.1) |
| 333.4 (0.2) | 324.4 (3.1) |
| 344.6 (0.0) | 339.8 (0.7) |
| 354.5 (14.9) | 347.0 (1.2) |
| 355.8 (1.3) | 358.7 (29.3) |
| 380.0 (8.7) | 374.9 (1.9) |
| 385.8 (0.4) | 379.8 (2.3) |
| 396.1 (35.0) | 387.8 (0.2) |
| 397.2 (5.9) | 395.6 (1.2) |
| 408.2 (0.0) | 418.2 (33.2) |
| 413.8 (2.2) | 427.6 (1.9) |
| 448.3 (11.0) | 444.9 (11.6) |
| 459.7 (35.3) | 449.1 (42.0) |
| 465.0 (10.0) | 456.8 (2.6) |
| 471.6 (7.3) | 465.7 (39.7) |
| 474.9 (17.0) | 470.7 (0.8) |
| 479.1 (14.0) | 482.6 (12.0) |
| 492.0 (2.0) | 490.9 (6.5) |

| | |
|---|---|
| 529.2 (1.0) | 515.4 (0.0) |
| 535.5 (246.9) | 519.3 (177.4) |
| 559.5 (88.0) | 544.0 (81.2) |
| 561.4 (82.9) | 559.6 (63.8) |
| 580.7 (22.9) | 574.6 (19.1) |
| 591.8 (46.0) | 589.5 (62.1) |
| 1904.2 (171.4) | 1823.9(120.4) |
| 1930.5 (329.7) | 1847.9 (232.4) |
| 2073.6 (1138.2) | 1985.4 (896.2) |
| 2098.0 (73.9) | 2006.6 (1.4) |
| 2105.8 (349.6) | 2014.2 (610.5) |
| 2119.3 (960.2) | 2026.7 (724.3) |
| 2143.4 (1278.2) | 2049.2 (946.3) |
| 2190.0 (163.4) | 2096.8 (144.8) |

**Table S22.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the tirplet structures of $[Co_2(BO)_2(CO)_6]$

| **26T-1**($C_s$) | | **26T-2**($C_s$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 11.3 (0.0) | 9.7 (0.0) | 11.0 (0.0) | 8.9 (0.0) |
| 19.9 (0.1) | 19.4 (0.1) | 18.6 (0.1) | 18.0 (0.1) |
| 37.9 (1.3) | 42.1 (0.2) | 36.7 (0.2) | 38.7 (0.0) |
| 47.1 (0.1) | 42.5 (0.3) | 40.9 (0.7) | 44.6 (0.1) |
| 52.1 (1.5) | 48.4 (1.5) | 54.7 (0.6) | 53.5 (0.8) |
| 53.9 (0.2) | 56.0 (0.0) | 59.7 (0.0) | 54.8 (0.2) |
| 62.5 (0.2) | 63.1 (0.0) | 62.7 (0.9) | 63.0 (0.5) |
| 66.1 (0.3) | 69.5 (0.1) | 67.5 (0.4) | 68.5 (0.2) |
| 68.1 (1.0) | 71.7 (1.4) | 68.7 (0.6) | 71.6 (0.3) |
| 73.8 (2.7) | 73.9 (1.8) | 73.9 (2.4) | 74.7 (1.5) |
| 84.0 (0.2) | 78.0 (0.2) | 83.2 (0.2) | 78.9 (0.2) |
| 87.3 (0.3) | 84.7 (0.1) | 88.3 (0.0) | 85.5 (0.0) |
| 109.5 (11.3) | 99.4 (5.5) | 112.3 (3.6) | 108.5 (1.9) |
| 112.7 (3.5) | 109.4 (1.9) | 117.3 (15.9) | 110.1 (11.7) |
| 145.2 (3.1) | 142.8 (2.2) | 145.2 (3.4) | 140.6 (2.3) |
| 264.0 (0.0) | 278.7 (0.0) | 262.6 (0.1) | 277.0 (0.0) |
| 285.6 (0.9) | 297.4 (0.0) | 285.0 (1.0) | 296.0 (0.0) |
| 288.8 (13.0) | 304.7 (2.6) | 286.9 (14.3) | 305.0 (2.7) |
| 298.0 (34.8) | 319.3 (33.8) | 297.0 (29.6) | 319.3 (27.0) |
| 323.9 (6.4) | 334.3 (0.1) | 321.8 (5.9) | 334.9 (0.2) |
| 340.6 (16.1) | 350.9 (0.5) | 339.7 (16.7) | 349.4 (0.6) |
| 342.6 (6.5) | 372.8 (0.4) | 342.5 (5.1) | 372.7 (0.1) |
| 357.2 (1.3) | 381.9 (6.3) | 356.0 (7.1) | 379.3 (9.9) |
| 357.4 (11.1) | 395.3 (3.4) | 356.4 (1.3) | 390.5 (3.8) |
| 383.4 (1.7) | 400.6 (15.4) | 382.2 (2.2) | 393.7 (12.1) |
| 395.0 (2.4) | 410.4 (1.2) | 389.5 (6.5) | 412.4 (21.8) |
| 402.2 (1.4) | 413.8 (20.3) | 402.7 (2.4) | 414.1 (2.3) |
| 411.2 (2.4) | 442.2 (12.6) | 410.6 (2.5) | 436.4 (16.6) |
| 420.3 (5.8) | 446.5 (5.2) | 420.6 (5.2) | 444.8 (3.3) |
| 425.6 (4.0) | 452.9 (1.9) | 424.8 (7.2) | 452.0 (2.3) |
| 437.2 (7.7) | 459.3 (2.4) | 432.6 (5.9) | 460.3 (6.6) |
| 463.8 (18.6) | 468.2 (43.4) | 458.0 (11.2) | 468.1 (23.9) |
| 472.9 (7.4) | 475.1 (2.4) | 478.6 (0.0) | 475.0 (4.6) |
| 478.7 (0.1) | 480.2 (2.8) | 487.7 (11.7) | 485.3 (0.3) |

| | | | |
|---|---|---|---|
| 508.1 (4.3) | 499.3 (17.7) | 504.2 (14.0) | 499.9 (7.5) |
| 515.0 (44.9) | 512.5 (6.4) | 515.5 (25.7) | 515.3 (5.1) |
| 523.9 (14.4) | 514.5 (72.0) | 526.8 (13.6) | 517.9 (57.1) |
| 573.0 (86.2) | 570.6 (81.6) | 578.6 (64.4) | 567.0 (97.8) |
| 580.5 (86.5) | 572.1 (80.4) | 579.8 (87.8) | 573.8 (81.0) |
| 587.5 (73.2) | 582.7 (57.0) | 581.0 (103.3) | 582.0 (57.0) |
| 1685.5 (569.4) | 1597.1 (382.1) | 1693.9 (473.8) | 1606.9 (387.2) |
| 1800.2 (940.5) | 1738.0 (457.5) | 1791.7 (1024.6) | 1725.9 (570.2) |
| 2076.1 (1001.2) | 2001.4(779.4) | 2073.5(1040.7) | 1998.5 (819.4) |
| 2081.3 (782.9) | 2004.5 (641.8) | 2082.2 (780.1) | 2004.9 (651.5) |
| 2130.6 (578.3) | 2025.5 (836.2) | 2130.3 (582.8) | 2026.7 (780.4) |
| 2141.7 (701.2) | 2031.9(798.1) | 2141.6 (774.3) | 2031.6 (786.6) |
| 2142.0 (782.9) | 2043.4(1198.0) | 2141.7 (681.4) | 2044.6 (998.8) |
| 2192.8 (217.4) | 2074.7 (215.4) | 2192.7 (216.9) | 2075.5 (236.0) |

**Table S23.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the triplet structures of $[Co_2(BO)_2(CO)_6]$

| **26T-3**($C_s$) | | **26T-4**($C_s$) | |
|---|---|---|---|
| B3LYP | BP86 | B3LYP | BP86 |
| 15.3 (0.0) | 13.6 (0.0) | 12.5 (0.0) | 12.3 (0.0) |
| 24.9 (0.2) | 22.5 (0.1) | 23.8 (5.4) | 37.6 (0.4) |
| 34.0 (0.4) | 35.8 (0.5) | 38.3 (0.2) | 40.0 (0.2) |
| 55.1 (0.1) | 53.4 (0.0) | 42.2 (0.6) | 50.6 (1.7) |
| 57.4 (0.5) | 56.8 (0.2) | 46.4 (1.0) | 54.6 (0.1) |
| 59.0 (0.0) | 57.8 (0.0) | 64.9 (0.9) | 63.3 (1.3) |
| 63.4 (0.2) | 63.5 (0.3) | 67.7 (0.1) | 71.3 (0.5) |
| 68.1 (0.1) | 68.0 (0.2) | 69.0 (0.8) | 72.3 (0.7) |
| 77.2 (0.3) | 76.4 (0.2) | 71.3 (3.5) | 73.2 (0.0) |
| 82.5 (1.7) | 79.1 (0.7) | 75.8 (1.5) | 77.5 (0.3) |
| 84.8 (0.2) | 81.8 (0.2) | 78.3 (1.8) | 83.2 (0.4) |
| 88.5 (0.0) | 83.6 (0.0) | 93.2 (0.2) | 89.5 (1.6) |
| 116.1 (12.2) | 111.3 (1.0) | 94.5 (2.3) | 90.8 (1.0) |
| 118.6 (2.0) | 111.6 (8.2) | 99.5 (0.3) | 96.5 (0.8) |
| 163.4 (11.7) | 163.5 (9.9) | 101.9 (1.0) | 102.9 (3.5) |
| 257.9 (5.0) | 275.7 (0.3) | 157.9 (16.4) | 170.1 (10.2) |
| 267.3 (12.5) | 280.3 (1.0) | 270.8 (0.0) | 293.3 (0.0) |
| 274.6 (3.9) | 295.6 (0.6) | 298.3 (1.7) | 315.2 (3.0) |
| 287.3 (19.5) | 302.1 (35.2) | 304.6 (1.7) | 319.0 (0.3) |
| 291.9 (26.2) | 326.0 (5.8) | 325.7 (8.3) | 331.1 (0.1) |
| 308.6 (33.8) | 334.7 (0.4) | 328.0 (0.2) | 336.3 (0.7) |
| 329.4 (7.8) | 352.0 (0.3) | 334.0 (0.9) | 344.0 (0.2) |
| 343.1 (0.1) | 363.7 (50.2) | 347.9 (10.8) | 354.5 (5.7) |
| 358.8 (1.4) | 375.9 (1.0) | 349.7 (3.3) | 356.9 (0.5) |
| 379.5 (1.1) | 385.8 (1.1) | 351.8 (13.8) | 390.2 (1.7) |
| 388.7 (1.8) | 393.3 (9.2) | 364.3 (0.2) | 394.5 (4.3) |
| 391.4 (1.7) | 403.8 (4.0) | 383.7 (16.3) | 404.4 (18.0) |
| 406.0 (1.2) | 416.0 (0.6) | 400.2 (1.4) | 422.3 (15.8) |
| 413.3 (9.5) | 422.1 (1.7) | 403.0 (0.0) | 433.7 (15.6) |
| 417.1 (3.9) | 442.9 (4.3) | 418.9 (3.5) | 439.5 (5.7) |
| 420.2 (3.3) | 459.1 (5.2) | 421.6 (2.1) | 447.8 (0.7) |
| 453.1 (22.3) | 464.8 (20.8) | 434.4 (5.4) | 454.1 (48.4) |
| 470.6 (0.2) | 473.9 (7.4) | 449.2 (0.2) | 457.1 (7.5) |
| 480.0 (0.2) | 479.0 (3.0) | 457.3 (0.2) | 473.1 (11.5) |

| | | | |
|---|---|---|---|
| 500.4 (2.1) | 496.2 (5.6) | 489.9 (25.3) | 481.0 (3.5) |
| 513.2 (19.3) | 507.8 (16.6) | 515.4 (15.2) | 499.5 (6.8) |
| 527.6 (11.9) | 516.5 (4.8) | 515.6 (3.7) | 501.6 (1.3) |
| 572.8 (86.5) | 571.1 (86.9) | 565.6 (72.6) | 550.8 (123.4) |
| 581.4 (82.2) | 572.7 (72.7) | 567.4 (132.3) | 554.9 (62.7) |
| 581.6 (89.0) | 574.9 (76.4) | 572.9 (62.0) | 557.8 (57.1) |
| 1721.7 (242.2) | 1637.4 (236.6) | 1867.7 (179.5) | 1755.7 (90.0) |
| 1782.8 (1095.5) | 1710.7 (954.9) | 1879.7 (244.7) | 1766.0 (137.3) |
| 2072.2 (953.9) | 1996.7(699.7) | 2095.1 (410.9) | 2011.9 (21.1) |
| 2079.8 (790.5) | 2001.6 (674.0) | 2105.9 (427.2) | 2016.7 (12.5) |
| 2128.0 (796.4) | 2025.8 (702.4) | 2137.9 (914.4) | 2031.0 (1134.4) |
| 2133.7 (377.0) | 2034.3(1275.9) | 2140.6 (924.9) | 2033.6 (1018.0) |
| 2153.8 (1104.4) | 2045.8 (511.7) | 2159.5 (799.7) | 2051.1 (1424.6) |
| 2199.5 (44.4) | 2083.4 (69.1) | 2196.6 (233.3) | 2080.8 (90.2) |

