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# Binuclear Manganese Carbonyl Thiocarbonyls: Metal-Metal Multiple Bonds versus Four-Electron Donor Thiocarbonyl Groups

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## Supporting Information

**Tables S1-S4:** The theoretical harmonic vibrational frequencies for $Mn_2(CS)_2(CO)_8$ (9 structures), $Mn_2(CS)_2(CO)_7$ (7 structures), $Mn_2(CS)_2(CO)_5$ (7 structures), $Mn_2(CS)_2(CO)_5$ (5 structures) using the BP86 method.

**Tables S6-S32:** The theoretical Cartesian coordinates for $Mn_2(CS)_2(CO)_8$ (9 structures), $Mn_2(CS)_2(CO)_7$ (7 structures), $Mn_2(CS)_2(CO)_5$ (7 structures), $Mn_2(CS)_2(CO)_5$ (5 structures) using the B3LYP method.

Complete Gaussian 03 reference (Reference 40)

**Table S1.** The theoretical harmonic vibrational frequencies (in $cm^{-1}$) for $Mn_2(CS)_2(CO)_8$ using the BP86/DZP method (infrared intensities in parentheses are in km/mol).

| **8-1**($D_{4d}$) | **8-2**($C_s$) | **8-3**($C_2$) | **8-4**($C_2$) | **8-5**($D_{4h}$) | **8-6**($C_s$) | **8-7**($C_{2h}$) | **8-8**($C_{2v}$) | **8-9**($D_{2h}$) |
|---|---|---|---|---|---|---|---|---|
| 39(e1, 0) | 33(a", 0) | 34(a, 0) | 33(a, 0) | -4(a1u, 0) | -20(a", 0) | -21(au, 0) | -16(a2, 0) | 14(au, 0) |
| 39(e1, 0) | 42(a', 0) | 47(b, 0) | 48(b, 0) | 35(eg, 0) | 33(a", 0) | 31(bg, 0) | 30(b2, 0) | 27(b1u, 0) |
| 41(b1, 0) | 43(a", 0) | 47(a, 0) | 48(a, 0) | 35(eg, 0) | 35(a', 0) | 33(ag, 0) | 33(a2, 0) | 41(b3g, 0) |
| 51(e3, 0) | 46(a", 0) | 49(b, 0) | 49(a, 0) | 46(eu, 0) | 43(a', 0) | 45(bu, 0) | 48(b2, 0) | 46(b1g, 0) |
| 51(e3, 0) | 49(a', 0) | 49(a, 0) | 50(b, 0) | 46(eu, 0) | 50(a", 0) | 58(au, 0) | 57(b1, 0) | 59(b2u, 0) |
| 58(e2, 0) | 57(a', 0) | 57(a, 0) | 58(b, 0) | 49(b2u, 0) | 51(a', 0) | 61(bu, 0) | 64(a1, 0) | 64(b3u, 1) |
| 58(e2, 0) | 57(a", 0) | 58(b, 0) | 59(a, 0) | 69(eg, 0) | 67(a", 0) | 68(bg, 0) | 66(a2, 0) | 79(b2g, 0) |
| 66(e3, 0) | 67(a", 0) | 69(b, 0) | 70(a, 0) | 69(eg, 0) | 73(a', 0) | 72(au, 0) | 75(b2, 0) | 86(au, 0) |
| 66(e3, 0) | 71(a', 0) | 72(a, 0) | 76(b, 0) | 89(b1u, 0) | 80(a", 0) | 73(ag, 0) | 76(b1, 0) | 89(b3g, 0) |
| 87(e1, 0) | 81(a", 0) | 82(a, 0) | 76(b, 0) | 91(b2g, 0) | 89(a", 0) | 84(bg, 0) | 82(a2, 0) | 92(b1u, 0) |
| 87(e1, 0) | 85(a', 0) | 87(b, 0) | 81(a, 0) | 92(eu, 0) | 91(a', 0) | 92(au, 0) | 92(b1, 0) | 94(ag, 0) |
| 92(a1, 0) | 90(a", 0) | 87(b, 0) | 90(a, 0) | 92(eu, 0) | 92(a", 0) | 92(bu, 1) | 93(a1, 0) | 96(b2u, 0) |
| 93(e1, 0) | 91(a', 0) | 90(a, 0) | 92(b, 0) | 94(eg, 0) | 96(a', 0) | 92(ag, 0) | 97(a1, 0) | 97(b1g, 0) |
| 93(e1, 0) | 93(a', 0) | 92(a, 0) | 93(a, 0) | 94(eg, 0) | 96(a", 0) | 101(bg, 0) | 98(b2, 0) | 107(ag, 0) |
| 94(e2, 0) | 93(a", 0) | 96(b, 0) | 97(b, 1) | 108(a1g, 0) | 103(a', 1) | 102(bu, 3) | 101(a2, 0) | 110(b3u, 0) |
| 94(e2, 0) | 94(a', 0) | 101(a, 0) | 98(a, 0) | 108(b1g, 0) | 109(a', 0) | 110(ag, 0) | 108(a1, 0) | 113(b1u, 0) |
| 95(e3, 0) | 98(a', 0) | 101(b, 0) | 101(a, 0) | 115(a2u, 6) | 113(a', 1) | 113(ag, 0) | 115(b2, 5) | 122(b2g, 0) |
| 95(e3, 0) | 101(a", 0) | 103(a, 0) | 102(b, 0) | 118(eu, 0) | 122(a', 3) | 125(au, 0) | 121(a1, 0) | 169(b1g, 0) |
| 108(b2, 6) | 110(a', 5) | 112(b, 5) | 112(b, 4) | 118(eu, 0) | 122(a", 0) | 128(bu, 3) | 126(b1, 0) | 170(b3u, 3) |
| 136(a1, 0) | 139(a', 0) | 141(a, 0) | 140(a, 0) | 134(a1g, 0) | 136(a', 0) | 135(ag, 0) | 135(a1, 0) | 193(ag, 0) |
| 367(e3, 0) | 348(a", 2) | 347(a, 3) | 347(a, 0) | 371(a2g, 0) | 349(a", 2) | 347(bg, 0) | 347(b1, 4) | 272(b1g, 0) |
| 367(e3, 0) | 355(a', 0) | 348(b, 0) | 348(b, 3) | 374(eg, 0) | 356(a', 0) | 350(au, 4) | 348(b2, 0) | 291(ag, 0) |
| 372(a2, 0) | 370(a", 2) | 354(a, 0) | 351(b, 0) | 374(eg, 0) | 370(a", 0) | 358(ag, 0) | 349(a2, 0) | 305(b2u, 3) |
| 374(b1, 0) | 371(a", 0) | 360(b, 1) | 360(a, 0) | 374(a1u, 0) | 372(a', 3) | 360(bu, 1) | 355(a1, 0) | 352(b3g, 0) |
| 377(e1, 5) | 372(a', 3) | 375(a, 0) | 376(b, 5) | 376(eu, 5) | 373(a", 2) | 380(ag, 0) | 380(a1, 0) | 366(b1u, 4) |
| 377(e1, 5) | 380(a', 2) | 379(b, 5) | 379(a, 0) | 376(eu, 5) | 384(a', 3) | 382(bu, 7) | 383(b2, 5) | 398(au, 0) |
| 417(b2, 9) | 405(a", 0) | 399(b, 0) | 399(a, 0) | 413(a2u, 8) | 405(a", 0) | 401(bg, 0) | 401(a2, 0) | 414(b2g, 0) |
| 423(b2, 2) | 419(a', 7) | 412(a, 0) | 411(b, 0) | 420(b1g, 0) | 415(a', 6) | 408(au, 0) | 409(b1, 0) | 415(b3u, 10) |
| 423(a1, 0) | 425(a', 1) | 424(b, 7) | 424(b, 7) | 420(a1g, 0) | 418(a', 0) | 420(ag, 0) | 422(b2, 8) | 420(ag, 0) |
| 424(e2, 0) | 425(a", 0) | 424(a, 0) | 426(a, 2) | 422(b2u, 0) | 422(a', 2) | 421(bu, 8) | 424(a1, 1) | 445(b1u, 21) |
| 424(e2, 0) | 426(a', 0) | 436(b, 5) | 435(b, 2) | 432(a2u, 4) | 434(a', 1) | 432(ag, 0) | 437(a1, 5) | 456(b3u, 276) |
| 431(a1, 0) | 436(a', 4) | 437(a, 1) | 439(a, 6) | 434(a1g, 0) | 437(a', 3) | 441(bu, 7) | 443(b2, 1) | 458(b2u, 0) |
| 454(e2, 0) | 453(a", 0) | 460(b, 0) | 462(a, 1) | 452(b1g, 0) | 459(a', 3) | 464(bg, 0) | 463(b1, 14) | 458(b3g, 0) |
| 454(e2, 0) | 462(a", 6) | 462(a, 8) | 463(b, 11) | 468(b2u, 0) | 465(a", 8) | 465(au, 14) | 464(a2, 0) | 468(b3u, 2) |
| 472(e3, 0) | 465(a', 7) | 463(a, 8) | 464(b, 5) | 479(eu, 13) | 470(a', 6) | 469(ag, 0) | 468(a1, 16) | 468(b1g, 0) |
| 472(e3, 0) | 471(a", 10) | 464(b, 18) | 466(a, 17) | 479(eu, 13) | 477(a", 7) | 472(bu, 11) | 471(b2, 0) | 477(b2u, 27) |
| 477(e1, 15) | 472(a', 10) | 488(b, 5) | 487(b, 4) | 479(eg, 0) | 477(a', 5) | 494(bu, 4) | 495(b2, 2) | 478(ag, 0) |
| 477(e1, 15) | 491(a', 2) | 496(a, 0) | 496(a, 0) | 479(eg, 0) | 496(a', 1) | 497(ag, 0) | 498(a1, 0) | 479(b1g, 0) |
| 510(e3, 0) | 513(a", 1) | 519(b, 0) | 518(a, 0) | 515(eg, 0) | 515(a', 0) | 520(bg, 0) | 522(b1, 1) | 484(b2g, 0) |
| 510(e3, 0) | 515(a', 0) | 522(a, 0) | 520(b, 0) | 515(eg, 0) | 516(a", 0) | 522(au, 0) | 522(a2, 0) | 510(b1u, 20) |
| 525(e1, 1) | 522(a", 0) | 533(b, 0) | 532(a, 0) | 523(eu, 0) | 522(a", 0) | 536(bg, 0) | 538(a2, 0) | 539(b3u, 4) |
| 525(e1, 1) | 536(a', 1) | 533(a, 0) | 532(b, 1) | 523(eu, 0) | 540(a", 0) | 538(ag, 0) | 539(b2, 1) | 544(ag, 0) |
| 540(e2, 0) | 537(a", 0) | 538(b, 1) | 540(a, 0) | 542(b2g, 0) | 540(a', 0) | 540(bu, 0) | 542(a1, 0) | 550(au, 0) |
| 540(e2, 0) | 539(a', 0) | 541(a, 0) | 541(b, 0) | 542(b1u, 0) | 542(a", 0) | 541(au, 1) | 544(b1, 1) | 554(b3g, 0) |
| 649(e3, 0) | 643(a", 49) | 643(b, 6) | 643(b, 67) | 650(eg, 0) | 645(a", 49) | 644(bg, 0) | 646(b2, 18) | 615(b2g, 0) |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 649(e3, 0) | 646(a', 65) | 643(a, 98) | 644(a, 6) | 650(eg, 0) | 648(a', 8) | 645(au, 139) | 647(a2, 0) | 633(b1u, 134) |
| 649(b2, 694) | 649(a", 93) | 646(a, 51) | 645(b, 112) | 654(eu, 143) | 650(a", 93) | 646(ag, 0) | 647(b1, 141) | 654(b2u, 153) |
| 652(e1, 140) | 650(a', 289) | 648(b, 185) | 648(a, 170) | 654(eu, 143) | 651(a', 161) | 649(bu, 183) | 651(a1, 181) | 655(b3u, 408) |
| 652(e1, 140) | 650(a', 380) | 653(b, 468) | 653(b, 456) | 661(a2u, 700) | 661(a', 566) | 662(bu, 493) | 664(b2, 474) | 656(b1g, 0) |
| 671(a1, 0) | 669(a', 13) | 671(a, 1) | 672(a, 3) | 672(a1g, 0) | 674(a', 22) | 674(ag, 0) | 675(a1, 6) | 671(ag, 0) |
| 1308(b2, 1758) | 1300(a', 684) | 1301(b, 1057) | 1289(b, 228) | 1310(a2u, 1753) | 1302(a', 706) | 1304(bu, 1251) | 1280(b2, 75) | 1125(b2u, 852) |
| 1317(a1, 0) | 1313(a', 752) | 1302(a, 165) | 1316(a, 859) | 1319(a1g, 0) | 1315(a', 736) | 1304(ag, 0) | 1320(a1, 923) | 1165(ag, 0) |
| 1970(e3, 0) | 1969(a", 18) | 1971(b, 84) | 1972(a, 88) | 1970(eg, 0) | 1969(a", 11) | 1969(bg, 0) | 1970(a2, 0) | 1975(b2g, 0) |
| 1970(e3, 0) | 1977(a', 110) | 1980(b, 824) | 1975(b, 411) | 1970(eg, 0) | 1976(a', 66) | 1979(bu, 604) | 1976(b2, 287) | 1999(b1g, 0) |
| 2001(e1, 2113) | 1985(a', 453) | 1985(a, 156) | 1988(a, 35) | 1993(b2u, 0) | 1985(a', 301) | 1986(ag, 0) | 1986(b2, 290) | 2001(b3u, 455) |
| 2001(e1, 2113) | 2001(a", 2023) | 1990(a, 222) | 1989(b, 599) | 2004(eu, 2085) | 1997(a', 847) | 1995(bu, 664) | 1989(a1, 43) | 2004(b2u, 1105) |
| 2004(e2, 0) | 2001(a', 1152) | 2003(a, 1451) | 2001(b, 1620) | 2004(eu, 2085) | 2004(a", 2069) | 1997(ag, 0) | 2004(b1, 2074) | 2004(b1u, 2108) |
| 2004(e2, 0) | 2006(a", 49) | 2003(b, 799) | 2003(a, 778) | 2014(a2u, 286) | 2012(a', 553) | 2003(au, 2075) | 2011(a1, 748) | 2010(ag, 0) |
| 2013(b2, 175) | 2020(a', 765) | 2023(b, 1393) | 2023(b, 1245) | 2016(b1g, 0) | 2021(a', 771) | 2023(bu, 1698) | 2022(b2, 1505) | 2044(b3u, 1422) |
| 2074(a1, 0) | 2069(a', 225) | 2064(a, 106) | 2067(a, 455) | 2074(a1g, 0) | 2069(a', 228) | 2064(ag, 0) | 2069(a1, 440) | 2075(ag, 0) |