**Table S24.** Theoretical harmonic vibrational frequencies (in $cm^{-1}$) for the triplet structures of $[Co_2(BO)_2(CO)_6]$

| **26T-5**($C_s$) | |
|---|---|
| B3LYP | BP86 |
| 19.1 (0.2) | 24.3 (0.7) |
| 26.4 (2.2) | 29.3 (1.7) |
| 41.3 (0.2) | 30.2 (0.0) |
| 47.4 (0.7) | 50.5 (0.8) |
| 55.4 (2.1) | 58.1 (0.1) |
| 67.0 (4.1) | 62.2 (2.5) |
| 68.4 (2.8) | 70.2 (0.4) |
| 68.9 (0.1) | 71.5 (1.0) |
| 73.2 (0.8) | 74.5 (0.4) |
| 79.5 (0.6) | 78.9 (0.4) |
| 79.7 (3.3) | 85.7 (0.2) |
| 94.0 (0.1) | 91.2 (0.0) |
| 96.7 (2.4) | 92.9 (0.9) |
| 100.8 (1.4) | 103.5 (1.1) |
| 115.9 (4.5) | 136.0 (6.7) |
| 162.4 (10.1) | 180.7 (6.3) |
| 267.2 (0.0) | 257.6 (0.4) |
| 299.2 (0.8) | 291.5 (0.0) |
| 305.6 (1.3) | 318.7 (0.2) |
| 316.5 (1.0) | 333.7 (4.9) |
| 336.0 (3.0) | 335.4 (0.5) |
| 338.0 (17.4) | 344.5 (3.1) |
| 341.6 (17.4) | 354.5 (0.7) |
| 347.7 (1.0) | 354.9 (0.0) |
| 350.2 (0.6) | 371.1 (1.4) |
| 366.1 (0.0) | 402.0 (6.3) |
| 369.7 (1.1) | 419.7 (11.0) |
| 393.8 (0.1) | 421.1 (18.0) |
| 419.0 (1.6) | 429.5 (10.1) |
| 420.8 (6.1) | 446.2 (35.7) |
| 423.0 (3.1) | 453.4 (5.0) |
| 435.1 (2.5) | 456.5 (2.8) |
| 447.9 (9.0) | 463.2 (19.5) |
| 485.7 (0.1) | 471.2 (0.0) |

| | |
|---|---|
| 506.3 (3.1) | 481.5 (11.5) |
| 516.9 (0.3) | 491.4 (5.9) |
| 531.8 (27.4) | 510.5 (7.6) |
| 560.1 (147.9) | 539.5 (65.1) |
| 568.4 (63.1) | 557.1 (60.6) |
| 591.2 (83.5) | 558.8 (93.7) |
| 1886.6 (200.9) | 1769.9 (67.4) |
| 1932.2 (168.7) | 1863.8 (183.4) |
| 2066.7 (1024.5) | 1993.4 (639.0) |
| 2096.9 (130.3) | 2010.3 (55.0) |
| 2144.8 (890.9) | 2031.7 (797.7) |
| 2149.2 (590.3) | 2036.7 (835.7) |
| 2155.2 (734.1) | 2050.9 (1019.8) |
| 2195.7 (266.1) | 2080.0 (120.7) |

**Table S25**. Theoretical Cartesian coordinates (in Å) for the structure **14S-1** using the BP86/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 1.783393 | -0.088422 |
| 2 | 6 | 0 | -1.544464 | -0.891697 | -0.088422 |
| 3 | 6 | 0 | 0.000000 | 0.000000 | 1.946798 |
| 4 | 27 | 0 | 0.000000 | 0.000000 | 0.141103 |
| 5 | 8 | 0 | 2.544765 | -1.469221 | -0.241169 |
| 6 | 8 | 0 | 0.000000 | 0.000000 | 3.109934 |
| 7 | 8 | 0 | 0.000000 | 2.938441 | -0.241169 |
| 8 | 8 | 0 | -2.544765 | -1.469221 | -0.241169 |
| 9 | 6 | 0 | 1.544464 | -0.891697 | -0.088422 |
| 10 | 5 | 0 | 0.000000 | 0.000000 | -1.780959 |
| 11 | 8 | 0 | 0.000000 | 0.000000 | -3.010701 |

**Table S26**. Theoretical Cartesian coordinates (in Å) for the structure **14S-2** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 1.505618 | 1.167729 |
| 2 | 6 | 0 | 0.000000 | -1.505618 | 1.167729 |
| 3 | 6 | 0 | 1.711121 | 0.000000 | -0.330759 |
| 4 | 27 | 0 | 0.000000 | 0.000000 | 0.149949 |
| 5 | 8 | 0 | 0.000000 | 0.000000 | -3.007586 |
| 6 | 8 | 0 | 2.839598 | 0.000000 | -0.627221 |
| 7 | 8 | 0 | 0.000000 | 2.479619 | 1.805455 |
| 8 | 8 | 0 | 0.000000 | -2.479619 | 1.805455 |
| 9 | 8 | 0 | -2.839598 | 0.000000 | -0.627221 |
| 10 | 6 | 0 | -1.711121 | 0.000000 | -0.330759 |
| 11 | 5 | 0 | 0.000000 | 0.000000 | -1.776667 |

**Table S27**. Theoretical Cartesian coordinates (in Å) for the structure **14S-3** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.000000 | 1.769325 | 0.434146 |
| 2 | 6 | 0 | 1.769325 | -0.000000 | 0.434146 |
| 3 | 27 | 0 | 0.000000 | 0.000000 | 0.200397 |
| 4 | 8 | 0 | 0.000000 | -2.930726 | 0.530791 |
| 5 | 8 | 0 | 2.930726 | -0.000000 | 0.530791 |
| 6 | 8 | 0 | 0.000000 | 0.000000 | -2.997609 |
| 7 | 8 | 0 | 0.000000 | 2.930726 | 0.530791 |
| 8 | 6 | 0 | -0.000000 | -1.769325 | 0.434146 |
| 9 | 8 | 0 | -2.930726 | 0.000000 | 0.530791 |
| 10 | 6 | 0 | -1.769325 | 0.000000 | 0.434146 |
| 11 | 5 | 0 | 0.000000 | 0.000000 | -1.766931 |

**Table S28**. Theoretical Cartesian coordinates (in Å) for the structure **13S-1** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.571070 | 1.159102 | 0.000000 |
| 2 | 6 | 0 | -0.042578 | -0.206270 | 1.707489 |
| 3 | 6 | 0 | -0.042578 | -0.206270 | -1.707489 |
| 4 | 27 | 0 | 0.009723 | 0.262128 | 0.000000 |
| 5 | 8 | 0 | 2.596542 | 1.711936 | 0.000000 |
| 6 | 8 | 0 | -0.042578 | -0.605227 | -2.804226 |
| 7 | 8 | 0 | -0.042578 | -0.605227 | 2.804226 |
| 8 | 5 | 0 | -1.609224 | -0.795719 | 0.000000 |
| 9 | 8 | 0 | -2.652873 | -1.448762 | 0.000000 |

**Table S29**. Theoretical Cartesian coordinates (in Å) for the structure **13S-2** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.555311 | -0.897959 | 0.392262 |
| 2 | 6 | 0 | 1.555311 | -0.897959 | 0.392262 |
| 3 | 27 | 0 | 0.000000 | 0.000000 | 0.524156 |
| 4 | 8 | 0 | 0.000000 | 2.954310 | 0.244083 |
| 5 | 8 | 0 | -2.558507 | -1.477155 | 0.244083 |
| 6 | 8 | 0 | 2.558507 | -1.477155 | 0.244083 |
| 7 | 6 | 0 | 0.000000 | 1.795918 | 0.392262 |
| 8 | 5 | 0 | 0.000000 | 0.000000 | -1.323448 |
| 9 | 8 | 0 | 0.000000 | 0.000000 | -2.556708 |

**Table S30**. Theoretical Cartesian coordinates (in Å) for the structure **13T-1** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.143407 | 0.815328 | 1.383700 |
| 2 | 6 | 0 | -1.623983 | -1.284448 | 0.000000 |
| 3 | 8 | 0 | -2.664790 | -1.804142 | 0.000000 |
| 4 | 8 | 0 | -0.143407 | 1.556887 | -2.281932 |
| 5 | 8 | 0 | 3.195700 | -0.211308 | 0.000000 |
| 6 | 8 | 0 | -0.143407 | 1.556887 | 2.281932 |
| 7 | 27 | 0 | -0.011161 | -0.353345 | 0.000000 |
| 8 | 5 | 0 | 1.962670 | -0.264708 | 0.000000 |
| 9 | 6 | 0 | -0.143407 | 0.815328 | -1.383700 |

**Table S31**. Theoretical Cartesian coordinates (in Å) for the structure **13T-2** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.658713 | -0.403253 | 1.793929 |
| 2 | 6 | 0 | 0.067819 | 1.605618 | 0.000000 |
| 3 | 6 | 0 | -0.658713 | -0.403253 | -1.793929 |
| 4 | 8 | 0 | -0.658713 | -0.574153 | 2.946570 |
| 5 | 8 | 0 | 0.478387 | 2.697106 | 0.000000 |
| 6 | 8 | 0 | 2.498752 | -1.255085 | 0.000000 |
| 7 | 8 | 0 | -0.658713 | -0.574153 | -2.946570 |
| 8 | 27 | 0 | -0.464621 | -0.116698 | 0.000000 |
| 9 | 5 | 0 | 1.352938 | -0.798709 | 0.000000 |

**Table S32**. Theoretical Cartesian coordinates (in Å) for the structure **12T-1** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.699836 | 1.076561 | 0.000000 |
| 2 | 8 | 0 | -2.778468 | 1.515175 | 0.000000 |
| 3 | 8 | 0 | 3.230118 | 0.186436 | 0.000000 |
| 4 | 8 | 0 | -0.254921 | -2.649507 | 0.000000 |
| 5 | 27 | 0 | 0.000000 | 0.326208 | 0.000000 |
| 6 | 5 | 0 | 1.997262 | 0.244553 | 0.000000 |
| 7 | 6 | 0 | -0.226854 | -1.484433 | 0.000000 |

**Table S33**. Theoretical Cartesian coordinates (in Å) for the structure **12T-2** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 1.818592 | 0.608665 |
| 2 | 6 | 0 | 0.000000 | -1.818592 | 0.608665 |
| 3 | 27 | 0 | 0.000000 | 0.000000 | 0.482231 |
| 4 | 8 | 0 | 0.000000 | -2.983491 | 0.547316 |
| 5 | 8 | 0 | 0.000000 | 2.983491 | 0.547316 |
| 6 | 5 | 0 | 0.000000 | 0.000000 | -1.477392 |
| 7 | 8 | 0 | 0.000000 | 0.000000 | -2.711791 |

**Table S34**. Theoretical Cartesian coordinates (in Å) for the structure **12T-3** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.654495 | 0.516942 | 1.417711 |
| 2 | 6 | 0 | 0.654495 | 0.516942 | -1.417711 |
| 3 | 8 | 0 | 0.654495 | 1.282291 | -2.299371 |
| 4 | 8 | 0 | -2.758823 | -0.898612 | 0.000000 |
| 5 | 8 | 0 | 0.654495 | 1.282291 | 2.299371 |
| 6 | 5 | 0 | -1.528949 | -0.782176 | 0.000000 |
| 7 | 27 | 0 | 0.421832 | -0.578526 | 0.000000 |

**Table S35**. Theoretical Cartesian coordinates (in Å) for the structure **12S-1** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.462242 | -0.001944 | 1.677455 |
| 2 | 6 | 0 | 0.462242 | -0.001944 | -1.677455 |
| 3 | 8 | 0 | 0.462242 | 0.518650 | -2.726686 |
| 4 | 8 | 0 | -2.374274 | 0.671660 | 0.000000 |
| 5 | 8 | 0 | 0.462242 | 0.518650 | 2.726686 |
| 6 | 5 | 0 | -1.230709 | 0.203651 | 0.000000 |
| 7 | 27 | 0 | 0.452036 | -0.543208 | 0.000000 |

**Table S36**. Theoretical Cartesian coordinates (in Å) for the structure **12S-2** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 1.746703 | 0.390116 |
| 2 | 6 | 0 | 0.000000 | -1.746703 | 0.390116 |
| 3 | 27 | 0 | 0.000000 | 0.000000 | 0.695247 |
| 4 | 8 | 0 | 0.000000 | -2.873947 | 0.081188 |
| 5 | 8 | 0 | 0.000000 | 2.873947 | 0.081188 |
| 6 | 5 | 0 | 0.000000 | 0.000000 | -1.143189 |
| 7 | 8 | 0 | 0.000000 | 0.000000 | -2.379515 |

**Table S37**. Theoretical Cartesian coordinates (in Å) for the structure **12S-3** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.787089 | 0.794863 | 0.000000 |
| 2 | 8 | 0 | -2.953937 | 0.835222 | 0.000000 |
| 3 | 8 | 0 | 3.089265 | -0.160505 | 0.000000 |
| 4 | 8 | 0 | 0.005719 | -2.307512 | 0.000000 |
| 5 | 27 | 0 | 0.000000 | 0.547950 | 0.000000 |
| 6 | 5 | 0 | 1.875265 | 0.057073 | 0.000000 |
| 7 | 6 | 0 | 0.036306 | -1.131137 | 0.000000 |

**Table S38**. Theoretical Cartesian coordinates (in Å) for the structure **11T-1** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 1.854351 |
| 2 | 27 | 0 | 0.000000 | 0.000000 | 0.018221 |
| 3 | 8 | 0 | 0.000000 | 0.000000 | 3.021063 |
| 4 | 5 | 0 | 0.000000 | 0.000000 | -1.993566 |
| 5 | 8 | 0 | 0.000000 | 0.000000 | -3.227345 |

**Table S39**. Theoretical Cartesian coordinates (in Å) for the structure **11S-1** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.096162 | -0.316983 | 0.000000 |
| 2 | 27 | 0 | 0.000000 | 0.932853 | 0.000000 |
| 3 | 8 | 0 | -1.877036 | -1.203296 | 0.000000 |
| 4 | 5 | 0 | 1.147504 | -0.486582 | 0.000000 |
| 5 | 8 | 0 | 1.981968 | -1.403233 | 0.000000 |

**Table S40**. Theoretical Cartesian coordinates (in Å) for the structure **28S-1** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.755871 | -0.618578 | 1.606504 |
| 2 | 6 | 0 | 3.595206 | 0.202049 | -0.745392 |
| 3 | 6 | 0 | 1.514522 | -1.305323 | -1.131902 |
| 4 | 6 | 0 | 1.640869 | 1.758122 | -0.033982 |
| 5 | 6 | 0 | -1.609333 | -1.911070 | -0.051416 |
| 6 | 6 | 0 | 0.142818 | -0.220271 | 0.957490 |
| 7 | 8 | 0 | 3.282701 | -0.998142 | 2.570618 |
| 8 | 8 | 0 | 4.624521 | 0.351838 | -1.266865 |
| 9 | 8 | 0 | -3.421334 | 0.042779 | 2.472893 |
| 10 | 8 | 0 | -4.407356 | -0.081953 | -1.504479 |
| 11 | 8 | 0 | 1.282343 | -2.152123 | -1.900868 |
| 12 | 8 | 0 | 1.518644 | 2.912833 | -0.105507 |
| 13 | 8 | 0 | -1.601220 | -3.067960 | 0.064051 |
| 14 | 8 | 0 | 0.027088 | -0.435190 | 2.125110 |
| 15 | 8 | 0 | -1.722312 | 2.866030 | 0.916759 |
| 16 | 6 | 0 | -0.900266 | 0.574088 | -1.675517 |
| 17 | 8 | 0 | -0.498724 | 1.065859 | -2.650236 |
| 18 | 27 | 0 | 1.984340 | -0.025534 | 0.057936 |
| 19 | 27 | 0 | -1.717170 | -0.103412 | -0.200756 |
| 20 | 5 | 0 | -2.695333 | 0.142774 | 1.483539 |
| 21 | 5 | 0 | -1.819607 | 1.671859 | 0.630076 |
| 22 | 6 | 0 | -3.358634 | -0.082914 | -1.006404 |

**Table S41.** Theoretical Cartesian coordinates (in Å) for the structure **28S-2** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.801824 | 2.805047 | 0.000000 |
| 2 | 6 | 0 | 3.614591 | 0.914249 | 0.000000 |
| 3 | 6 | 0 | 1.707342 | 0.136883 | 1.601049 |
| 4 | 6 | 0 | 1.707342 | 0.136883 | -1.601049 |
| 5 | 6 | 0 | -1.570455 | -0.367250 | 1.742289 |
| 6 | 6 | 0 | -0.262135 | 1.064546 | 0.000000 |
| 7 | 6 | 0 | -1.570455 | -0.367250 | -1.742289 |
| 8 | 8 | 0 | 1.840775 | 3.966835 | 0.000000 |
| 9 | 8 | 0 | 4.776837 | 0.870213 | 0.000000 |
| 10 | 8 | 0 | -4.487477 | 0.010626 | -0.000000 |
| 11 | 8 | 0 | -3.240743 | -3.432062 | -0.000000 |
| 12 | 8 | 0 | 1.707342 | -0.391280 | 2.640591 |
| 13 | 8 | 0 | 1.707342 | -0.391280 | -2.640591 |
| 14 | 8 | 0 | -1.706268 | -0.121209 | 2.871231 |
| 15 | 8 | 0 | -0.894635 | 2.074066 | 0.000000 |
| 16 | 8 | 0 | -1.706268 | -0.121209 | -2.871231 |
| 17 | 6 | 0 | -0.165410 | -2.105164 | -0.000000 |
| 18 | 8 | 0 | 0.586085 | -2.992399 | -0.000000 |
| 19 | 27 | 0 | 1.796677 | 0.979421 | 0.000000 |
| 20 | 27 | 0 | -1.432961 | -0.806180 | -0.000000 |
| 21 | 5 | 0 | -2.680699 | -2.336801 | -0.000000 |
| 22 | 5 | 0 | -3.331320 | -0.415916 | -0.000000 |

**Table S42**. Theoretical Cartesian coordinates (in Å) for the structure **28S-3** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.090320 | 2.533006 | 0.000000 |
| 2 | 6 | 0 | 3.644291 | 0.454416 | 0.000000 |
| 3 | 6 | 0 | 1.704229 | -0.137137 | 1.598082 |
| 4 | 6 | 0 | 1.704229 | -0.137137 | -1.598082 |
| 5 | 6 | 0 | -1.615129 | -0.322752 | 1.753324 |
| 6 | 8 | 0 | 2.279234 | 3.680086 | 0.000000 |
| 7 | 8 | 0 | 4.793910 | 0.282899 | 0.000000 |
| 8 | 8 | 0 | -4.228871 | 1.272726 | 0.000000 |
| 9 | 8 | 0 | -3.490893 | -3.028880 | 0.000000 |
| 10 | 8 | 0 | 1.684927 | -0.656245 | 2.638465 |
| 11 | 8 | 0 | 1.684927 | -0.656245 | -2.638465 |
| 12 | 8 | 0 | -1.615129 | -0.124043 | 2.900808 |
| 13 | 8 | 0 | -0.681408 | 2.125293 | 0.000000 |
| 14 | 8 | 0 | -1.615129 | -0.124043 | -2.900808 |
| 15 | 8 | 0 | 0.622738 | -2.842699 | 0.000000 |
| 16 | 27 | 0 | 1.852353 | 0.723892 | 0.000000 |
| 17 | 27 | 0 | -1.697707 | -0.666071 | 0.000000 |
| 18 | 5 | 0 | -3.233802 | 0.552244 | 0.000000 |
| 19 | 6 | 0 | -2.796089 | -2.097518 | 0.000000 |
| 20 | 6 | 0 | -1.615129 | -0.322752 | -1.753324 |
| 21 | 5 | 0 | -0.275822 | -2.000202 | 0.000000 |
| 22 | 6 | 0 | -0.133688 | 1.071178 | 0.000000 |

**Table S43**. Theoretical Cartesian coordinates (in Å) for the structure **28S-4** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.090320 | 2.533006 | 0.000000 |
| 2 | 6 | 0 | 3.644291 | 0.454416 | 0.000000 |
| 3 | 6 | 0 | 1.704229 | -0.137137 | 1.598082 |
| 4 | 6 | 0 | 1.704229 | -0.137137 | -1.598082 |
| 5 | 6 | 0 | -1.615129 | -0.322752 | 1.753324 |
| 6 | 8 | 0 | 2.279234 | 3.680086 | 0.000000 |
| 7 | 8 | 0 | 4.793910 | 0.282899 | 0.000000 |
| 8 | 8 | 0 | -4.228871 | 1.272726 | 0.000000 |
| 9 | 8 | 0 | -3.490893 | -3.028880 | 0.000000 |
| 10 | 8 | 0 | 1.684927 | -0.656245 | 2.638465 |
| 11 | 8 | 0 | 1.684927 | -0.656245 | -2.638465 |
| 12 | 8 | 0 | -1.615129 | -0.124043 | 2.900808 |
| 13 | 8 | 0 | -0.681408 | 2.125293 | 0.000000 |
| 14 | 8 | 0 | -1.615129 | -0.124043 | -2.900808 |
| 15 | 8 | 0 | 0.622738 | -2.842699 | 0.000000 |
| 16 | 27 | 0 | 1.852353 | 0.723892 | 0.000000 |
| 17 | 27 | 0 | -1.697707 | -0.666071 | 0.000000 |
| 18 | 5 | 0 | -3.233802 | 0.552244 | 0.000000 |
| 19 | 6 | 0 | -2.796089 | -2.097518 | 0.000000 |
| 20 | 6 | 0 | -1.615129 | -0.322752 | -1.753324 |
| 21 | 5 | 0 | -0.275822 | -2.000202 | 0.000000 |
| 22 | 6 | 0 | -0.133688 | 1.071178 | 0.000000 |

**Table S44**. Theoretical Cartesian coordinates (in Å) for the structure **28S-5** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.116132 | -1.446990 | 0.000000 |
| 2 | 8 | 0 | -0.000000 | -3.513195 | 2.277969 |
| 3 | 8 | 0 | -0.000000 | -3.513195 | -2.277969 |
| 4 | 8 | 0 | 0.000000 | 3.513195 | 2.277969 |
| 5 | 8 | 0 | 0.000000 | 3.513195 | -2.277969 |
| 6 | 8 | 0 | -3.267035 | -1.581938 | 0.000000 |
| 7 | 8 | 0 | 2.908600 | -1.571551 | 0.000000 |
| 8 | 8 | 0 | -2.908600 | 1.571551 | 0.000000 |
| 9 | 8 | 0 | 0.000000 | 0.000000 | 2.442324 |
| 10 | 8 | 0 | 3.267035 | 1.581938 | 0.000000 |
| 11 | 8 | 0 | 0.000000 | 0.000000 | -2.442324 |
| 12 | 27 | 0 | -0.262687 | -1.578969 | 0.000000 |
| 13 | 27 | 0 | 0.262687 | 1.578969 | 0.000000 |
| 14 | 6 | 0 | 0.159572 | 2.803559 | -1.374317 |
| 15 | 6 | 0 | 0.000000 | 0.000000 | -1.243747 |
| 16 | 6 | 0 | -0.159572 | -2.803559 | 1.374317 |
| 17 | 5 | 0 | -1.678341 | 1.574473 | 0.000000 |
| 18 | 6 | 0 | -0.159572 | -2.803559 | -1.374317 |
| 19 | 6 | 0 | 0.159572 | 2.803559 | 1.374317 |
| 20 | 6 | 0 | 2.116132 | 1.446990 | 0.000000 |
| 21 | 5 | 0 | 1.678341 | -1.574473 | 0.000000 |
| 22 | 6 | 0 | 0.000000 | 0.000000 | 1.243747 |