**Table S2.** The theoretical harmonic vibrational frequencies (in $cm^{-1}$) for $Mn_2(CS)_2(CO)_7$ using the BP86/DZP method (infrared intensities in parentheses are in km/mol).

| **7-1**($C_s$) | **7-2**($C_s$) | **7-3**($C_s$) | **7-4**($C_1$) | **7-5**($C_s$) | **7-6**($C_s$) | **7-7**($C_s$) |
|---|---|---|---|---|---|---|
| 17(a", 0) | 19(a", 0) | 20(a", 0) | 17(a, 0) | 17(a", 0) | 21(a", 0) | 9(a", 0) |
| 44(a', 0) | 39(a', 0) | 42(a', 0) | 44(a, 0) | 42(a', 1) | 36(a', 0) | 16(a", 0) |
| 52(a', 0) | 49(a', 0) | 47(a', 0) | 50(a, 0) | 54(a', 0) | 40(a', 0) | 23(a', 0) |
| 60(a", 0) | 53(a", 0) | 50(a", 0) | 56(a, 0) | 60(a', 0) | 46(a", 0) | 51(a', 0) |
| 62(a', 0) | 60(a', 0) | 62(a', 0) | 63(a, 0) | 64(a", 0) | 55(a', 0) | 54(a", 0) |
| 69(a", 0) | 71(a", 0) | 70(a", 0) | 69(a, 0) | 69(a", 0) | 70(a", 0) | 60(a", 0) |
| 75(a", 0) | 78(a", 0) | 81(a', 0) | 75(a, 0) | 70(a', 0) | 75(a', 0) | 64(a", 0) |
| 75(a', 0) | 80(a', 0) | 81(a", 0) | 80(a, 0) | 71(a", 0) | 75(a", 0) | 72(a', 1) |
| 87(a', 0) | 82(a', 0) | 85(a', 0) | 86(a, 0) | 77(a", 0) | 80(a', 0) | 82(a', 0) |
| 88(a", 0) | 90(a', 0) | 89(a", 0) | 87(a, 0) | 86(a', 0) | 86(a", 0) | 84(a", 0) |
| 93(a', 0) | 90(a", 0) | 91(a', 0) | 93(a, 0) | 92(a', 1) | 90(a', 0) | 86(a', 2) |
| 96(a', 0) | 94(a", 0) | 93(a", 0) | 97(a, 0) | 96(a', 0) | 92(a', 1) | 88(a", 0) |
| 98(a", 0) | 97(a', 0) | 93(a', 0) | 97(a, 1) | 100(a", 0) | 93(a", 0) | 91(a', 0) |
| 99(a', 0) | 99(a", 0) | 98(a', 1) | 99(a, 0) | 101(a', 0) | 95(a', 1) | 97(a', 1) |
| 107(a", 0) | 101(a', 0) | 105(a", 0) | 107(a, 0) | 105(a", 0) | 99(a", 0) | 97(a", 0) |
| 116(a", 0) | 124(a", 0) | 118(a", 0) | 120(a, 0) | 143(a", 0) | 146(a', 0) | 112(a', 0) |
| 158(a', 1) | 158(a', 1) | 154(a', 1) | 160(a, 1) | 150(a', 0) | 148(a", 0) | 123(a', 3) |
| 219(a', 1) | 231(a', 1) | 224(a', 2) | 228(a, 1) | 247(a', 3) | 250(a', 7) | 152(a', 2) |
| 336(a", 1) | 334(a", 1) | 336(a", 0) | 331(a, 1) | 340(a', 1) | 351(a', 2) | 330(a", 3) |
| 345(a', 4) | 345(a', 4) | 355(a', 6) | 359(a, 8) | 345(a", 1) | 361(a", 1) | 358(a', 0) |
| 383(a', 3) | 365(a', 6) | 382(a', 13) | 365(a, 0) | 372(a', 1) | 375(a', 1) | 363(a", 1) |
| 386(a", 2) | 379(a", 2) | 386(a", 4) | 375(a, 2) | 380(a", 3) | 376(a", 4) | 366(a', 5) |
| 393(a', 3) | 407(a", 0) | 396(a', 4) | 393(a, 3) | 387(a', 0) | 387(a", 0) | 374(a", 0) |
| 403(a", 0) | 410(a', 0) | 405(a", 1) | 394(a, 2) | 404(a", 0) | 405(a', 2) | 389(a', 4) |
| 414(a', 2) | 418(a', 3) | 410(a', 0) | 406(a, 1) | 411(a", 1) | 407(a", 0) | 395(a", 0) |
| 416(a", 2) | 424(a", 0) | 416(a", 1) | 427(a, 8) | 412(a', 4) | 411(a', 0) | 413(a", 0) |
| 430(a', 2) | 425(a', 1) | 429(a', 4) | 430(a, 3) | 429(a', 2) | 429(a', 0) | 416(a', 2) |
| 435(a', 1) | 436(a', 8) | 431(a', 2) | 442(a, 37) | 434(a', 3) | 430(a', 2) | 422(a', 8) |
| 452(a", 24) | 448(a', 30) | 452(a', 23) | 453(a, 15) | 442(a', 10) | 445(a', 8) | 444(a", 3) |
| 454(a', 5) | 450(a", 20) | 452(a", 22) | 458(a, 14) | 451(a", 29) | 458(a", 27) | 466(a', 27) |
| 457(a', 20) | 465(a', 12) | 459(a', 5) | 460(a, 0) | 467(a", 0) | 469(a', 18) | 475(a", 1) |
| 471(a", 3) | 475(a", 10) | 470(a", 5) | 475(a, 1) | 478(a', 6) | 473(a", 0) | 478(a', 6) |
| 480(a', 5) | 480(a', 2) | 486(a', 10) | 486(a, 1) | 481(a', 12) | 476(a', 32) | 482(a", 7) |
| 496(a', 1) | 488(a', 2) | 496(a', 2) | 495(a, 2) | 490(a', 8) | 485(a', 34) | 497(a', 7) |
| 500(a', 4) | 499(a', 0) | 502(a', 1) | 498(a, 5) | 505(a', 1) | 511(a', 2) | 509(a", 1) |
| 516(a', 5) | 517(a", 5) | 516(a', 7) | 514(a, 4) | 523(a", 0) | 519(a', 9) | 512(a', 4) |
| 527(a", 2) | 522(a', 7) | 526(a", 6) | 528(a, 3) | 528(a', 6) | 524(a", 3) | 524(a", 0) |
| 537(a", 1) | 530(a", 0) | 536(a", 1) | 550(a, 2) | 535(a", 0) | 535(a", 2) | 531(a', 93) |
| 558(a", 6) | 567(a", 2) | 557(a", 2) | 558(a, 3) | 555(a", 2) | 542(a", 1) | 539(a', 1) |
| 602(a", 39) | 612(a", 50) | 610(a", 27) | 609(a, 56) | 605(a", 40) | 619(a", 16) | 589(a", 19) |
| 630(a', 66) | 626(a", 70) | 634(a', 126) | 624(a, 75) | 629(a', 82) | 631(a", 98) | 611(a', 39) |
| 634(a", 81) | 640(a', 258) | 636(a", 92) | 635(a, 79) | 632(a", 76) | 635(a', 111) | 645(a", 83) |
| 652(a', 169) | 645(a', 14) | 654(a', 107) | 649(a, 137) | 651(a', 158) | 653(a', 434) | 647(a', 70) |
| 663(a', 91) | 656(a', 83) | 664(a', 107) | 663(a, 97) | 664(a', 113) | 661(a', 10) | 658(a', 308) |
| 669(a', 117) | 675(a', 120) | 670(a', 141) | 670(a, 123) | 667(a', 165) | 672(a', 89) | 680(a', 24) |