**Table S45**. Theoretical Cartesian coordinates (in Å) for the structure **28S-6** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 2.289930 | 3.492549 | -0.291896 |
| 2 | 8 | 0 | -2.289930 | 3.492549 | -0.291896 |
| 3 | 8 | 0 | 2.289930 | -3.492549 | -0.291896 |
| 4 | 8 | 0 | -2.289930 | -3.492549 | -0.291896 |
| 5 | 8 | 0 | -0.000000 | 1.723739 | -3.051291 |
| 6 | 8 | 0 | 0.000000 | 1.679947 | 3.116507 |
| 7 | 8 | 0 | -0.000000 | -1.723739 | -3.051291 |
| 8 | 8 | 0 | 2.436614 | -0.000000 | -0.083779 |
| 9 | 8 | 0 | -0.000000 | -1.679947 | 3.116507 |
| 10 | 8 | 0 | -2.436614 | 0.000000 | -0.083779 |
| 11 | 27 | 0 | 0.000000 | 1.596944 | 0.124519 |
| 12 | 27 | 0 | -0.000000 | -1.596944 | 0.124519 |
| 13 | 6 | 0 | -1.380220 | -2.805282 | -0.080950 |
| 14 | 6 | 0 | -1.239435 | 0.000000 | -0.026358 |
| 15 | 6 | 0 | 1.380220 | 2.805282 | -0.080950 |
| 16 | 5 | 0 | -0.000000 | -1.566919 | -1.833414 |
| 17 | 6 | 0 | -1.380220 | 2.805282 | -0.080950 |
| 18 | 6 | 0 | 1.380220 | -2.805282 | -0.080950 |
| 19 | 6 | 0 | 0.000000 | -1.573123 | 1.958908 |
| 20 | 6 | 0 | 1.239435 | -0.000000 | -0.026358 |
| 21 | 6 | 0 | 0.000000 | 1.573123 | 1.958908 |
| 22 | 5 | 0 | 0.000000 | 1.566919 | -1.833414 |

**Table S46**. Theoretical Cartesian coordinates (in Å) for the structure **28S-7** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 2.849545 | 1.428544 |
| 2 | 6 | 0 | -1.786874 | 1.650594 | -0.161754 |
| 3 | 6 | 0 | -1.786874 | -1.650594 | -0.161754 |
| 4 | 8 | 0 | 0.000000 | 3.955285 | -2.101091 |
| 5 | 8 | 0 | 0.000000 | 3.608654 | 2.305520 |
| 6 | 8 | 0 | -0.000000 | -3.955285 | -2.101091 |
| 7 | 8 | 0 | -0.000000 | -3.608654 | 2.305520 |
| 8 | 8 | 0 | -2.927504 | 1.785875 | -0.349342 |
| 9 | 8 | 0 | 2.927504 | 1.785875 | -0.349342 |
| 10 | 8 | 0 | -2.927504 | -1.785875 | -0.349342 |
| 11 | 8 | 0 | 0.000000 | 0.000000 | -2.389933 |
| 12 | 8 | 0 | 2.927504 | -1.785875 | -0.349342 |
| 13 | 8 | 0 | 0.000000 | 0.000000 | 2.578550 |
| 14 | 27 | 0 | 0.000000 | 1.603149 | 0.088495 |
| 15 | 27 | 0 | -0.000000 | -1.603149 | 0.088495 |
| 16 | 5 | 0 | 0.000000 | -3.048856 | -1.272342 |
| 17 | 6 | 0 | -0.000000 | -2.849545 | 1.428544 |
| 18 | 6 | 0 | 1.786874 | -1.650594 | -0.161754 |
| 19 | 6 | 0 | 0.000000 | 0.000000 | -1.202686 |
| 20 | 6 | 0 | 0.000000 | 0.000000 | 1.383257 |
| 21 | 5 | 0 | 0.000000 | 3.048856 | -1.272342 |
| 22 | 6 | 0 | 1.786874 | 1.650594 | -0.161754 |

**Table S47**. Theoretical Cartesian coordinates (in Å) for the structure **27S-1** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.429574 | 2.160597 | 0.770448 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.566161 |
| 3 | 6 | 0 | 0.000000 | -2.015610 | -1.582399 |
| 4 | 6 | 0 | 1.429574 | 2.160597 | 0.770448 |
| 5 | 6 | 0 | -1.429574 | -2.160597 | 0.770448 |
| 6 | 6 | 0 | 0.000000 | 2.015610 | -1.582399 |
| 7 | 6 | 0 | 1.429574 | -2.160597 | 0.770448 |
| 8 | 8 | 0 | -2.310976 | 2.789621 | 1.190204 |
| 9 | 8 | 0 | 2.495426 | 0.000000 | -1.456097 |
| 10 | 8 | 0 | 0.000000 | 0.000000 | 2.750771 |
| 11 | 8 | 0 | 0.000000 | -2.534619 | -2.619702 |
| 12 | 8 | 0 | -2.495426 | 0.000000 | -1.456097 |
| 13 | 8 | 0 | 2.310976 | 2.789621 | 1.190204 |
| 14 | 8 | 0 | -2.310976 | -2.789621 | 1.190204 |
| 15 | 8 | 0 | 0.000000 | 2.534619 | -2.619702 |
| 16 | 8 | 0 | 2.310976 | -2.789621 | 1.190204 |
| 17 | 27 | 0 | 0.000000 | -1.263629 | 0.078828 |
| 18 | 27 | 0 | 0.000000 | 1.263629 | 0.078828 |
| 19 | 5 | 0 | 1.441345 | 0.000000 | -0.803556 |
| 20 | 5 | 0 | -1.441345 | 0.000000 | -0.803556 |

**Table S48**. Theoretical Cartesian coordinates (in Å) for the structure **27S-2** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.913567 | 1.747503 | 0.000000 |
| 2 | 6 | 0 | -1.844117 | -1.262792 | 0.000000 |
| 3 | 6 | 0 | 1.712530 | -1.197964 | 0.000000 |
| 4 | 6 | 0 | -0.035841 | 0.768250 | 1.733849 |
| 5 | 6 | 0 | -0.035841 | 0.768250 | -1.733849 |
| 6 | 6 | 0 | -0.035841 | -2.463093 | 1.512791 |
| 7 | 6 | 0 | -0.035841 | -2.463093 | -1.512791 |
| 8 | 8 | 0 | -2.876917 | 1.991268 | 0.000000 |
| 9 | 8 | 0 | 2.986355 | 2.195685 | 0.000000 |
| 10 | 8 | 0 | -3.004860 | -1.214098 | 0.000000 |
| 11 | 8 | 0 | 2.880403 | -1.173069 | 0.000000 |
| 12 | 8 | 0 | -0.183504 | 0.614697 | 2.880978 |
| 13 | 8 | 0 | -0.183504 | 0.614697 | -2.880978 |
| 14 | 8 | 0 | -0.022395 | -3.171938 | 2.437425 |
| 15 | 8 | 0 | -0.123645 | 4.329657 | 0.000000 |
| 16 | 8 | 0 | -0.022395 | -3.171938 | -2.437425 |
| 17 | 27 | 0 | 0.190476 | 1.186910 | 0.000000 |
| 18 | 27 | 0 | -0.051695 | -1.485922 | 0.000000 |
| 19 | 5 | 0 | -0.178049 | 3.099484 | 0.000000 |
| 20 | 5 | 0 | -1.656965 | 1.814775 | 0.000000 |

**Table S49**. Theoretical Cartesian coordinates (in Å) for the structure **27S-3** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.015643 | -0.000077 | 1.582354 |
| 2 | 6 | 0 | -2.015674 | -0.000117 | 1.582394 |
| 3 | 8 | 0 | 0.000025 | 2.495344 | 1.456236 |
| 4 | 8 | 0 | 2.789632 | -2.310939 | -1.190309 |
| 5 | 8 | 0 | -2.789459 | 2.311127 | -1.190143 |
| 6 | 8 | 0 | 0.000034 | -2.495477 | 1.456026 |
| 7 | 8 | 0 | 2.534640 | -0.000116 | 2.619662 |
| 8 | 8 | 0 | -0.000038 | 0.000076 | -2.750773 |
| 9 | 8 | 0 | -2.534704 | -0.000210 | 2.619686 |
| 10 | 8 | 0 | 2.789588 | 2.311095 | -1.189977 |
| 11 | 8 | 0 | -2.789615 | -2.310903 | -1.190323 |
| 12 | 27 | 0 | 1.263618 | -0.000024 | -0.078859 |
| 13 | 27 | 0 | -1.263641 | 0.000023 | -0.078806 |
| 14 | 5 | 0 | -0.000082 | 1.441304 | 0.803631 |
| 15 | 6 | 0 | 2.160550 | 1.429643 | -0.770344 |
| 16 | 6 | 0 | -2.160579 | -1.429529 | -0.770526 |
| 17 | 6 | 0 | -0.000003 | 0.000058 | -1.566163 |
| 18 | 6 | 0 | 2.160592 | -1.429548 | -0.770551 |
| 19 | 6 | 0 | -2.160535 | 1.429644 | -0.770404 |
| 20 | 5 | 0 | 0.000047 | -1.441383 | 0.803510 |

**Table S50**. Theoretical Cartesian coordinates (in Å) for the structure **27S-4** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.810721 | -0.232720 | 1.676649 |
| 2 | 6 | 0 | -2.049515 | 1.758019 | -0.083416 |
| 3 | 6 | 0 | 1.894492 | -1.217052 | -1.062902 |
| 4 | 8 | 0 | -2.084756 | -0.425814 | 2.792104 |
| 5 | 8 | 0 | 0.003019 | 0.967611 | -2.479061 |
| 6 | 8 | 0 | 1.824035 | -1.480671 | 2.590088 |
| 7 | 8 | 0 | -0.481312 | -2.955004 | 0.221509 |
| 8 | 8 | 0 | -2.531279 | 2.816454 | -0.095892 |
| 9 | 8 | 0 | 2.395256 | -1.991389 | -1.769525 |
| 10 | 8 | 0 | 1.132236 | 2.673726 | 1.328912 |
| 11 | 8 | 0 | -3.378600 | -1.261946 | -1.826753 |
| 12 | 8 | 0 | 3.904607 | 1.366405 | -0.835739 |
| 13 | 27 | 0 | -1.405783 | 0.059745 | -0.060862 |
| 14 | 27 | 0 | 1.208347 | 0.011035 | 0.056444 |
| 15 | 5 | 0 | 2.841676 | 0.848276 | -0.500843 |
| 16 | 6 | 0 | -2.586699 | -0.745158 | -1.148568 |
| 17 | 6 | 0 | 1.153185 | 1.627377 | 0.814927 |
| 18 | 6 | 0 | -0.082248 | 0.550617 | -1.374325 |
| 19 | 6 | 0 | 1.536925 | -0.926633 | 1.611856 |
| 20 | 5 | 0 | -0.695154 | -1.742825 | 0.122607 |

**Table S51.** Theoretical Cartesian coordinates (in Å) for the structure **27S-5** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.994268 | 1.557341 | -0.646279 |
| 2 | 6 | 0 | -0.231711 | -1.403689 | 0.755962 |
| 3 | 6 | 0 | -0.041526 | 0.053098 | -1.487305 |
| 4 | 6 | 0 | 1.977283 | -0.314565 | 1.681902 |
| 5 | 6 | 0 | -2.436307 | -1.258132 | -0.893181 |
| 6 | 6 | 0 | -2.113723 | 0.206794 | 1.582808 |
| 7 | 6 | 0 | 2.146632 | -1.384031 | -0.857855 |
| 8 | 8 | 0 | -2.478040 | 2.544885 | -1.017549 |
| 9 | 8 | 0 | -0.292049 | -2.422854 | 1.355097 |
| 10 | 8 | 0 | 0.014279 | 0.191485 | -2.660931 |
| 11 | 8 | 0 | 2.529739 | -0.413285 | 2.698663 |
| 12 | 8 | 0 | 0.622800 | 2.793582 | 1.090110 |
| 13 | 8 | 0 | -3.177335 | -1.993169 | -1.407659 |
| 14 | 8 | 0 | 3.199675 | 1.874632 | -1.285513 |
| 15 | 8 | 0 | -2.634712 | 0.376159 | 2.607307 |
| 16 | 8 | 0 | 2.844013 | -2.110169 | -1.437347 |
| 17 | 27 | 0 | 1.172486 | -0.169217 | 0.067344 |
| 18 | 27 | 0 | -1.361257 | -0.058952 | -0.062434 |
| 19 | 5 | 0 | 0.910251 | 1.702417 | 0.588538 |
| 20 | 5 | 0 | 2.336066 | 1.235491 | -0.685800 |