| | | | | | | |
|---|---|---|---|---|---|---|
| 1176(a', 320) | 1171(a', 394) | 1180(a', 355) | 1178(a, 334) | 1286(a', 105) | 1305(a', 1531) | 1278(a', 591) |
| 1300(a', 515) | 1313(a', 759) | 1311(a', 802) | 1297(a, 595) | 1322(a', 873) | 1315(a', 138) | 1309(a', 875) |
| 1972(a", 20) | 1963(a', 163) | 1966(a', 10) | 1964(a, 103) | 1774(a', 311) | 1766(a', 386) | 1957(a', 25) |
| 1976(a', 782) | 1971(a", 143) | 1973(a", 18) | 1978(a, 546) | 1971(a", 24) | 1970(a', 76) | 1962(a", 176) |
| 1990(a', 531) | 1989(a', 499) | 1981(a', 859) | 1983(a, 407) | 1983(a', 776) | 1973(a", 30) | 1981(a", 1556) |
| 1998(a', 109) | 2002(a", 2003) | 2001(a", 2130) | 1994(a, 1116) | 1991(a', 209) | 2000(a', 841) | 1982(a', 1136) |
| 2001(a", 2109) | 2004(a', 741) | 2002(a', 597) | 2002(a, 694) | 2001(a", 2117) | 2001(a", 2138) | 1997(a", 181) |
| 2029(a', 1133) | 2027(a', 644) | 2026(a', 493) | 2021(a, 1515) | 2025(a', 1001) | 2020(a', 181) | 2005(a', 937) |
| 2065(a', 68) | 2066(a', 348) | 2067(a', 420) | 2062(a, 415) | 2059(a', 160) | 2060(a', 182) | 2050(a', 374) |

**Table S3.** The theoretical harmonic vibrational frequencies (in $cm^{-1}$) for $Mn_2(CS)_2(CO)_6$ using the BP86/DZP method (infrared intensities in parentheses are in km/mol).

| **6-1**($C_1$) | **6-2**($C_s$) | **6-3**($C_s$) | **6-4**($C_2$) | **6-5**($C_{2v}$) | **6-6**($C_s$) | **6-7**($C_2$) |
|---|---|---|---|---|---|---|
| 14(a, 0) | 29(a", 0) | -12(a", 0) | 32(a, 0) | 32(b1, 0) | 8(a", 0) | 29(a, 0) |
| 46(a, 0) | 49(a", 0) | 41(a', 0) | 51(a, 0) | 48(a2, 0) | 23(a", 0) | 30(b, 0) |
| 51(a, 0) | 51(a', 0) | 42(a", 0) | 51(b, 0) | 58(b1, 0) | 39(a', 0) | 39(a, 0) |
| 63(a, 0) | 67(a", 0) | 60(a", 0) | 67(a, 0) | 63(b2, 0) | 56(a", 0) | 55(a, 0) |
| 66(a, 0) | 75(a', 0) | 61(a', 0) | 70(b, 0) | 81(b2, 0) | 56(a', 0) | 60(b, 0) |
| 68(a, 0) | 81(a', 0) | 65(a', 0) | 78(a, 0) | 82(a1, 1) | 72(a", 0) | 64(b, 0) |
| 73(a, 0) | 83(a", 0) | 70(a", 0) | 82(b, 0) | 88(b1, 0) | 75(a", 0) | 66(a, 0) |
| 77(a, 0) | 89(a', 0) | 75(a", 0) | 86(b, 0) | 94(b2, 0) | 76(a', 0) | 68(b, 2) |
| 86(a, 0) | 90(a", 0) | 76(a', 0) | 89(a, 0) | 97(a1, 0) | 83(a', 1) | 69(a, 0) |
| 90(a, 0) | 95(a', 0) | 89(a", 0) | 95(a, 0) | 100(b1, 0) | 91(a', 1) | 80(a, 0) |
| 91(a, 0) | 104(a', 0) | 90(a', 0) | 99(b, 0) | 100(a2, 0) | 92(a", 0) | 80(b, 1) |
| 99(a, 0) | 114(a", 0) | 96(a', 0) | 104(b, 0) | 106(b2, 0) | 93(a', 0) | 85(a, 0) |
| 102(a, 1) | 136(a', 0) | 101(a", 0) | 117(a, 0) | 142(b2, 0) | 114(a', 0) | 90(b, 0) |
| 104(a, 0) | 178(a", 0) | 102(a', 1) | 191(a, 0) | 193(a1, 2) | 121(a", 0) | 90(a, 0) |
| 165(a, 1) | 200(a', 1) | 160(a', 0) | 195(b, 2) | 209(a1, 4) | 167(a', 2) | 100(b, 6) |
| 246(a, 0) | 225(a', 2) | 246(a', 1) | 201(a, 1) | 269(b1, 0) | 209(a', 1) | 199(a, 0) |
| 332(a, 1) | 303(a", 1) | 329(a", 0) | 321(a, 0) | 273(b1, 1) | 306(a", 0) | 347(b, 3) |
| 345(a, 3) | 336(a", 0) | 373(a', 1) | 348(b, 11) | 306(a2, 0) | 353(a', 1) | 349(a, 1) |
| 366(a, 12) | 358(a', 13) | 379(a", 3) | 351(a, 1) | 340(a1, 37) | 368(a", 4) | 350(b, 7) |
| 385(a, 2) | 368(a', 6) | 401(a", 0) | 353(b, 8) | 380(b2, 3) | 381(a', 9) | 365(a, 5) |
| 399(a, 0) | 389(a", 1) | 405(a', 1) | 400(b, 8) | 389(b1, 1) | 398(a", 0) | 378(b, 1) |
| 411(a, 5) | 412(a", 2) | 411(a", 1) | 422(b, 0) | 413(a1, 1) | 401(a', 7) | 391(a, 0) |
| 428(a, 3) | 432(a", 0) | 411(a', 6) | 426(a, 3) | 420(b2, 4) | 417(a', 4) | 415(a, 0) |
| 441(a, 1) | 440(a', 14) | 428(a', 2) | 431(b, 18) | 431(a1, 3) | 418(a", 0) | 420(b, 27) |
| 450(a, 2) | 452(a", 3) | 434(a', 7) | 431(a, 0) | 437(b2, 29) | 420(a', 2) | 430(b, 2) |
| 454(a, 9) | 452(a', 8) | 457(a", 10) | 436(a, 3) | 445(a2, 0) | 447(a', 17) | 434(a, 1) |
| 463(a, 2) | 471(a', 3) | 457(a', 2) | 471(b, 6) | 460(b1, 14) | 451(a", 12) | 456(b, 6) |
| 481(a, 6) | 475(a", 0) | 482(a', 14) | 477(a, 0) | 465(b2, 16) | 476(a', 15) | 457(a, 5) |
| 492(a, 6) | 482(a', 4) | 490(a", 0) | 480(b, 4) | 469(a1, 66) | 486(a", 6) | 475(a, 1) |
| 500(a, 7) | 503(a", 1) | 493(a', 1) | 492(a, 0) | 483(b1, 3) | 498(a', 2) | 478(b, 2) |
| 508(a, 6) | 503(a', 7) | 514(a', 9) | 505(a, 7) | 497(a1, 0) | 502(a", 2) | 493(b, 211) |
| 517(a, 2) | 515(a', 8) | 520(a", 1) | 516(b, 1) | 515(a2, 0) | 514(a', 6) | 495(a, 0) |
| 527(a, 8) | 524(a", 3) | 523(a', 3) | 535(a, 7) | 520(a1, 7) | 519(a", 10) | 499(b, 0) |
| 552(a, 2) | 532(a', 9) | 553(a", 2) | 536(b, 6) | 540(b2, 12) | 543(a', 101) | 527(a, 2) |
| 576(a, 18) | 571(a", 27) | 585(a", 12) | 609(b, 12) | 601(b2, 64) | 581(a", 15) | 555(b, 43) |
| 597(a, 73) | 615(a', 61) | 596(a', 98) | 616(a, 74) | 615(b2, 24) | 611(a", 51) | 557(a, 31) |
| 635(a, 81) | 626(a', 157) | 633(a", 89) | 619(b, 110) | 631(a1, 171) | 630(a', 155) | 607(a, 53) |
| 639(a, 23) | 635(a", 72) | 660(a', 98) | 625(a, 27) | 636(b1, 24) | 636(a', 12) | 607(b, 53) |
| 663(a, 129) | 646(a', 101) | 665(a', 126) | 641(b, 204) | 653(a1, 7) | 649(a', 129) | 624(b, 172) |
| 673(a, 123) | 660(a', 38) | 682(a', 62) | 646(a, 0) | 672(b1, 57) | 681(a', 52) | 639(a, 0) |

| | | | | | | |
|---|---|---|---|---|---|---|
| 1150(a, 316) | 1146(a", 174) | 1140(a', 344) | 1157(a, 194) | 1125(b1, 349) | 1171(a', 309) | 1301(b, 953) |
| 1305(a, 515) | 1201(a', 360) | 1301(a', 754) | 1181(b, 408) | 1176(a1, 303) | 1306(a', 923) | 1305(a, 329) |
| 1951(a, 179) | 1965(a", 261) | 1947(a", 294) | 1970(b, 289) | 1958(b2, 384) | 1950(a', 12) | 1960(a, 559) |
| 1981(a, 787) | 1972(a', 366) | 1971(a', 67) | 1975(a, 37) | 1972(a1, 1145) | 1954(a", 431) | 1962(b, 922) |
| 1993(a, 890) | 1984(a', 708) | 1985(a', 1081) | 1980(a, 818) | 1983(a1, 112) | 1975(a', 1077) | 1975(b, 235) |
| 1997(a, 1297) | 1998(a", 847) | 1997(a", 1518) | 1990(b, 1145) | 1996(b2, 1812) | 1990(a", 1451) | 1981(a, 874) |
| 2007(a, 709) | 2010(a', 1894) | 2001(a', 463) | 2008(b, 1760) | 2021(a1, 1092) | 2008(a', 1077) | 1995(b, 1322) |
| 2060(a, 419) | 2047(a', 496) | 2060(a', 643) | 2045(a, 505) | 2055(a1, 13) | 2046(a', 212) | 2035(a, 161) |

**Table S4.** The theoretical harmonic vibrational frequencies (in $cm^{-1}$) for $Mn_2(CS)_2(CO)_5$ using the BP86/DZP method (infrared intensities in parentheses are in km/mol).

| **5-1**($C_1$) | **5-2**($C_s$) | **5-3**($C_1$) | **5-4**($C_1$) | **5-5**($C_1$) |
|---|---|---|---|---|
| 38(a, 1) | 30(a", 0) | 28(a, 0) | 30(a, 0) | 29(a, 0) |
| 48(a, 0) | 45(a', 0) | 30(a, 0) | 40(a, 0) | 37(a, 1) |
| 58(a, 0) | 53(a", 0) | 48(a, 0) | 57(a, 0) | 54(a, 0) |
| 69(a, 0) | 76(a', 0) | 53(a, 0) | 75(a, 0) | 64(a, 0) |
| 78(a, 0) | 80(a", 0) | 64(a, 0) | 77(a, 0) | 70(a, 2) |
| 83(a, 0) | 84(a', 0) | 67(a, 0) | 80(a, 0) | 75(a, 0) |
| 85(a, 1) | 91(a', 1) | 74(a, 0) | 86(a, 0) | 78(a, 0) |
| 91(a, 0) | 93(a", 0) | 84(a, 0) | 92(a, 1) | 85(a, 0) |
| 93(a, 0) | 99(a', 0) | 87(a, 0) | 95(a, 0) | 91(a, 0) |
| 95(a, 0) | 106(a", 0) | 91(a, 1) | 110(a, 0) | 93(a, 1) |
| 112(a, 0) | 132(a', 0) | 99(a, 0) | 143(a, 0) | 111(a, 0) |
| 173(a, 0) | 210(a', 1) | 113(a, 0) | 213(a, 0) | 133(a, 2) |
| 228(a, 2) | 229(a', 1) | 182(a, 2) | 230(a, 1) | 191(a, 1) |
| 236(a, 0) | 283(a", 0) | 249(a, 0) | 266(a, 2) | 211(a, 5) |
| 352(a, 4) | 288(a", 1) | 283(a, 0) | 314(a, 4) | 336(a, 1) |
| 358(a, 0) | 309(a", 0) | 355(a, 3) | 332(a, 2) | 361(a, 12) |
| 371(a, 2) | 357(a', 11) | 383(a, 1) | 343(a, 4) | 374(a, 5) |
| 390(a, 67) | 374(a', 6) | 395(a, 2) | 363(a, 7) | 397(a, 49) |
| 413(a, 3) | 392(a", 0) | 403(a, 3) | 398(a, 2) | 404(a, 5) |
| 416(a, 2) | 426(a', 4) | 409(a, 5) | 418(a, 9) | 407(a, 0) |
| 425(a, 3) | 435(a', 4) | 415(a, 1) | 431(a, 5) | 413(a, 8) |
| 429(a, 5) | 445(a', 8) | 442(a, 8) | 445(a, 24) | 427(a, 5) |
| 445(a, 21) | 461(a", 19) | 446(a, 8) | 460(a, 15) | 438(a, 3) |
| 466(a, 4) | 474(a", 0) | 469(a, 25) | 466(a, 15) | 454(a, 26) |
| 482(a, 25) | 483(a', 30) | 475(a, 2) | 478(a, 26) | 468(a, 56) |
| 503(a, 6) | 501(a', 6) | 486(a, 2) | 489(a, 8) | 501(a, 1) |
| 509(a, 1) | 513(a", 8) | 513(a, 9) | 496(a, 8) | 508(a, 2) |
| 525(a, 7) | 522(a", 3) | 520(a, 4) | 513(a, 10) | 514(a, 4) |
| 548(a, 9) | 525(a', 13) | 546(a, 2) | 526(a, 0) | 530(a, 9) |
| 575(a, 18) | 549(a', 7) | 572(a, 3) | 565(a, 6) | 564(a, 13) |
| 603(a, 53) | 576(a', 7) | 585(a, 34) | 574(a, 11) | 602(a, 50) |
| 618(a, 12) | 613(a', 81) | 599(a, 67) | 601(a, 83) | 615(a, 116) |
| 623(a, 98) | 632(a', 129) | 647(a, 31) | 623(a, 159) | 628(a, 39) |
| 653(a, 14) | 660(a', 20) | 668(a, 60) | 656(a, 48) | 656(a, 20) |
| 679(a, 88) | 680(a", 43) | 677(a, 46) | 683(a, 44) | 663(a, 153) |
| 1124(a, 125) | 1098(a", 268) | 1103(a, 417) | 1121(a, 410) | 1182(a, 285) |
| 1168(a, 376) | 1158(a', 296) | 1281(a, 430) | 1300(a, 796) | 1303(a, 892) |
| 1954(a, 410) | 1943(a', 409) | 1939(a, 364) | 1717(a, 297) | 1782(a, 384) |

| | | | | |
|---|---|---|---|---|
| 1980(a, 1440) | 1973(a', 961) | 1959(a, 485) | 1942(a, 453) | 1945(a, 536) |
| 1991(a, 970) | 1993(a', 1448) | 1964(a, 882) | 1993(a, 1281) | 1984(a, 1314) |
| 1992(a, 1120) | 1997(a', 917) | 1994(a, 1962) | 1997(a, 1259) | 1992(a, 1363) |
| 2047(a, 219) | 2045(a', 317) | 2016(a, 175) | 2038(a, 72) | 2037(a, 21) |

**Table S5**. The theoretical Cartesian coordinates (in Å) for the structure **28-1** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | 0.000000 | 0.000000 | 1.501301 |
| 2 | 25 | 0 | 0.000000 | 0.000000 | -1.501301 |
| 3 | 6 | 0 | 0.000000 | 0.000000 | 3.288083 |
| 4 | 6 | 0 | 0.000000 | -1.862028 | 1.385361 |
| 5 | 6 | 0 | -1.862028 | 0.000000 | 1.385361 |
| 6 | 6 | 0 | 1.862028 | 0.000000 | 1.385361 |
| 7 | 6 | 0 | 0.000000 | 1.862028 | 1.385361 |
| 8 | 6 | 0 | -1.316652 | 1.316652 | -1.385361 |
| 9 | 6 | 0 | -1.316652 | -1.316652 | -1.385361 |
| 10 | 6 | 0 | 0.000000 | 0.000000 | -3.288083 |
| 11 | 6 | 0 | 1.316652 | -1.316652 | -1.385361 |
| 12 | 6 | 0 | 1.316652 | 1.316652 | -1.385361 |
| 13 | 8 | 0 | 0.000000 | 3.016383 | 1.364243 |
| 14 | 8 | 0 | -3.016383 | 0.000000 | 1.364243 |
| 15 | 8 | 0 | -2.132905 | 2.132905 | -1.364243 |
| 16 | 8 | 0 | -2.132905 | -2.132905 | -1.364243 |
| 17 | 8 | 0 | 0.000000 | -3.016383 | 1.364243 |
| 18 | 8 | 0 | 2.132905 | -2.132905 | -1.364243 |
| 19 | 8 | 0 | 3.016383 | 0.000000 | 1.364243 |
| 20 | 8 | 0 | 2.132905 | 2.132905 | -1.364243 |
| 21 | 16 | 0 | 0.000000 | 0.000000 | 4.843617 |
| 22 | 16 | 0 | 0.000000 | 0.000000 | -4.843617 |

**Table S6**. The theoretical Cartesian coordinates (in Å) for the structure **8-2** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -0.320434 | -1.632130 | 0.000000 |
| 2 | 25 | 0 | -0.013431 | 1.368307 | 0.000000 |
| 3 | 6 | 0 | -1.332156 | 1.399839 | 1.321344 |
| 4 | 6 | 0 | 1.510762 | -1.766978 | 0.000000 |
| 5 | 6 | 0 | 1.289109 | 1.113191 | 1.313185 |
| 6 | 6 | 0 | 0.180867 | 3.143593 | 0.000000 |
| 7 | 6 | 0 | -1.332156 | 1.399839 | -1.321344 |
| 8 | 6 | 0 | 1.289109 | 1.113191 | -1.313185 |
| 9 | 6 | 0 | -0.276355 | -1.500791 | -1.857686 |
| 10 | 6 | 0 | -2.163947 | -1.269447 | 0.000000 |
| 11 | 6 | 0 | -0.276355 | -1.500791 | 1.857686 |
| 12 | 6 | 0 | -0.547247 | -3.429089 | 0.000000 |
| 13 | 8 | 0 | -0.233616 | -1.458161 | -3.011104 |
| 14 | 8 | 0 | -3.304577 | -1.088358 | 0.000000 |
| 15 | 8 | 0 | -2.141792 | 1.468044 | 2.140997 |
| 16 | 8 | 0 | -0.669306 | -4.579761 | 0.000000 |
| 17 | 8 | 0 | -0.233616 | -1.458161 | 3.011104 |
| 18 | 8 | 0 | -2.141792 | 1.468044 | -2.140997 |
| 19 | 8 | 0 | 2.104044 | 1.013109 | 2.123924 |
| 20 | 8 | 0 | 2.104044 | 1.013109 | -2.123924 |
| 21 | 16 | 0 | 3.049092 | -1.979756 | 0.000000 |
| 22 | 16 | 0 | 0.352766 | 4.689587 | 0.000000 |