**Table S52**. Theoretical Cartesian coordinates (in Å) for the structure **27S-6** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 1.483382 | -1.877628 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.397789 |
| 3 | 6 | 0 | 0.000000 | -1.483382 | -1.877628 |
| 4 | 6 | 0 | 1.729457 | 1.677362 | 0.221455 |
| 5 | 6 | 0 | -1.729457 | 1.677362 | 0.221455 |
| 6 | 6 | 0 | 1.729457 | -1.677362 | 0.221455 |
| 7 | 6 | 0 | -1.729457 | -1.677362 | 0.221455 |
| 8 | 8 | 0 | 0.000000 | 1.662494 | -3.027071 |
| 9 | 8 | 0 | 0.000000 | 0.000000 | 2.581505 |
| 10 | 8 | 0 | 0.000000 | -1.662494 | -3.027071 |
| 11 | 8 | 0 | 2.855909 | 1.926191 | 0.385965 |
| 12 | 8 | 0 | -2.855909 | 1.926191 | 0.385965 |
| 13 | 8 | 0 | 2.855909 | -1.926191 | 0.385965 |
| 14 | 8 | 0 | -2.855909 | -1.926191 | 0.385965 |
| 15 | 8 | 0 | 0.000000 | 4.203780 | 1.222609 |
| 16 | 8 | 0 | 0.000000 | -4.203780 | 1.222609 |
| 17 | 27 | 0 | 0.000000 | 1.328779 | -0.050783 |
| 18 | 27 | 0 | 0.000000 | -1.328779 | -0.050783 |
| 19 | 5 | 0 | 0.000000 | -3.071400 | 0.744061 |
| 20 | 5 | 0 | 0.000000 | 3.071400 | 0.744061 |

**Table S53**. Theoretical Cartesian coordinates (in Å) for the structure **27S-7** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.210079 | 1.526151 | 0.591593 |
| 2 | 6 | 0 | 2.223739 | 1.679704 | -0.061746 |
| 3 | 6 | 0 | -1.958430 | -1.073288 | 1.276931 |
| 4 | 6 | 0 | -0.226326 | 1.108853 | -1.134325 |
| 5 | 6 | 0 | 0.628246 | 0.372342 | 1.666517 |
| 6 | 8 | 0 | -2.824212 | 2.436291 | 0.976395 |
| 7 | 8 | 0 | -0.028275 | -2.789421 | -0.543176 |
| 8 | 8 | 0 | 2.935079 | 2.597308 | -0.076310 |
| 9 | 8 | 0 | -2.411497 | -1.775552 | 2.084420 |
| 10 | 8 | 0 | -0.227968 | 1.882897 | -2.029695 |
| 11 | 8 | 0 | 0.436029 | 0.550075 | 2.806244 |
| 12 | 8 | 0 | 2.512034 | -1.219135 | -2.283993 |
| 13 | 8 | 0 | -3.021542 | -0.885472 | -2.314689 |
| 14 | 8 | 0 | 3.217914 | -1.692987 | 1.560491 |
| 15 | 27 | 0 | -1.360177 | 0.038024 | -0.036689 |
| 16 | 27 | 0 | 1.202698 | 0.174632 | -0.018971 |
| 17 | 5 | 0 | 2.400573 | -1.011921 | 0.947422 |
| 18 | 6 | 0 | -2.346552 | -0.524157 | -1.439612 |
| 19 | 6 | 0 | 1.949310 | -0.692889 | -1.414967 |
| 20 | 5 | 0 | -0.162174 | -1.578888 | -0.315626 |

**Table S54**. Theoretical Cartesian coordinates (in Å) for the structure **27S-8** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.238699 | -1.398415 | 1.716823 |
| 2 | 6 | 0 | -0.117864 | 1.690326 | -1.722134 |
| 3 | 8 | 0 | 2.454123 | -3.002138 | 0.000000 |
| 4 | 8 | 0 | -2.684728 | 0.368810 | 0.000000 |
| 5 | 8 | 0 | 3.110528 | 0.975564 | 0.000000 |
| 6 | 8 | 0 | 0.537383 | -1.477805 | -2.841886 |
| 7 | 8 | 0 | 0.537383 | -1.477805 | 2.841886 |
| 8 | 8 | 0 | -0.256809 | 1.989079 | -2.839906 |
| 9 | 8 | 0 | -0.256809 | 1.989079 | 2.839906 |
| 10 | 8 | 0 | -2.405142 | -3.377776 | 0.000000 |
| 11 | 8 | 0 | -0.616272 | 4.324783 | 0.000000 |
| 12 | 27 | 0 | -0.242596 | -1.343736 | 0.000000 |
| 13 | 27 | 0 | 0.119972 | 1.271382 | 0.000000 |
| 14 | 5 | 0 | -0.346496 | 3.125249 | 0.000000 |
| 15 | 6 | 0 | -1.574749 | -2.564611 | 0.000000 |
| 16 | 6 | 0 | -0.117864 | 1.690326 | 1.722134 |
| 17 | 6 | 0 | -1.518391 | 0.167814 | 0.000000 |
| 18 | 6 | 0 | 1.953410 | 1.072911 | 0.000000 |
| 19 | 5 | 0 | 1.414892 | -2.345330 | 0.000000 |
| 20 | 6 | 0 | 0.238699 | -1.398415 | -1.716823 |

**Table S55**. Theoretical Cartesian coordinates (in Å) for the structure **27S-9** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.808350 | -2.152214 | 1.339909 |
| 2 | 6 | 0 | -0.772292 | 0.044169 | -1.313759 |
| 3 | 6 | 0 | -0.772292 | 0.044169 | 1.313759 |
| 4 | 6 | 0 | 0.752389 | 2.200073 | -1.342561 |
| 5 | 6 | 0 | -1.695426 | -2.173295 | 0.000000 |
| 6 | 6 | 0 | 0.808350 | -2.152214 | -1.339909 |
| 7 | 8 | 0 | 1.350776 | -2.760019 | 2.165719 |
| 8 | 8 | 0 | -1.301827 | 0.034747 | -2.371225 |
| 9 | 8 | 0 | -1.301827 | 0.034747 | 2.371225 |
| 10 | 8 | 0 | 1.158164 | 2.887072 | -2.185142 |
| 11 | 8 | 0 | 2.994337 | -0.104990 | 0.000000 |
| 12 | 8 | 0 | -2.664570 | -2.814635 | 0.000000 |
| 13 | 8 | 0 | 1.158164 | 2.887072 | 2.185142 |
| 14 | 8 | 0 | 1.350776 | -2.760019 | -2.165719 |
| 15 | 8 | 0 | -2.644102 | 2.881473 | 0.000000 |
| 16 | 27 | 0 | 0.071581 | 1.204278 | 0.000000 |
| 17 | 27 | 0 | -0.107764 | -1.287234 | 0.000000 |
| 18 | 5 | 0 | 1.788195 | 0.160949 | 0.000000 |
| 19 | 5 | 0 | -1.610390 | 2.217385 | 0.000000 |
| 20 | 6 | 0 | 0.752389 | 2.200073 | 1.342561 |

**Table S56**. Theoretical Cartesian coordinates (in Å) for the structure **27S-10** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 1.608899 |
| 2 | 6 | 0 | 1.292710 | 0.915544 | -1.041788 |
| 3 | 6 | 0 | -1.711064 | 1.779344 | 0.407917 |
| 4 | 6 | 0 | -1.292710 | -0.915544 | -1.041788 |
| 5 | 6 | 0 | 1.711064 | -1.779344 | 0.407917 |
| 6 | 6 | 0 | -0.900165 | -2.517443 | 1.137811 |
| 7 | 6 | 0 | 0.900165 | 2.517443 | 1.137811 |
| 8 | 8 | 0 | 0.770196 | -2.994380 | -2.440689 |
| 9 | 8 | 0 | 0.000000 | 0.000000 | 2.791621 |
| 10 | 8 | 0 | 2.168820 | 0.770734 | -1.800556 |
| 11 | 8 | 0 | -2.804626 | 2.131893 | 0.599928 |
| 12 | 8 | 0 | -2.168820 | -0.770734 | -1.800556 |
| 13 | 8 | 0 | 2.804626 | -2.131893 | 0.599928 |
| 14 | 8 | 0 | -0.770196 | 2.994380 | -2.440689 |
| 15 | 8 | 0 | -1.458948 | -3.332765 | 1.749395 |
| 16 | 8 | 0 | 1.458948 | 3.332765 | 1.749395 |
| 17 | 27 | 0 | 0.000000 | 1.316262 | 0.127295 |
| 18 | 27 | 0 | 0.000000 | -1.316262 | 0.127295 |
| 19 | 5 | 0 | -0.471528 | 2.311479 | -1.463680 |
| 20 | 5 | 0 | 0.471528 | -2.311479 | -1.463680 |

**Table S57**. Theoretical Cartesian coordinates (in Å) for the structure **27S-11** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.642143 | -0.151533 | 1.389794 |
| 2 | 6 | 0 | -1.759102 | 0.992424 | 0.000000 |
| 3 | 6 | 0 | 1.592080 | -2.376725 | 0.000000 |
| 4 | 6 | 0 | 0.642143 | -0.151533 | -1.389794 |
| 5 | 6 | 0 | 1.541441 | 2.071165 | 0.000000 |
| 6 | 8 | 0 | -0.717565 | 3.058149 | -2.418457 |
| 7 | 8 | 0 | 1.148624 | -0.175857 | 2.457293 |
| 8 | 8 | 0 | -2.923100 | 0.940631 | 0.000000 |
| 9 | 8 | 0 | 2.530937 | -3.064377 | 0.000000 |
| 10 | 8 | 0 | 1.148624 | -0.175857 | -2.457293 |
| 11 | 8 | 0 | -0.717565 | 3.058149 | 2.418457 |
| 12 | 8 | 0 | -1.605823 | -2.719052 | -2.101898 |
| 13 | 8 | 0 | 2.494109 | 2.736461 | 0.000000 |
| 14 | 8 | 0 | -1.605823 | -2.719052 | 2.101898 |
| 15 | 27 | 0 | 0.062341 | -1.406758 | 0.000000 |
| 16 | 27 | 0 | 0.014001 | 1.149074 | 0.000000 |
| 17 | 5 | 0 | -0.438683 | 2.307794 | -1.487919 |
| 18 | 6 | 0 | -0.970498 | -2.161404 | -1.303022 |
| 19 | 6 | 0 | -0.970498 | -2.161404 | 1.303022 |
| 20 | 5 | 0 | -0.438683 | 2.307794 | 1.487919 |

**Table S58**. Theoretical Cartesian coordinates (in Å) for the structure **26S-1** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.220508 | 2.216432 | 1.571903 |
| 2 | 6 | 0 | -2.321379 | 2.655068 | 0.000000 |
| 3 | 8 | 0 | -0.220508 | -2.696620 | 2.543004 |
| 4 | 8 | 0 | 0.220508 | 2.696620 | 2.543004 |
| 5 | 8 | 0 | -1.994277 | -0.175941 | 0.000000 |
| 6 | 8 | 0 | 3.287412 | -3.301965 | -0.000000 |
| 7 | 8 | 0 | 1.994277 | 0.175941 | 0.000000 |
| 8 | 8 | 0 | -3.287412 | 3.301965 | -0.000000 |
| 9 | 8 | 0 | -0.220508 | -2.696620 | -2.543004 |
| 10 | 8 | 0 | 0.220508 | 2.696620 | -2.543004 |
| 11 | 27 | 0 | 0.820369 | -1.652031 | -0.000000 |
| 12 | 27 | 0 | -0.820369 | 1.652031 | -0.000000 |
| 13 | 6 | 0 | -0.220508 | 2.216432 | -1.571903 |
| 14 | 6 | 0 | 0.220508 | -2.216432 | -1.571903 |
| 15 | 5 | 0 | -0.807517 | -0.611114 | -0.000000 |
| 16 | 6 | 0 | 2.321379 | -2.655068 | 0.000000 |
| 17 | 6 | 0 | 0.220508 | -2.216432 | 1.571903 |
| 18 | 5 | 0 | 0.807517 | 0.611114 | -0.000000 |

**Table S59**. Theoretical Cartesian coordinates (in Å) for the structure **26S-2** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 27 | 0 | 1.115412 | -0.024704 | 0.045887 |
| 2 | 27 | 0 | -1.318396 | -0.097875 | -0.334182 |
| 3 | 6 | 0 | 1.780190 | -1.244871 | 1.218178 |
| 4 | 8 | 0 | 2.119282 | 2.484685 | 1.315407 |
| 5 | 8 | 0 | -3.625603 | -1.910912 | 0.030678 |
| 6 | 8 | 0 | 3.120428 | -0.335469 | -2.125164 |
| 7 | 8 | 0 | 2.268553 | -1.987078 | 1.965688 |
| 8 | 8 | 0 | -2.832338 | 2.405548 | 0.196222 |
| 9 | 8 | 0 | -0.710004 | 0.244741 | 2.678062 |
| 10 | 8 | 0 | -0.013608 | 2.123186 | -2.036344 |
| 11 | 8 | 0 | 0.047412 | -2.572260 | -1.149466 |
| 12 | 6 | 0 | -0.147768 | -1.489395 | -0.711467 |
| 13 | 6 | 0 | 2.322216 | -0.222872 | -1.289176 |
| 14 | 6 | 0 | -2.212000 | 1.446947 | -0.018995 |
| 15 | 6 | 0 | 1.703419 | 1.520228 | 0.820580 |
| 16 | 5 | 0 | -0.478812 | 0.118123 | 1.465887 |
| 17 | 5 | 0 | 0.100901 | 1.254294 | -1.160219 |
| 18 | 6 | 0 | -2.716529 | -1.205365 | -0.143294 |