**Table S7**. The theoretical Cartesian coordinates (in Å) for the structure **8-3** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -0.010535 | 1.515368 | 0.117364 |
| 2 | 25 | 0 | 0.010535 | -1.515368 | 0.117364 |
| 3 | 6 | 0 | 0.022643 | 3.325588 | 0.127202 |
| 4 | 6 | 0 | -1.703912 | 1.460112 | -0.591409 |
| 5 | 6 | 0 | 0.680709 | 1.380283 | -1.609392 |
| 6 | 6 | 0 | -0.747063 | 1.389475 | 1.824757 |
| 7 | 6 | 0 | 1.721910 | 1.353126 | 0.831691 |
| 8 | 6 | 0 | 1.703912 | -1.460112 | -0.591409 |
| 9 | 6 | 0 | -0.680709 | -1.380283 | -1.609392 |
| 10 | 6 | 0 | -0.022643 | -3.325588 | 0.127202 |
| 11 | 6 | 0 | -1.721910 | -1.353126 | 0.831691 |
| 12 | 6 | 0 | 0.747063 | -1.389475 | 1.824757 |
| 13 | 8 | 0 | 2.788827 | 1.305865 | 1.269421 |
| 14 | 8 | 0 | 1.092689 | 1.341885 | -2.686994 |
| 15 | 8 | 0 | -1.092689 | -1.341885 | -2.686994 |
| 16 | 8 | 0 | -2.788827 | -1.305865 | 1.269421 |
| 17 | 8 | 0 | -1.220207 | 1.347204 | 2.877117 |
| 18 | 8 | 0 | 1.220207 | -1.347204 | 2.877117 |
| 19 | 8 | 0 | 0.022643 | 4.482737 | 0.124159 |
| 20 | 8 | 0 | -0.022643 | -4.482737 | 0.124159 |
| 21 | 16 | 0 | 3.133875 | -1.507130 | -1.193801 |
| 22 | 16 | 0 | -3.133875 | 1.507130 | -1.193801 |

**Table S8**. The theoretical Cartesian coordinates (in Å) for the structure **8-4** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -0.009313 | 1.518177 | -0.278307 |
| 2 | 25 | 0 | 0.009313 | -1.518177 | -0.278307 |
| 3 | 6 | 0 | 0.009313 | 3.328111 | -0.315828 |
| 4 | 6 | 0 | 1.688651 | 1.381076 | 0.479794 |
| 5 | 6 | 0 | -0.719584 | 1.473425 | 1.415082 |
| 6 | 6 | 0 | 0.722545 | 1.355074 | -2.002352 |
| 7 | 6 | 0 | -1.736614 | 1.387432 | -0.966136 |
| 8 | 6 | 0 | -1.688651 | -1.381076 | 0.479794 |
| 9 | 6 | 0 | 0.719584 | -1.473425 | 1.415082 |
| 10 | 6 | 0 | -0.009313 | -3.328111 | -0.315828 |
| 11 | 6 | 0 | 1.736614 | -1.387432 | -0.966136 |
| 12 | 6 | 0 | -0.722545 | -1.355074 | -2.002352 |
| 13 | 8 | 0 | -2.816938 | 1.341273 | -1.370912 |
| 14 | 8 | 0 | -2.732410 | -1.342609 | 0.971318 |
| 15 | 8 | 0 | 2.732410 | 1.342609 | 0.971318 |
| 16 | 8 | 0 | 2.816938 | -1.341273 | -1.370912 |
| 17 | 8 | 0 | 1.174289 | 1.298314 | -3.063263 |
| 18 | 8 | 0 | -1.174289 | -1.298314 | -3.063263 |
| 19 | 8 | 0 | 0.012557 | 4.485227 | -0.317716 |
| 20 | 8 | 0 | -0.012557 | -4.485227 | -0.317716 |
| 21 | 16 | 0 | 1.316263 | -1.538893 | 2.846181 |
| 22 | 16 | 0 | -1.316263 | 1.538893 | 2.846181 |

**Table S9**. The theoretical Cartesian coordinates (in Å) for the structure **8-5** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | 0.000000 | 0.000000 | 1.559176 |
| 2 | 25 | 0 | 0.000000 | 0.000000 | -1.559176 |
| 3 | 6 | 0 | 0.000000 | 0.000000 | 3.342019 |
| 4 | 6 | 0 | 0.000000 | 1.864003 | 1.481523 |
| 5 | 6 | 0 | 1.864003 | 0.000000 | 1.481523 |
| 6 | 6 | 0 | -1.864003 | 0.000000 | 1.481523 |
| 7 | 6 | 0 | 0.000000 | -1.864003 | 1.481523 |
| 8 | 6 | 0 | 1.864003 | 0.000000 | -1.481523 |
| 9 | 6 | 0 | 0.000000 | 1.864003 | -1.481523 |
| 10 | 6 | 0 | 0.000000 | 0.000000 | -3.342019 |
| 11 | 6 | 0 | -1.864003 | 0.000000 | -1.481523 |
| 12 | 6 | 0 | 0.000000 | -1.864003 | -1.481523 |
| 13 | 8 | 0 | 0.000000 | -3.017440 | 1.527074 |
| 14 | 8 | 0 | 3.017440 | 0.000000 | 1.527074 |
| 15 | 8 | 0 | 3.017440 | 0.000000 | -1.527074 |
| 16 | 8 | 0 | 0.000000 | 3.017440 | -1.527074 |
| 17 | 8 | 0 | 0.000000 | 3.017440 | 1.527074 |
| 18 | 8 | 0 | -3.017440 | 0.000000 | -1.527074 |
| 19 | 8 | 0 | -3.017440 | 0.000000 | 1.527074 |
| 20 | 8 | 0 | 0.000000 | -3.017440 | -1.527074 |
| 21 | 16 | 0 | 0.000000 | 0.000000 | 4.897650 |
| 22 | 16 | 0 | 0.000000 | 0.000000 | -4.897650 |

**Table S10**. The theoretical Cartesian coordinates (in Å) for the structure **8-6** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -0.325078 | -1.686121 | 0.000000 |
| 2 | 25 | 0 | -0.007980 | 1.442483 | 0.000000 |
| 3 | 6 | 0 | -1.866910 | 1.605245 | 0.000000 |
| 4 | 6 | 0 | 1.500455 | -1.896251 | 0.000000 |
| 5 | 6 | 0 | -0.016441 | 1.364044 | 1.865115 |
| 6 | 6 | 0 | 0.208478 | 3.211105 | 0.000000 |
| 7 | 6 | 0 | -0.016441 | 1.364044 | -1.865115 |
| 8 | 6 | 0 | 1.835382 | 1.147965 | 0.000000 |
| 9 | 6 | 0 | -0.276360 | -1.594506 | -1.860138 |
| 10 | 6 | 0 | -2.171420 | -1.337452 | 0.000000 |
| 11 | 6 | 0 | -0.276360 | -1.594506 | 1.860138 |
| 12 | 6 | 0 | -0.583273 | -3.473743 | 0.000000 |
| 13 | 8 | 0 | -0.232806 | -1.622715 | -3.013691 |
| 14 | 8 | 0 | -3.319912 | -1.216703 | 0.000000 |
| 15 | 8 | 0 | -3.004254 | 1.799851 | 0.000000 |
| 16 | 8 | 0 | -0.724708 | -4.622369 | 0.000000 |
| 17 | 8 | 0 | -0.232806 | -1.622715 | 3.013691 |
| 18 | 8 | 0 | -0.010354 | 1.409472 | -3.018139 |
| 19 | 8 | 0 | -0.010354 | 1.409472 | 3.018139 |
| 20 | 8 | 0 | 2.987145 | 1.074702 | 0.000000 |
| 21 | 16 | 0 | 3.016802 | -2.226964 | 0.000000 |
| 22 | 16 | 0 | 0.401209 | 4.754671 | 0.000000 |

**Table S11**. The theoretical Cartesian coordinates (in Å) for the structure **8-7** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -0.071656 | 1.585302 | 0.000000 |
| 2 | 25 | 0 | 0.071656 | -1.585302 | 0.000000 |
| 3 | 6 | 0 | -0.272214 | 3.379553 | 0.000000 |
| 4 | 6 | 0 | 1.758711 | 1.746830 | 0.000000 |
| 5 | 6 | 0 | -0.024010 | 1.490359 | 1.861122 |
| 6 | 6 | 0 | -0.024010 | 1.490359 | -1.861122 |
| 7 | 6 | 0 | -1.930818 | 1.303894 | 0.000000 |
| 8 | 6 | 0 | 0.024010 | -1.490359 | 1.861122 |
| 9 | 6 | 0 | 1.930818 | -1.303894 | 0.000000 |
| 10 | 6 | 0 | 0.272214 | -3.379553 | 0.000000 |
| 11 | 6 | 0 | 0.024010 | -1.490359 | -1.861122 |
| 12 | 6 | 0 | -1.758711 | -1.746830 | 0.000000 |
| 13 | 8 | 0 | -3.083818 | 1.244029 | 0.000000 |
| 14 | 8 | 0 | 0.024010 | 1.515450 | 3.014164 |
| 15 | 8 | 0 | -0.024010 | -1.515450 | 3.014164 |
| 16 | 8 | 0 | 3.083818 | -1.244029 | 0.000000 |
| 17 | 8 | 0 | -0.024010 | -1.515450 | -3.014164 |
| 18 | 8 | 0 | 0.024010 | 1.515450 | -3.014164 |
| 19 | 8 | 0 | -0.378518 | 4.531932 | 0.000000 |
| 20 | 8 | 0 | 0.378518 | -4.531932 | 0.000000 |
| 21 | 16 | 0 | 3.283694 | 2.031155 | 0.000000 |
| 22 | 16 | 0 | -3.283694 | -2.031155 | 0.000000 |