**Table S60**. Theoretical Cartesian coordinates (in Å) for the structure **26S-3** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.130686 | 1.637538 | 1.697627 |
| 2 | 6 | 0 | -0.130686 | 1.637538 | -1.697627 |
| 3 | 6 | 0 | 2.077398 | -2.087308 | -0.000000 |
| 4 | 6 | 0 | -2.077398 | 2.087308 | -0.000000 |
| 5 | 8 | 0 | 0.130686 | 1.987046 | 2.778826 |
| 6 | 8 | 0 | 0.130686 | 1.987046 | -2.778826 |
| 7 | 8 | 0 | 2.657950 | 0.896039 | -0.000000 |
| 8 | 8 | 0 | -0.130686 | -1.987046 | 2.778826 |
| 9 | 8 | 0 | -2.657950 | -0.896039 | -0.000000 |
| 10 | 8 | 0 | 3.072966 | -2.687072 | -0.000000 |
| 11 | 8 | 0 | -3.072966 | 2.687072 | -0.000000 |
| 12 | 8 | 0 | -0.130686 | -1.987046 | -2.778826 |
| 13 | 27 | 0 | -0.496520 | 1.230878 | 0.000000 |
| 14 | 27 | 0 | 0.496520 | -1.230878 | 0.000000 |
| 15 | 5 | 0 | -1.425880 | -0.753388 | 0.000000 |
| 16 | 6 | 0 | 0.130686 | -1.637538 | 1.697627 |
| 17 | 6 | 0 | 0.130686 | -1.637538 | -1.697627 |
| 18 | 5 | 0 | 1.425880 | 0.753388 | 0.000000 |

**Table S61**. Theoretical Cartesian coordinates (in Å) for the structure **26S-4** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.387873 | 0.015284 | 0.000000 |
| 2 | 6 | 0 | 0.006554 | 1.620190 | 1.748565 |
| 3 | 6 | 0 | -0.702889 | -1.792716 | -1.618829 |
| 4 | 6 | 0 | -0.702889 | -1.792716 | 1.618829 |
| 5 | 6 | 0 | 1.167912 | -2.671825 | 0.000000 |
| 6 | 8 | 0 | -2.628034 | 0.513939 | 0.000000 |
| 7 | 8 | 0 | 2.570621 | 0.047794 | 0.000000 |
| 8 | 8 | 0 | 0.046426 | 1.900834 | 2.877195 |
| 9 | 8 | 0 | 0.046426 | 1.900834 | -2.877195 |
| 10 | 8 | 0 | -1.130114 | -2.119127 | -2.654056 |
| 11 | 8 | 0 | -1.130114 | -2.119127 | 2.654056 |
| 12 | 8 | 0 | 0.595467 | 4.311318 | 0.000000 |
| 13 | 8 | 0 | 1.936956 | -3.544377 | 0.000000 |
| 14 | 27 | 0 | -0.064517 | -1.370457 | 0.000000 |
| 15 | 27 | 0 | -0.046144 | 1.238065 | 0.000000 |
| 16 | 5 | 0 | 0.334381 | 3.108814 | 0.000000 |
| 17 | 5 | 0 | -1.624764 | -0.219327 | 0.000000 |
| 18 | 6 | 0 | 0.006554 | 1.620190 | -1.748565 |

**Table S62**. Theoretical Cartesian coordinates (in Å) for the structure **26S-5** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 27 | 0 | -1.301494 | 0.045898 | -0.082338 |
| 2 | 27 | 0 | 1.261560 | -0.045667 | -0.261293 |
| 3 | 6 | 0 | -1.619689 | 1.833324 | -0.057843 |
| 4 | 8 | 0 | -2.249560 | -0.504270 | 2.686587 |
| 5 | 8 | 0 | 2.180100 | 2.789944 | -0.056380 |
| 6 | 8 | 0 | -3.432804 | -1.356554 | -1.560964 |
| 7 | 8 | 0 | -1.839842 | 2.976978 | -0.069604 |
| 8 | 8 | 0 | 3.737363 | -1.648636 | -0.457291 |
| 9 | 8 | 0 | 1.524507 | 0.051735 | 2.837358 |
| 10 | 8 | 0 | -0.041491 | -2.636617 | 0.261216 |
| 11 | 8 | 0 | 0.639004 | 0.213105 | -2.499631 |
| 12 | 6 | 0 | -2.580901 | -0.825407 | -0.968896 |
| 13 | 6 | 0 | 2.759798 | -1.022243 | -0.389096 |
| 14 | 6 | 0 | -1.850878 | -0.294257 | 1.616579 |
| 15 | 5 | 0 | 1.414812 | 0.005541 | 1.611453 |
| 16 | 6 | 0 | 1.800109 | 1.696794 | -0.170102 |
| 17 | 6 | 0 | 0.061821 | -1.472385 | 0.057633 |
| 18 | 5 | 0 | -0.311124 | 0.277129 | -1.687837 |

**Table S63**. Theoretical Cartesian coordinates (in Å) for the structure **26S-6** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 27 | 0 | 1.364609 | 0.004090 | -0.078297 |
| 2 | 27 | 0 | -1.295353 | 0.132054 | -0.019327 |
| 3 | 6 | 0 | 1.424424 | 1.666842 | 0.542195 |
| 4 | 8 | 0 | 1.637962 | -2.611038 | 1.268523 |
| 5 | 8 | 0 | 0.697223 | -0.139561 | -2.419124 |
| 6 | 8 | 0 | 4.223121 | 0.013045 | -0.693130 |
| 7 | 8 | 0 | 1.557568 | 2.700109 | 1.074867 |
| 8 | 8 | 0 | -4.189638 | -0.333469 | -0.343809 |
| 9 | 8 | 0 | -1.237921 | -2.889191 | -0.940674 |
| 10 | 8 | 0 | -0.968059 | -0.330701 | 2.897911 |
| 11 | 8 | 0 | -1.453271 | 3.044127 | -0.605714 |
| 12 | 6 | 0 | -1.349172 | 1.916175 | -0.340521 |
| 13 | 6 | 0 | 3.089745 | 0.009875 | -0.423703 |
| 14 | 6 | 0 | -1.067557 | -0.143288 | 1.752874 |
| 15 | 6 | 0 | -3.048481 | -0.147224 | -0.213794 |
| 16 | 6 | 0 | 1.461052 | -1.630411 | 0.661935 |
| 17 | 5 | 0 | -1.177609 | -1.694545 | -0.640695 |
| 18 | 5 | 0 | -0.235564 | -0.172304 | -1.589084 |

**Table S64**. Theoretical Cartesian coordinates (in Å) for the structure **26S-7** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 0.150102 | -0.094501 | 2.569620 |
| 2 | 8 | 0 | 0.669220 | 0.211033 | -2.554970 |
| 3 | 8 | 0 | 1.278947 | -3.038155 | -0.205864 |
| 4 | 8 | 0 | 1.781090 | 3.075178 | 0.103696 |
| 5 | 8 | 0 | -2.151377 | 2.667074 | -1.022512 |
| 6 | 8 | 0 | -2.132603 | -2.580239 | -1.239082 |
| 7 | 8 | 0 | 4.053481 | -0.624200 | 0.663023 |
| 8 | 8 | 0 | -3.401705 | -0.129159 | 1.996311 |
| 9 | 27 | 0 | -1.293603 | 0.005040 | -0.069660 |
| 10 | 27 | 0 | 1.316891 | 0.122850 | -0.048516 |
| 11 | 6 | 0 | 2.962758 | -0.340170 | 0.361092 |
| 12 | 5 | 0 | 1.305378 | -1.809894 | -0.140009 |
| 13 | 6 | 0 | 1.567661 | 1.935685 | 0.036230 |
| 14 | 6 | 0 | 0.143027 | -0.024678 | 1.388393 |
| 15 | 6 | 0 | -1.778032 | 1.630640 | -0.636764 |
| 16 | 6 | 0 | -1.744130 | -1.589629 | -0.766864 |
| 17 | 5 | 0 | -0.144095 | 0.097735 | -1.619528 |
| 18 | 6 | 0 | -2.553358 | -0.076599 | 1.202355 |

**Table S65**. Theoretical Cartesian coordinates (in Å) for the structure **26S-8** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 2.817185 | -0.484020 | 0.000000 |
| 2 | 8 | 0 | -2.728660 | 0.017521 | 0.000000 |
| 3 | 8 | 0 | 0.107029 | -1.354435 | 2.956157 |
| 4 | 8 | 0 | 0.107029 | -1.354435 | -2.956157 |
| 5 | 8 | 0 | 0.948924 | 2.172724 | -2.597304 |
| 6 | 8 | 0 | 0.948924 | 2.172724 | 2.597304 |
| 7 | 8 | 0 | -0.559363 | -4.278583 | 0.000000 |
| 8 | 8 | 0 | -1.462947 | 3.870044 | 0.000000 |
| 9 | 27 | 0 | 0.032402 | 1.108958 | 0.000000 |
| 10 | 27 | 0 | -0.066032 | -1.387350 | 0.000000 |
| 11 | 6 | 0 | -0.366873 | -3.129609 | 0.000000 |
| 12 | 6 | 0 | 0.022504 | -1.347173 | -1.798408 |
| 13 | 6 | 0 | 0.579247 | 1.722378 | 1.586724 |
| 14 | 6 | 0 | -1.588028 | 0.301397 | 0.000000 |
| 15 | 6 | 0 | 0.022504 | -1.347173 | 1.798408 |
| 16 | 5 | 0 | 1.673083 | -0.011605 | 0.000000 |
| 17 | 5 | 0 | -0.874793 | 2.789824 | 0.000000 |
| 18 | 6 | 0 | 0.579247 | 1.722378 | -1.586724 |

**Table S66**. Theoretical Cartesian coordinates (in Å) for the structure **26S-9** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 0.275667 | -0.009577 | 2.789463 |
| 2 | 8 | 0 | 0.275667 | -0.009577 | -2.789463 |
| 3 | 8 | 0 | 1.895624 | 2.772640 | 0.000000 |
| 4 | 8 | 0 | -3.239517 | -0.189990 | 0.000000 |
| 5 | 8 | 0 | -1.564351 | -3.277037 | 0.000000 |
| 6 | 8 | 0 | 3.404647 | -0.184731 | 0.000000 |
| 7 | 8 | 0 | -2.140142 | 3.822206 | 0.000000 |
| 8 | 8 | 0 | 2.163537 | -3.593545 | 0.000000 |
| 9 | 27 | 0 | 0.346529 | -1.001498 | 0.000000 |
| 10 | 27 | 0 | -0.684098 | 1.290050 | 0.000000 |
| 11 | 6 | 0 | -1.551862 | 2.813837 | 0.000000 |
| 12 | 6 | 0 | -2.206990 | 0.348357 | 0.000000 |
| 13 | 6 | 0 | 0.917166 | 2.151357 | 0.000000 |
| 14 | 5 | 0 | 2.271480 | -0.672063 | 0.000000 |
| 15 | 6 | 0 | 0.275667 | -0.363978 | -1.674383 |
| 16 | 6 | 0 | 0.275667 | -0.363978 | 1.674383 |
| 17 | 6 | 0 | -0.854289 | -2.354486 | 0.000000 |
| 18 | 5 | 0 | 1.611146 | -2.492070 | 0.000000 |

**Table S67**. Theoretical Cartesian coordinates (in Å) for the structure **26T-1** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.912579 | 0.820446 | 1.485934 |
| 2 | 6 | 0 | 1.940438 | -2.041214 | -1.411333 |
| 3 | 6 | 0 | -2.912579 | 0.820446 | -1.485934 |
| 4 | 6 | 0 | 1.940438 | -2.041214 | 1.411333 |
| 5 | 6 | 0 | -1.783544 | 2.902524 | 0.000000 |
| 6 | 6 | 0 | 3.785812 | -0.401388 | 0.000000 |
| 7 | 8 | 0 | -3.517248 | 0.608467 | 2.463490 |
| 8 | 8 | 0 | 1.940438 | -2.813082 | -2.278569 |
| 9 | 8 | 0 | -3.517248 | 0.608467 | -2.463490 |
| 10 | 8 | 0 | 1.184183 | 0.963516 | 0.000000 |
| 11 | 8 | 0 | 1.940438 | -2.813082 | 2.278569 |
| 12 | 8 | 0 | -1.639073 | 4.063216 | 0.000000 |
| 13 | 8 | 0 | -0.644734 | -1.740921 | 0.000000 |
| 14 | 8 | 0 | 4.924880 | -0.170861 | 0.000000 |
| 15 | 27 | 0 | 1.976027 | -0.835646 | 0.000000 |
| 16 | 27 | 0 | -1.949412 | 1.128174 | 0.000000 |
| 17 | 5 | 0 | -1.197980 | -0.619167 | 0.000000 |
| 18 | 5 | 0 | -0.089940 | 1.038843 | 0.000000 |