**Table S12**. The theoretical Cartesian coordinates (in Å) for the structure **8-8** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | 0.000000 | 1.597965 | -0.298266 |
| 2 | 25 | 0 | 0.000000 | -1.597965 | -0.298266 |
| 3 | 6 | 0 | 0.000000 | 3.402214 | -0.345742 |
| 4 | 6 | 0 | 0.000000 | 1.596431 | 1.538893 |
| 5 | 6 | 0 | -1.861400 | 1.497751 | -0.260716 |
| 6 | 6 | 0 | 1.861400 | 1.497751 | -0.260716 |
| 7 | 6 | 0 | 0.000000 | 1.476639 | -2.173520 |
| 8 | 6 | 0 | -1.861400 | -1.497751 | -0.260716 |
| 9 | 6 | 0 | 0.000000 | -1.596431 | 1.538893 |
| 10 | 6 | 0 | 0.000000 | -3.402214 | -0.345742 |
| 11 | 6 | 0 | 1.861400 | -1.497751 | -0.260716 |
| 12 | 6 | 0 | 0.000000 | -1.476639 | -2.173520 |
| 13 | 8 | 0 | 0.000000 | 1.498891 | -3.327628 |
| 14 | 8 | 0 | -3.014530 | 1.515865 | -0.215389 |
| 15 | 8 | 0 | -3.014530 | -1.515865 | -0.215389 |
| 16 | 8 | 0 | 3.014530 | -1.515865 | -0.215389 |
| 17 | 8 | 0 | 3.014530 | 1.515865 | -0.215389 |
| 18 | 8 | 0 | 0.000000 | -1.498891 | -3.327628 |
| 19 | 8 | 0 | 0.000000 | 4.559442 | -0.348135 |
| 20 | 8 | 0 | 0.000000 | -4.559442 | -0.348135 |
| 21 | 16 | 0 | 0.000000 | -1.754136 | 3.082486 |
| 22 | 16 | 0 | 0.000000 | 1.754136 | 3.082486 |

**Table S13**. The theoretical Cartesian coordinates (in Å) for the structure **8-9** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -1.389023 | 0.000000 | 0.000000 |
| 2 | 25 | 0 | 1.389023 | 0.000000 | 0.000000 |
| 3 | 6 | 0 | 0.000000 | 1.539880 | 0.000000 |
| 4 | 6 | 0 | 0.000000 | -1.539880 | 0.000000 |
| 5 | 6 | 0 | 1.478322 | 0.000000 | 1.873957 |
| 6 | 6 | 0 | 2.642548 | 1.345198 | 0.000000 |
| 7 | 6 | 0 | 1.478322 | 0.000000 | -1.873957 |
| 8 | 6 | 0 | 2.642548 | -1.345198 | 0.000000 |
| 9 | 6 | 0 | -1.478322 | 0.000000 | -1.873957 |
| 10 | 6 | 0 | -2.642548 | 1.345198 | 0.000000 |
| 11 | 6 | 0 | -1.478322 | 0.000000 | 1.873957 |
| 12 | 6 | 0 | -2.642548 | -1.345198 | 0.000000 |
| 13 | 8 | 0 | -1.622994 | 0.000000 | -3.016495 |
| 14 | 8 | 0 | -3.420767 | 2.196397 | 0.000000 |
| 15 | 8 | 0 | -3.420767 | -2.196397 | 0.000000 |
| 16 | 8 | 0 | -1.622994 | 0.000000 | 3.016495 |
| 17 | 8 | 0 | 1.622994 | 0.000000 | -3.016495 |
| 18 | 8 | 0 | 1.622994 | 0.000000 | 3.016495 |
| 19 | 8 | 0 | 3.420767 | -2.196397 | 0.000000 |
| 20 | 8 | 0 | 3.420767 | 2.196397 | 0.000000 |
| 21 | 16 | 0 | 0.000000 | 3.129433 | 0.000000 |
| 22 | 16 | 0 | 0.000000 | -3.129433 | 0.000000 |

**Table S14**. The theoretical Cartesian coordinates (in Å) for the structure **7-1** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | 0.537537 | 1.294950 | 0.000000 |
| 2 | 25 | 0 | -0.214811 | -1.587470 | 0.000000 |
| 3 | 6 | 0 | 0.483945 | 1.338721 | 1.876215 |
| 4 | 6 | 0 | 0.483945 | 1.338721 | -1.876215 |
| 5 | 6 | 0 | 1.125985 | 3.025471 | 0.000000 |
| 6 | 6 | 0 | -1.209695 | 1.680734 | 0.000000 |
| 7 | 6 | 0 | -2.080795 | -1.543310 | 0.000000 |
| 8 | 6 | 0 | -0.221216 | -1.650181 | 1.863719 |
| 9 | 6 | 0 | -0.221216 | -1.650181 | -1.863719 |
| 10 | 6 | 0 | 1.356756 | -0.686001 | 0.000000 |
| 11 | 6 | 0 | 0.126390 | -3.367432 | 0.000000 |
| 12 | 8 | 0 | 1.493177 | 4.121256 | 0.000000 |
| 13 | 8 | 0 | 0.411440 | 1.449484 | -3.020822 |
| 14 | 8 | 0 | 0.411440 | 1.449484 | 3.020822 |
| 15 | 8 | 0 | -0.221216 | -1.751010 | 3.012451 |
| 16 | 8 | 0 | 0.404365 | -4.491367 | 0.000000 |
| 17 | 8 | 0 | -3.233197 | -1.471415 | 0.000000 |
| 18 | 8 | 0 | -0.221216 | -1.751010 | -3.012451 |
| 19 | 16 | 0 | 2.738912 | 0.131330 | 0.000000 |
| 20 | 16 | 0 | -2.707106 | 2.115568 | 0.000000 |

**Table S15**. The theoretical Cartesian coordinates (in Å) for the structure **7-2** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -0.109223 | -1.664740 | 0.000000 |
| 2 | 25 | 0 | 0.148120 | 1.304232 | 0.000000 |
| 3 | 6 | 0 | -0.088617 | -1.697541 | 1.876283 |
| 4 | 6 | 0 | -0.088617 | -1.697541 | -1.876283 |
| 5 | 6 | 0 | -0.335897 | -3.477845 | 0.000000 |
| 6 | 6 | 0 | 1.706452 | -1.659620 | 0.000000 |
| 7 | 6 | 0 | 2.002105 | 1.557943 | 0.000000 |
| 8 | 6 | 0 | 0.116030 | 1.398760 | 1.862573 |
| 9 | 6 | 0 | 0.116030 | 1.398760 | -1.862573 |
| 10 | 6 | 0 | -1.241689 | 0.141288 | 0.000000 |
| 11 | 6 | 0 | -0.441588 | 2.989795 | 0.000000 |
| 12 | 8 | 0 | -0.492181 | -4.623580 | 0.000000 |
| 13 | 8 | 0 | -0.048149 | -1.783203 | -3.024999 |
| 14 | 8 | 0 | -0.048149 | -1.783203 | 3.024999 |
| 15 | 8 | 0 | 0.070251 | 1.530035 | 3.006863 |
| 16 | 8 | 0 | 3.148649 | 1.688033 | 0.000000 |
| 17 | 8 | 0 | 2.865222 | -1.704794 | 0.000000 |
| 18 | 8 | 0 | 0.070251 | 1.530035 | -3.006863 |
| 19 | 16 | 0 | -2.465553 | -0.900695 | 0.000000 |
| 20 | 16 | 0 | -1.032250 | 4.429579 | 0.000000 |

**Table S16**. The theoretical Cartesian coordinates (in Å) for the structure **7-3** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic \Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | 0.039435 | 1.228758 | 0.000000 |
| 2 | 25 | 0 | 0.025120 | -1.748251 | 0.000000 |
| 3 | 6 | 0 | 0.031758 | 1.300585 | 1.876645 |
| 4 | 6 | 0 | 0.031758 | 1.300585 | -1.876645 |
| 5 | 6 | 0 | 0.088145 | 3.024528 | 0.000000 |
| 6 | 6 | 0 | -1.771931 | 1.077160 | 0.000000 |
| 7 | 6 | 0 | -1.798784 | -2.145276 | 0.000000 |
| 8 | 6 | 0 | 0.031758 | -1.795189 | 1.863698 |
| 9 | 6 | 0 | 0.031758 | -1.795189 | -1.863698 |
| 10 | 6 | 0 | 1.336375 | -0.504902 | 0.000000 |
| 11 | 6 | 0 | 0.769545 | -3.402488 | 0.000000 |
| 12 | 8 | 0 | -0.000313 | 1.432139 | -3.020772 |
| 13 | 8 | 0 | -0.000313 | 1.432139 | 3.020772 |
| 14 | 8 | 0 | 0.054105 | -1.874326 | 3.014059 |
| 15 | 8 | 0 | 1.303176 | -4.429804 | 0.000000 |
| 16 | 8 | 0 | -2.935193 | -2.350599 | 0.000000 |
| 17 | 8 | 0 | -2.930174 | 1.042720 | 0.000000 |
| 18 | 8 | 0 | 0.054105 | -1.874326 | -3.014059 |
| 19 | 16 | 0 | 2.454720 | 0.647145 | 0.000000 |
| 20 | 16 | 0 | 0.140323 | 4.578161 | 0.000000 |

**Table S17**. The theoretical Cartesian coordinates (in Å) for the structure **7-4** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -1.606723 | 0.119948 | -0.054461 |
| 2 | 25 | 0 | 1.326704 | -0.383350 | -0.017272 |
| 3 | 6 | 0 | -1.340299 | 1.966023 | -0.075624 |
| 4 | 6 | 0 | -1.996474 | -1.702564 | -0.057891 |
| 5 | 6 | 0 | -3.209586 | 0.403442 | -0.851426 |
| 6 | 6 | 0 | -2.054611 | 0.210366 | 1.755798 |
| 7 | 6 | 0 | 1.153835 | -0.266003 | 1.785603 |
| 8 | 6 | 0 | 1.761789 | 1.400080 | -0.044892 |
| 9 | 6 | 0 | 1.014152 | -2.258077 | 0.076915 |
| 10 | 6 | 0 | 3.117657 | -0.727508 | -0.067916 |
| 11 | 8 | 0 | -4.204802 | 0.580189 | -1.416175 |
| 12 | 8 | 0 | -2.294360 | -2.816545 | -0.081921 |
| 13 | 8 | 0 | -1.247160 | 3.114853 | -0.107214 |
| 14 | 8 | 0 | 4.256589 | -0.921565 | -0.112350 |
| 15 | 8 | 0 | 1.094208 | -0.176449 | 2.939766 |
| 16 | 8 | 0 | -2.292453 | 0.259688 | 2.884674 |
| 17 | 8 | 0 | 0.909173 | -3.400407 | 0.179987 |
| 18 | 6 | 0 | -0.346758 | -0.120495 | -1.333989 |
| 19 | 16 | 0 | 0.788102 | -0.368682 | -2.440922 |
| 20 | 16 | 0 | 2.251441 | 2.870893 | -0.035346 |

**Table S18**. The theoretical Cartesian coordinates (in Å) for the structure **7-5** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -0.488386 | -1.486061 | 0.000000 |
| 2 | 25 | 0 | -0.452451 | 1.494136 | 0.000000 |
| 3 | 6 | 0 | -0.411176 | -1.494629 | 1.876265 |
| 4 | 6 | 0 | -0.411176 | -1.494629 | -1.876265 |
| 5 | 6 | 0 | -0.859048 | -3.272948 | 0.000000 |
| 6 | 6 | 0 | 1.285869 | -1.660539 | 0.000000 |
| 7 | 6 | 0 | 1.352351 | 1.780150 | 0.000000 |
| 8 | 6 | 0 | -0.378139 | 1.561727 | 1.858833 |
| 9 | 6 | 0 | -0.378139 | 1.561727 | -1.858833 |
| 10 | 6 | 0 | -1.805905 | 0.268628 | 0.000000 |
| 11 | 6 | 0 | -1.145373 | 3.176846 | 0.000000 |
| 12 | 8 | 0 | -1.072824 | -4.408580 | 0.000000 |
| 13 | 8 | 0 | -0.296012 | -1.580962 | -3.019488 |
| 14 | 8 | 0 | -0.296012 | -1.580962 | 3.019488 |
| 15 | 8 | 0 | -0.307585 | 1.671207 | 3.005321 |
| 16 | 8 | 0 | -1.605809 | 4.238285 | 0.000000 |
| 17 | 8 | 0 | -2.562342 | -0.653915 | 0.000000 |
| 18 | 8 | 0 | -0.307585 | 1.671207 | -3.005321 |
| 19 | 16 | 0 | 2.833206 | -1.833317 | 0.000000 |
| 20 | 16 | 0 | 2.892462 | 1.982684 | 0.000000 |

**Table S19**. The theoretical Cartesian coordinates (in Å) for the structure **7-6** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -0.138076 | -1.465987 | 0.000000 |
| 2 | 25 | 0 | 0.001505 | 1.501517 | 0.000000 |
| 3 | 6 | 0 | -0.113815 | -1.501045 | 1.878533 |
| 4 | 6 | 0 | -0.113815 | -1.501045 | -1.878533 |
| 5 | 6 | 0 | -0.484441 | -3.227098 | 0.000000 |
| 6 | 6 | 0 | 1.670229 | -1.613875 | 0.000000 |
| 7 | 6 | 0 | 1.853380 | 1.643936 | 0.000000 |
| 8 | 6 | 0 | 0.007602 | 1.595562 | 1.859527 |
| 9 | 6 | 0 | 0.007602 | 1.595562 | -1.859527 |
| 10 | 6 | 0 | -1.379910 | 0.323309 | 0.000000 |
| 11 | 6 | 0 | -0.547629 | 3.208283 | 0.000000 |
| 12 | 8 | 0 | -0.066404 | -1.609470 | -3.024498 |
| 13 | 8 | 0 | -0.066404 | -1.609470 | 3.024498 |
| 14 | 8 | 0 | 0.003920 | 1.725771 | 3.006022 |
| 15 | 8 | 0 | -2.177955 | -0.565883 | 0.000000 |
| 16 | 8 | 0 | 3.006679 | 1.717021 | 0.000000 |
| 17 | 8 | 0 | 2.821658 | -1.735081 | 0.000000 |
| 18 | 8 | 0 | 0.003920 | 1.725771 | -3.006022 |
| 19 | 16 | 0 | -1.079597 | 4.670669 | 0.000000 |
| 20 | 16 | 0 | -0.806920 | -4.746858 | 0.000000 |

**Table S20**. The theoretical Cartesian coordinates (in Å) for the structure **7-7** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | 0.328883 | -1.523225 | 0.000000 |
| 2 | 25 | 0 | 0.018950 | 1.256696 | 0.000000 |
| 3 | 6 | 0 | 0.483605 | -2.784886 | 1.292611 |
| 4 | 6 | 0 | 0.483605 | -2.784886 | -1.292611 |
| 5 | 6 | 0 | -1.494442 | -1.682071 | 0.000000 |
| 6 | 6 | 0 | 1.324151 | 1.296336 | 1.326940 |
| 7 | 6 | 0 | -1.257552 | 0.968383 | -1.325714 |
| 8 | 6 | 0 | -1.257552 | 0.968383 | 1.325714 |
| 9 | 6 | 0 | 1.324151 | 1.296336 | -1.326940 |
| 10 | 6 | 0 | 2.175735 | -1.168833 | 0.000000 |
| 11 | 6 | 0 | -0.207066 | 3.035234 | 0.000000 |
| 12 | 8 | 0 | 0.551702 | -3.552270 | 2.155912 |
| 13 | 8 | 0 | 0.551702 | -3.552270 | -2.155912 |
| 14 | 8 | 0 | 3.324904 | -1.049364 | 0.000000 |
| 15 | 8 | 0 | 2.120315 | 1.375020 | 2.161501 |
| 16 | 8 | 0 | -2.047745 | 0.859449 | -2.162116 |
| 17 | 8 | 0 | -2.047745 | 0.859449 | 2.162116 |
| 18 | 8 | 0 | 2.120315 | 1.375020 | -2.161501 |
| 19 | 16 | 0 | -3.016406 | -1.998408 | 0.000000 |
| 20 | 16 | 0 | -0.404294 | 4.578345 | 0.000000 |

**Table S21**. The theoretical Cartesian coordinates (in Å) for the structure **6-1** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | 1.495292 | 0.001890 | -0.062641 |
| 2 | 25 | 0 | -1.347226 | -0.517523 | -0.072227 |
| 3 | 6 | 0 | 1.777431 | -1.596084 | 0.860790 |
| 4 | 6 | 0 | 0.334726 | -0.828412 | -1.166591 |
| 5 | 6 | 0 | -1.820940 | 1.171196 | -0.066704 |
| 6 | 6 | 0 | -3.101171 | -1.041909 | 0.005757 |
| 7 | 6 | 0 | -1.132902 | -0.434581 | 1.719456 |
| 8 | 6 | 0 | 3.190507 | -0.098738 | -0.707725 |
| 9 | 6 | 0 | 1.748180 | 0.984599 | 1.504235 |
| 10 | 6 | 0 | 1.250250 | 1.587528 | -1.020720 |
| 11 | 8 | 0 | -1.050147 | -0.403497 | 2.876861 |
| 12 | 8 | 0 | -4.213219 | -1.352936 | 0.054263 |
| 13 | 8 | 0 | 1.973115 | -2.589763 | 1.411991 |
| 14 | 8 | 0 | 1.131586 | 2.557090 | -1.631329 |
| 15 | 8 | 0 | 1.856759 | 1.594701 | 2.478112 |
| 16 | 8 | 0 | 4.247075 | -0.198780 | -1.169826 |
| 17 | 16 | 0 | -0.783378 | -1.568721 | -2.081770 |
| 18 | 16 | 0 | -2.262840 | 2.667142 | -0.140722 |

**Table S22**. The theoretical Cartesian coordinates (in Å) for the structure **6-2** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | 0.042810 | 1.300387 | 0.000000 |
| 2 | 25 | 0 | -0.118316 | -1.482574 | 0.000000 |
| 3 | 6 | 0 | -0.943442 | -0.305783 | 1.117283 |
| 4 | 6 | 0 | -0.943442 | -0.305783 | -1.117283 |
| 5 | 6 | 0 | 1.058792 | -2.078752 | -1.330514 |
| 6 | 6 | 0 | 1.058792 | -2.078752 | 1.330514 |
| 7 | 6 | 0 | -1.187434 | -2.942920 | 0.000000 |
| 8 | 6 | 0 | 1.351747 | 1.319645 | 1.267803 |
| 9 | 6 | 0 | -0.158332 | 3.122499 | 0.000000 |
| 10 | 6 | 0 | 1.351747 | 1.319645 | -1.267803 |
| 11 | 8 | 0 | -1.936273 | -3.825846 | 0.000000 |
| 12 | 8 | 0 | 1.788542 | -2.413493 | -2.159312 |
| 13 | 8 | 0 | 1.788542 | -2.413493 | 2.159312 |
| 14 | 8 | 0 | 2.197800 | 1.344174 | -2.055867 |
| 15 | 8 | 0 | -0.284563 | 4.270948 | 0.000000 |
| 16 | 8 | 0 | 2.197800 | 1.344174 | 2.055867 |
| 17 | 16 | 0 | -1.676803 | 0.931380 | -1.809152 |
| 18 | 16 | 0 | -1.676803 | 0.931380 | 1.809152 |