**Table S68**. Theoretical Cartesian coordinates (in Å) for the structure **26T-2** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.915416 | 2.673207 | 1.411467 |
| 2 | 6 | 0 | -1.413932 | 3.494387 | 0.000000 |
| 3 | 8 | 0 | -1.476880 | -3.139443 | 2.466777 |
| 4 | 8 | 0 | 1.589109 | 3.048920 | 2.279117 |
| 5 | 8 | 0 | -1.430318 | 0.594346 | 0.000000 |
| 6 | 8 | 0 | 2.384996 | -3.839984 | 0.000000 |
| 7 | 8 | 0 | 1.791525 | 0.284702 | 0.000000 |
| 8 | 8 | 0 | -2.161130 | 4.383995 | 0.000000 |
| 9 | 8 | 0 | -1.476880 | -3.139443 | -2.466777 |
| 10 | 8 | 0 | 1.589109 | 3.048920 | -2.279117 |
| 11 | 27 | 0 | -0.102527 | -2.244708 | 0.000000 |
| 12 | 27 | 0 | -0.155074 | 2.114654 | 0.000000 |
| 13 | 6 | 0 | 0.915416 | 2.673207 | -1.411467 |
| 14 | 6 | 0 | -0.931743 | -2.797631 | -1.490089 |
| 15 | 5 | 0 | -0.905179 | -0.567902 | 0.000000 |
| 16 | 6 | 0 | 1.389317 | -3.227240 | 0.000000 |
| 17 | 6 | 0 | -0.931743 | -2.797631 | 1.490089 |
| 18 | 5 | 0 | 1.069698 | -0.738988 | 0.000000 |

**Table S69**. Theoretical Cartesian coordinates (in Å) for the structure **26T-3** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 27 | 0 | 2.154093 | -0.529735 | 0.000000 |
| 2 | 27 | 0 | -2.051176 | 0.360200 | 0.000000 |
| 3 | 6 | 0 | 2.040913 | -0.847623 | 1.874790 |
| 4 | 8 | 0 | 2.040913 | -0.964135 | -3.027345 |
| 5 | 8 | 0 | 0.973175 | 1.222434 | 0.000000 |
| 6 | 8 | 0 | 4.745496 | 1.019292 | 0.000000 |
| 7 | 8 | 0 | 2.040913 | -0.964135 | 3.027345 |
| 8 | 8 | 0 | -3.340882 | -0.622311 | -2.481271 |
| 9 | 8 | 0 | 0.132272 | -1.904973 | 0.000000 |
| 10 | 8 | 0 | -3.340882 | -0.622311 | 2.481271 |
| 11 | 8 | 0 | -2.715339 | 3.235781 | 0.000000 |
| 12 | 6 | 0 | -2.473084 | 2.091152 | 0.000000 |
| 13 | 6 | 0 | 3.759161 | 0.403238 | 0.000000 |
| 14 | 6 | 0 | -2.843480 | -0.230883 | 1.497527 |
| 15 | 6 | 0 | -2.843480 | -0.230883 | -1.497527 |
| 16 | 6 | 0 | 2.040913 | -0.847623 | -1.874790 |
| 17 | 5 | 0 | -0.776199 | -1.033990 | 0.000000 |
| 18 | 5 | 0 | -0.253752 | 0.905201 | 0.000000 |

**Table S70**. Theoretical Cartesian coordinates (in Å) for the structure **26T-4** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.095959 | 1.607846 | 1.390388 |
| 2 | 8 | 0 | 1.830317 | -1.938981 | 2.263619 |
| 3 | 8 | 0 | -1.660549 | 3.856397 | 0.000000 |
| 4 | 8 | 0 | -1.916488 | -0.253877 | 1.937598 |
| 5 | 8 | 0 | 1.830317 | -1.938981 | -2.263619 |
| 6 | 8 | 0 | -1.916488 | -0.253877 | -1.937598 |
| 7 | 8 | 0 | 1.803203 | 1.758466 | 2.304212 |
| 8 | 8 | 0 | -1.783651 | -3.745530 | -0.000000 |
| 9 | 8 | 0 | 1.803203 | 1.758466 | -2.304212 |
| 10 | 27 | 0 | -0.027994 | 1.384115 | 0.000000 |
| 11 | 27 | 0 | -0.029526 | -1.288127 | -0.000000 |
| 12 | 6 | 0 | 1.095959 | 1.607846 | -1.390388 |
| 13 | 6 | 0 | -1.010922 | 2.890170 | 0.000000 |
| 14 | 6 | 0 | -1.136990 | -2.782809 | -0.000000 |
| 15 | 5 | 0 | -1.189450 | 0.362966 | 1.140669 |
| 16 | 6 | 0 | 1.105384 | -1.674694 | -1.393113 |
| 17 | 6 | 0 | 1.105384 | -1.674694 | 1.393113 |
| 18 | 5 | 0 | -1.189450 | 0.362966 | -1.140669 |

**Table S71**. Theoretical Cartesian coordinates (in Å) for the structure **26T-5** using the BP86/DZP method.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 27 | 0 | 0.107994 | -1.232246 | 0.000000 |
| 2 | 27 | 0 | -0.146134 | 1.194237 | 0.000000 |
| 3 | 6 | 0 | -0.472294 | -2.320038 | 1.378618 |
| 4 | 8 | 0 | 3.048214 | -1.872404 | 0.000000 |
| 5 | 8 | 0 | 0.854912 | 0.761983 | 2.746238 |
| 6 | 8 | 0 | -0.837719 | -3.009883 | -2.237454 |
| 7 | 8 | 0 | -0.837719 | -3.009883 | 2.237454 |
| 8 | 8 | 0 | -2.153241 | 3.362016 | 0.000000 |
| 9 | 8 | 0 | 2.080695 | 3.433768 | 0.000000 |
| 10 | 8 | 0 | 0.854912 | 0.761983 | -2.746238 |
| 11 | 8 | 0 | -2.923588 | -0.417064 | 0.000000 |
| 12 | 6 | 0 | -0.472294 | -2.320038 | -1.378618 |
| 13 | 6 | 0 | -1.368988 | 2.502134 | 0.000000 |
| 14 | 6 | 0 | 1.914996 | -1.617202 | 0.000000 |
| 15 | 5 | 0 | 1.213863 | 2.561414 | 0.000000 |
| 16 | 6 | 0 | 0.456998 | 0.880053 | 1.653114 |
| 17 | 6 | 0 | 0.456998 | 0.880053 | -1.653114 |
| 18 | 5 | 0 | -1.764750 | 0.021057 | 0.000000 |

**Table S72.** ν(CO) and ν(BO) frequencies ($cm^{-1}$) for the mononuclear $Co(BO)(CO)_n$ ($n$ = 4, 3, 2, 1) structures (BP86 method). Infrared intensities in parentheses are in km $mol^{-1}$.

| | ν(CO) | ν(BO) |
|---|---|---|
| **14S-1** ($C_{3v}$) | 2026(893),2026(893),2039(471),2095(90) | 1869(235) |
| $Fe(CS)(CO)_4$ ($C_{3v}$) | 1991(1067),1991(1067),2010(367),2063(346) | — |
| $Mn(NO)(CO)_4$ ($C_{3v}$) | 1978(1170),1978(1170),1997(366),2058(125) | — |
| **14S-2** ($C_{2v}$) | 2020(1072),2029(857),2033(373),2089(64) | 1854(235) |
| **14S-3** ($C_{4v}$) | 2025(1146),2025(1146),2035(0),2101(63) | 1863(178) |
| **13S-1** ($C_{2v}/C_s$) | 2005(1292),2024(614),2081(122) | 1854(228) |
| **13T-1** ($C_s$) | 2015(732),2016(816),2059(294) | 1824(90) |
| **13T-2** ($C_s$) | 2002(1290),2009(631),2054(66) | 1833(97) |
| **13S-2** ($C_{3v}$) | 1997(939),1997(938),2060(10) | 1846(176) |
| **12T-1** ($C_s$) | 2009(864),2052(412) | 1835(107) |
| **12T-2** ($C_{2v}$) | 1992(1488),2052(63) | 1835(106) |
| **12T-3** ($C_s$) | 1988(953),2029(360) | 1821(93) |
| **12S-1** ($C_s$) | 1975(1297),2044(73) | 1832(173) |
| **12S-2** ($C_{2v}$) | 1981(1473),2061(0) | 1829(172) |
| **12S-3** ($C_s$) | 1986(731),2042(472) | 1834(211) |
| **11T-1** ($C_{\infty v}$) | 2038(621) | 1847(125) |
| **11S-1** ($C_s$) | 1982(439) | 1806(185) |

**Table S73** ν(CO) and ν(BO) frequencies ($cm^{-1}$) for the binuclear $Co_2(BO)_2(CO)_8$ structures (BP86 method). Infrared intensities in parentheses are in km $mol^{-1}$ and bridging ν(CO) and ν(CO) frequencies are in **bold** type.

| | ν(CO) | ν(BO) |
|---|---|---|
| **28S-1**($C_1$) | **1806(172)**,2003(508),2024(356),2030(241), 2035(994),2040(396),2070(981),2089(135) | 1834(148), 1854(236) |
| **28S-2**($C_s$) | **1817(155)**,2003(187),2017(262),2032(403), 2032(1399),2038(663),2064(416),2089(205) | 1837(225), 1855(217) |
| **28S-3**($C_s$) | **1837(192)**,2015(23),2030(635),2034(372), 2037(1528),2043(161),2070(767),2095(113) | 1849(154), 1873(129), |
| **28S-4**($C_s$) | **1804(189)**,2021(796),2024(384),2031(382), 2041(612),2055(605),2081(798),2100(51) | 1862(249), 1875(15) |
| **28S-5**($C_{2h}$) | **1789(506),1800(0)**,2040(0),2048(1106), 2051(824),2051(0),2074(1444),2094(0) | 1858(0), 1859(288) |
| **28S-6**($C_{2v}$) | **1789(503),1800(5)**,2022(0),2043(0), 2043(772),2051(1087),2071(1354),2093(126) | 1865(6), 1871(297) |
| **28S-7**($C_{2v}$) | **1812(354),1857(77)**,2011(0),2033(12), 2034(1766),2049(455),2059(1020),2090(138) | 1865(188), 1870(262) |

**Table S74**. ν(CO) and ν(BO) frequencies ($cm^{-1}$) for the binuclear $Co_2(BO)_2(CO)_7$ structures (BP86 method). Infrared intensities in parentheses are in km $mol^{-1}$ and bridging ν(CO) and ν(CO) frequencies are in **bold** type.

| | ν(CO) | ν(BO) |
|---|---|---|
| **27S-1**($C_{2v}$) | **1895(402)**,2043(0),2045(1181),2048(94), 2053(1023),2076(1068),2101(2) | **1771(286), 1779(122)** |
| **27S-2**($C_s$) | 2002(140),2004(338),2027(265),2027(1417), 2037(327),2053(1046),2092(126) | 1829(108), 1852(223) |
| **27S-3**($C_1$) | **1895(402)**,2043(0),2045(1181),2048(94), 2053(1023),2076(1068),2101(2) | **1771(286), 1779(122)** |
| **27S-4**($C_1$) | **1895(442)**,2020(169),2024(433),2037(996), 2050(683),2062(969),2094(30) | 1822(175), 1864(177) |
| **27S-5**($C_1$) | **1891(598),1906(174)**,2032(563),2042(405), 2047(769),2065(1188),2091(78) | 1819(130), 1852(225) |
| **27S-6**($C_{2v}$) | **1896(462)**,2012(0),2019(55),2029(1732), 2043(846),2048(416),2089(79) | 1860(327), 1861(30) |
| **27S-7**($C_1$) | **1898(334)**,2001(284),2032(632),2039(752), 2049(553),2064(1143),2093(44) | **1779(185)**, 1871(255) |
| **27S-8**($C_s$) | **1895(324)**,2004(52),2026(1631),2029(145), 2040(349),2056(948),2088(14) | 1858(206), 1860(251) |
| **27S-9**($C_s$) | **1899(585),1910(235)**,2040(658),2048(305), 2056(725),2073(1074),2097(62) | 1812(203), 1871(133) |
| **27S-10**($C_2$) | **1898(195)**,2005(380),2011(518),2032(1057), 2039(314),2056(970),2085(89) | 1862(369), 1863(161) |
| **27S-11**($C_s$) | **1895(533),1916(178)**,2025(37),2029(542), 2035(1338),2061(981),2090(31) | 1871(302), 1878(162) |

**Table S75.** ν(CO) and ν(BO) frequencies ($cm^{-1}$) for the binuclear $Co_2(BO)_2(CO)_6$ structures (BP86 method ). Infrared intensities in parentheses are in km $mol^{-1}$ and bridging ν(CO) and ν(BO) frequencies are in **bold** type.

| | ν(CO) | ν(BO) |
|---|---|---|
| **26T-1**($C_s$) | 2001(779),2005(642),2026(836),2032(798),2043(1198),2075(215) | **1597(382),1738(458)** |
| **26T-2**($C_s$) | 1999(819),2005(652),2027(780)2032(787),2045(999),2076(236) | **1607(387),1726(570)** |
| **26T-3**($C_s$) | 1997(700),2002(674),2026(702),2034(1276),2046(512),2083(69) | 1637(237),1711(955) |
| **26T-4**($C_s$) | 2012(21),2017(13),2031(1134),2034(1018),2051(1425),2081(90) | **1756(90),1766(137)** |
| **26T-5**($C_s$) | 1993(639),2010(55),2032(798),2037(836),2051(1020),2080(128) | **1770(67)**,1864(183) |
| **26S-1**($C_{2h}$) | 1994(0),2002(1844),2019(718),2023(0),2063(1418),2079(0) | **1664(0),1671(255)** |
| **26S-2**($C_s$/$C_1$) | **1896(459)**,2033(599),2045(596),2047(611),2057(1343),2093(97) | **1767(190),1777(104)** |
| **26S-3**($C_{2h}$) | 1997(0),2021(1827),2029(489),2037(0),2056(1701),2089(0) | **1766(0),1768(195)** |
| **26S-4**($C_s$) | **1898(332)**,2010(117),2024(1681),2029(353),2058(811),2086(116) | **1767(107)**,1854(233) |
| **26S-5**($C_1$) | **1880(415)**,2017(122),2032(993),2038(757),2057(1140),2084(91) | **1724(120)**,1851(148) |
| **26S-6**($C_1$) | 1988(549),2011(184),2032(819),2036(386),2057(1316),2084(139) | **1737(145)**,1837(170) |
| **26S-7**($C_1$) | **1898(319)**,2013(481),2027(894),2035(454),2056(1268),2084(161) | **1755(106)**,1854(148) |
| **26S-8**($C_s$) | **1956(496)**,2010(132),2036(1565),2036(819),2044(371),2100(117) | **1788(111)**,1866(195) |
| **26S-9**($C_s$) | 1985(896),2007(1),2014(611),2027(724),2049(946),2097(145) | 1824(120),1848(232) |

**Table S76.** Total energies (*E*, in Hartree), relative energies (Δ*E,* in kcal/mol), and the numbers of imaginary frequencies ($N_{Imag}$) for the three $Co(BO)(CO)_4$ structures

| Species | B3LYP | | | BP86 | | |
|---|---|---|---|---|---|---|
| | $-E_{total}$ | ΔE | $N_{Imag}$ | $-E_{total}$ | ΔE | $N_{Imag}$ |
| **14S-1**($C_{3v}$) | 1936.43262 | 0.0 | 0 | 1936.69101 | 0.0 | 0 |
| **14S-2**($C_{2v}$) | 1936.42422 | 5.3 | 1 (29*i*) | 1936.68423 | 4.3 | 1 (27*i*) |
| **14S-3**($C_{4v}$) | 1936.40103 | 19.8 | 1(176*i*) | 1936.65546 | 22.3 | 1(204*i*) |

**Table S77.** Total energies (*E*, in Hartree), relative energies (Δ*E,* in kcal/mol), and numbers of imaginary frequencies ($N_{Imag}$) for the four optimized $Co(BO)(CO)_3$ structures.

| | B3LYP | | | BP86 | | |
|---|---|---|---|---|---|---|
| Species | $-E_{total}$ | ΔE | $N_{Imag}$ | $-E_{total}$ | ΔE | $N_{Imag}$ |
| **13S-1**($C_{2v}$/$C_s$) | 1823.05346 | 0.0 | 0 | 1823.29781 | 0.0 | 0 |
| **13T-1** ($C_s$) | 1823.03997 | 8.5 | 0 | 1823.26360 | 21.6 | 0 |
| **13T-2** ($C_s$) | 1823.03744 | 10.1 | 0 | 1823.26741 | 19.1 | 0 |
| **13S-2** ($C_{3v}$) | 1823.03572 | 11.1 | 0 | 1823.28440 | 8.4 | 0 |

**Table S78.** Total energies ($E$, in Hartree), relative energies ($\Delta E$, in kcal/mol), and numbers of imaginary vibrational frequencies ($N_{Imag}$) for the six energetically low-lying $Co(BO)(CO)_2$ structures.

| Species | B3LYP | | | BP86 | | |
|---|---|---|---|---|---|---|
| | $-E_{total}$ | ΔE | $N_{Imag}$ | $-E_{total}$ | ΔE | $N_{Imag}$ |
| **12T-1** ($C_s$) | 1709.67383 | 0.0 | 0 | 1709.87808 | 0.0 | 0 |
| **12T-2** ($C_{2v}$) | 1709.66975 | 2.6 | 0 | 1709.87982 | -1.1 | 0 |
| **12T-3** ($C_s$) | 1709.66733 | 4.1 | 0 | 1709.87826 | -0.1 | 0 |
| **12S-1** ($C_s$) | 1709.65825 | 9.8 | 0 | 1709.89551 | -10.9 | 0 |
| **12S-2** ($C_{2v}$) | 1709.65790 | 10.0 | 1 (33$i$) | 1709.89320 | -9.5 | 1 (62$i$) |
| **12S-3** ($C_s$) | 1709.65130 | 14.1 | 0 | 1709.88615 | -5.1 | 0 |

**Table S79** Total energies ($E$, in Hartree), relative energies ($\Delta E$, in kcal/mol), and numbers of imaginary vibrational frequencies ($N_{Imag}$) for the Co(BO)(CO) structures.

| Species | B3LYP | | | BP86 | | |
|---|---|---|---|---|---|---|
| | $-E_{total}$ | ΔE | $N_{Imag}$ | $-E_{total}$ | ΔE | $N_{Imag}$ |
| **11T-1** ($C_{\infty v}$) | 1596.27528 | 0.0 | 0 | 1596.49828 | 0.0 | 0 |
| **11S-1** ($C_s$) | 1596.26005 | 9.6 | 0 | 1596.48520 | 8.2 | 0 |

**Table S80** Total energies ($E$, in hartree), relative energies ($\Delta E$, in kcal $mol^{-1}$), and numbers of imaginary vibrational frequencies ($N_{Imag}$) for the optimized $Co_2(BO)_2(CO)_8$ structures.

| Species | B3LYP | | | BP86 | | |
|---|---|---|---|---|---|---|
| | $-E_{total}$ | ΔE | $N_{Imag}$ | $-E_{total}$ | ΔE | $N_{Imag}$ |
| **28S-1**($C_1$) | 3872.80508 | 0.0 | 0 | 3873.33149 | 0.0 | 0 |
| **28S-2**($C_s$) | 3872.80337 | 1.1 | 0 | 3873.33026 | 0.8 | 0 |
| **28S-3**($C_s$) | 3872.80196 | 2.0 | 0 | 3873.32319 | 5.2 | 0 |
| **28S-4**($C_s$) | 3872.79680 | 5.2 | 0 | 3873.31718 | 9.0 | 1 (10$i$) |
| **28S-5**($C_{2h}$) | 3872.77561 | 18.5 | 0 | 3873.30526 | 16.5 | 0 |
| **28S-6**($C_{2v}$) | 3872.76500 | 25.2 | 0 | 3873.29689 | 21.7 | 1 (11$i$) |
| **28S-7**($C_{2v}$) | 3872.76158 | 27.3 | 0 | 3873.29405 | 23.5 | 0 |

**Table S81** Total energies ($E$, in hartree), relative energies ($\Delta E$, in kcal mol$^{-1}$), and numbers of imaginary vibrational frequencies ($N_{Imag}$) for the optimized $Co_2(BO)_2(CO)_7$ structures.

| | B3LYP | | | BP86 | | |
|---|---|---|---|---|---|---|
| Species | $-E_{total}$ | ΔE | $N_{Imag}$ | $-E_{total}$ | ΔE | $N_{Imag}$ |
| **27S-1** ($C_{2v}$) | 3759.49671 | 0.0 | 0 | 3760.02411 | 0.0 | 0 |
| **27S-2** ($C_s$) | 3759.48717 | 6.0 | 0 | 3760.00536 | 11.8 | 0 |
| **27S-3** ($C_1$) | 3759.48685 | 6.2 | 0 | 3760.02411 | 0.0 | 0 |
| **27S-4** ($C_1$) | 3759.48664 | 6.3 | 0 | 3760.00706 | 10.7 | 0 |
| **27S-5** ($C_1$) | 3759.48520 | 7.2 | 0 | 3760.01225 | 7.4 | 0 |
| **27S-6** ($C_{2v}$) | 3759.48196 | 9.3 | 0 | 3760.00235 | 13.7 | 0 |
| **27S-7** ($C_1$) | 3759.48149 | 9.6 | 0 | 3760.00649 | 11.1 | 0 |
| **27S-8** ($C_s$) | 3759.48095 | 9.9 | 0 | 3760.00218 | 13.8 | 0 |
| **27S-9** ($C_s$) | 3759.47912 | 11.0 | 0 | 3760.00389 | 12.7 | 0 |
| **27S-10** ($C_2$) | 3759.47556 | 13.3 | 0 | 3759.99938 | 15.5 | 0 |
| **27S-11** ($C_s$) | 3759.47497 | 13.6 | 0 | 3760.00000 | 15.1 | 0 |

**Table S82.** Total energies ($E$, in hartree), relative energies ($\Delta E$, in kcal mol$^{-1}$), and numbers of imaginary vibrational frequencies ($N_{Imag}$) for the optimized $Co_2(BO)_2(CO)_6$ structures.

| Species | B3LYP | | | BP86 | | |
|---|---|---|---|---|---|---|
| | $-E_{total}$ | ΔE | $N_{Imag}$ | $-E_{total}$ | ΔE | $N_{Imag}$ |
| **26T-1**($C_s$) | 3646.17080 | 0.0 | 0 | 3646.63943 | 0.0 | 0 |
| **26T-2**($C_s$) | 3646.17048 | 0.2 | 0 | 3646.63883 | 0.4 | 0 |
| **26T-3**($C_s$) | 3646.15999 | 6.8 | 0 | 3646.62409 | 9.6 | 0 |
| **26T-4**($C_s$) | 3646.15229 | 11.6 | 0 | 3646.63166 | 4.9 | 0 |
| **26T-5**($C_s$) | 3646.14549 | 15.9 | 0 | 3646.62301 | 10.3 | 0 |
| **26S-1**($C_{2h}$) | 3646.14262 | 17.7 | 0 | 3646.65136 | − 7.5 | 0 |
| **26S-2**($C_s$/$C_1$) | 3646.13216 | 24.2 | 0 | 3646.64620 | − 4.2 | 0 |
| **26S-3**($C_{2h}$) | 3646.12967 | 25.8 | 0 | 3646.63709 | 1.5 | 1 (27*i*) |
| **26S-4**($C_s$) | 3646.12825 | 26.7 | 0 | 3646.64098 | − 1.0 | 0 |
| **26S-5**($C_1$) | 3646.12744 | 27.2 | 0 | 3646.63963 | − 0.1 | 0 |
| **26S-6**($C_1$) | 3646.12744 | 27.2 | 0 | 3646.63646 | 1.9 | 0 |
| **26S-7**($C_1$) | 3646.12617 | 28.0 | 0 | 3646.63845 | 0.6 | 0 |
| **26S-8**($C_s$) | 3646.12600 | 28.1 | 0 | 3646.63382 | 3.5 | 0 |
| **26S-9**($C_s$) | 3646.12484 | 28.8 | 0 | 3646.63067 | 5.5 | 1 (28*i*) |

**Complete Gaussian 03 reference (Reference 52)**

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