**Table S23**. The theoretical Cartesian coordinates (in Å) for the structure **6-3** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -0.563896 | -1.524036 | 0.000000 |
| 2 | 25 | 0 | 0.646495 | 1.108438 | 0.000000 |
| 3 | 6 | 0 | 1.116949 | -0.878175 | 0.000000 |
| 4 | 6 | 0 | -0.612838 | -3.341847 | 0.000000 |
| 5 | 6 | 0 | -2.375638 | -1.084834 | 0.000000 |
| 6 | 8 | 0 | -3.483149 | -0.757350 | 0.000000 |
| 7 | 8 | 0 | -0.577842 | -4.498902 | 0.000000 |
| 8 | 16 | 0 | 2.588153 | -0.185334 | 0.000000 |
| 9 | 6 | 0 | 1.416555 | 2.732721 | 0.000000 |
| 10 | 6 | 0 | -0.543919 | 1.571416 | 1.270513 |
| 11 | 6 | 0 | -0.543919 | 1.571416 | -1.270513 |
| 12 | 16 | 0 | 2.081392 | 4.138065 | 0.000000 |
| 13 | 8 | 0 | -1.264753 | 1.892152 | 2.120813 |
| 14 | 8 | 0 | -1.264753 | 1.892152 | -2.120813 |
| 15 | 6 | 0 | -0.543919 | -1.558630 | -1.866481 |
| 16 | 6 | 0 | -0.543919 | -1.558630 | 1.866481 |
| 17 | 8 | 0 | -0.516865 | -1.612424 | -3.017645 |
| 18 | 8 | 0 | -0.516865 | -1.612424 | 3.017645 |

**Table S24**. The theoretical Cartesian coordinates (in Å) for the structure **6-4** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | 0.031027 | 1.386926 | -0.047942 |
| 2 | 25 | 0 | -0.031027 | -1.386926 | -0.047942 |
| 3 | 6 | 0 | 1.139327 | -0.316244 | -0.930480 |
| 4 | 6 | 0 | -1.139327 | 0.316244 | -0.930480 |
| 5 | 6 | 0 | 1.143123 | -1.549328 | 1.326664 |
| 6 | 6 | 0 | -1.425303 | -1.837297 | 1.144233 |
| 7 | 6 | 0 | 0.313586 | -3.052874 | -0.697852 |
| 8 | 6 | 0 | -0.313586 | 3.052874 | -0.697852 |
| 9 | 6 | 0 | 1.425303 | 1.837297 | 1.144233 |
| 10 | 6 | 0 | -1.143123 | 1.549328 | 1.326664 |
| 11 | 8 | 0 | 0.576056 | -4.084806 | -1.150421 |
| 12 | 8 | 0 | 1.892089 | -1.657297 | 2.202305 |
| 13 | 8 | 0 | -2.255948 | -2.091554 | 1.902903 |
| 14 | 8 | 0 | -1.892089 | 1.657297 | 2.202305 |
| 15 | 8 | 0 | 2.255948 | 2.091554 | 1.902903 |
| 16 | 8 | 0 | -0.576056 | 4.084806 | -1.150421 |
| 17 | 16 | 0 | 1.892089 | 0.848016 | -1.718445 |
| 18 | 16 | 0 | -1.892089 | -0.848016 | -1.718445 |

**Table S25**. The theoretical Cartesian coordinates (in Å) for the structure **6-5** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | 0.000000 | 0.000000 | 1.492699 |
| 2 | 25 | 0 | 0.000000 | 0.000000 | -1.224019 |
| 3 | 6 | 0 | 0.000000 | 1.853703 | 1.681057 |
| 4 | 6 | 0 | -1.464931 | 0.000000 | 0.458629 |
| 5 | 6 | 0 | 1.464931 | 0.000000 | 0.458629 |
| 6 | 6 | 0 | 0.000000 | 0.000000 | 3.339940 |
| 7 | 6 | 0 | 0.000000 | -1.883921 | -1.346072 |
| 8 | 6 | 0 | 0.000000 | 1.883921 | -1.346072 |
| 9 | 6 | 0 | 0.000000 | 0.000000 | -3.052306 |
| 10 | 6 | 0 | 0.000000 | -1.853703 | 1.681057 |
| 11 | 8 | 0 | 0.000000 | 2.992031 | 1.868864 |
| 12 | 8 | 0 | 0.000000 | 0.000000 | 4.497697 |
| 13 | 8 | 0 | 0.000000 | -2.992031 | 1.868864 |
| 14 | 8 | 0 | 0.000000 | 0.000000 | -4.209500 |
| 15 | 8 | 0 | 0.000000 | 3.020873 | -1.530558 |
| 16 | 8 | 0 | 0.000000 | -3.020873 | -1.530558 |
| 17 | 16 | 0 | -2.457835 | 0.000000 | -0.802645 |
| 18 | 16 | 0 | 2.457835 | 0.000000 | -0.802645 |

**Table S26**. The theoretical Cartesian coordinates (in Å) for the structure **6-6** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -0.018939 | 1.098670 | 0.000000 |
| 2 | 6 | 0 | -0.004840 | 1.093559 | 1.879361 |
| 3 | 6 | 0 | -1.353996 | -0.473452 | 0.000000 |
| 4 | 6 | 0 | 1.773503 | 0.828219 | 0.000000 |
| 5 | 6 | 0 | -0.004840 | 1.093559 | -1.879361 |
| 6 | 6 | 0 | 0.054157 | 2.913771 | 0.000000 |
| 7 | 6 | 0 | 1.786623 | -2.278646 | 0.000000 |
| 8 | 8 | 0 | 2.932758 | 0.761906 | 0.000000 |
| 9 | 8 | 0 | 0.030176 | 1.134932 | -3.030959 |
| 10 | 8 | 0 | 0.030176 | 1.134932 | 3.030959 |
| 11 | 8 | 0 | 2.865651 | -2.690752 | 0.000000 |
| 12 | 16 | 0 | -2.483412 | 0.664951 | 0.000000 |
| 13 | 16 | 0 | 0.115858 | 4.464488 | 0.000000 |
| 14 | 25 | 0 | 0.011912 | -1.666725 | 0.000000 |
| 15 | 6 | 0 | -0.574143 | -2.807894 | -1.269796 |
| 16 | 6 | 0 | -0.574143 | -2.807894 | 1.269796 |
| 17 | 8 | 0 | -0.964219 | -3.497820 | -2.114968 |
| 18 | 8 | 0 | -0.964219 | -3.497820 | 2.114968 |

**Table S27**. The theoretical Cartesian coordinates (in Å) for the structure **6-7** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | 0.014795 | 1.194443 | 0.218938 |
| 2 | 25 | 0 | -0.014795 | -1.194443 | 0.218938 |
| 3 | 6 | 0 | 1.278510 | -1.003397 | -1.104000 |
| 4 | 6 | 0 | -1.278510 | 1.003397 | -1.104000 |
| 5 | 6 | 0 | 0.793869 | -2.588178 | 1.084438 |
| 6 | 6 | 0 | -1.327883 | -0.907284 | 1.501912 |
| 7 | 6 | 0 | -1.008793 | -2.332909 | -0.727651 |
| 8 | 6 | 0 | 1.008793 | 2.332909 | -0.727651 |
| 9 | 6 | 0 | 1.327883 | 0.907284 | 1.501912 |
| 10 | 6 | 0 | -0.793869 | 2.588178 | 1.084438 |
| 11 | 8 | 0 | 1.327883 | -3.441511 | 1.653368 |
| 12 | 8 | 0 | -2.168930 | -0.807911 | 2.292208 |
| 13 | 8 | 0 | 2.070845 | -0.956770 | -1.946031 |
| 14 | 8 | 0 | -2.070845 | 0.956770 | -1.946031 |
| 15 | 8 | 0 | -1.327883 | 3.441511 | 1.653368 |
| 16 | 8 | 0 | 2.168930 | 0.807911 | 2.292208 |
| 17 | 16 | 0 | 1.940981 | 3.197578 | -1.624876 |
| 18 | 16 | 0 | -1.940981 | -3.197578 | -1.624876 |

**Table S28**. The theoretical Cartesian coordinates (in Å) for the structure **5-1** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -1.348186 | -0.172749 | -0.032344 |
| 2 | 25 | 0 | 1.227430 | -0.022246 | -0.004622 |
| 3 | 6 | 0 | -2.040342 | 1.474714 | -0.164544 |
| 4 | 6 | 0 | -0.370303 | 0.234425 | 1.382843 |
| 5 | 6 | 0 | 2.999467 | -0.071219 | -0.483178 |
| 6 | 6 | 0 | 1.443084 | -1.808909 | 0.530303 |
| 7 | 6 | 0 | 1.244639 | 1.798655 | -0.498946 |
| 8 | 6 | 0 | -2.967857 | -0.819563 | 0.536049 |
| 9 | 8 | 0 | -3.958241 | -1.252420 | 0.949773 |
| 10 | 8 | 0 | -2.464344 | 2.548322 | -0.272928 |
| 11 | 8 | 0 | 1.637437 | -2.906117 | 0.825019 |
| 12 | 8 | 0 | 1.303935 | 2.898961 | -0.831495 |
| 13 | 8 | 0 | 4.095723 | -0.119193 | -0.850345 |
| 14 | 6 | 0 | 0.159478 | -0.503334 | -1.353062 |
| 15 | 16 | 0 | -1.067982 | -1.019080 | -2.278288 |
| 16 | 16 | 0 | 0.773844 | 0.624695 | 2.444986 |

**Table S29**. The theoretical Cartesian coordinates (in Å) for the structure **5-2** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -0.309187 | 1.356933 | 0.000000 |
| 2 | 25 | 0 | 0.115966 | -1.233187 | 0.000000 |
| 3 | 6 | 0 | 1.509039 | 1.816928 | 0.000000 |
| 4 | 6 | 0 | -2.159015 | 1.218500 | 0.000000 |
| 5 | 6 | 0 | -0.621495 | 3.179539 | 0.000000 |
| 6 | 6 | 0 | -0.196815 | 0.295301 | 1.438539 |
| 7 | 6 | 0 | -0.196815 | 0.295301 | -1.438539 |
| 8 | 6 | 0 | 1.890321 | -1.418729 | 0.000000 |
| 9 | 6 | 0 | -0.093870 | -3.060133 | 0.000000 |
| 10 | 8 | 0 | -0.816850 | 4.321012 | 0.000000 |
| 11 | 8 | 0 | 2.613842 | 2.144504 | 0.000000 |
| 12 | 8 | 0 | -3.313455 | 1.182076 | 0.000000 |
| 13 | 8 | 0 | -0.236473 | -4.207492 | 0.000000 |
| 14 | 8 | 0 | 3.045498 | -1.523087 | 0.000000 |
| 15 | 16 | 0 | -0.196815 | -1.012188 | -2.382451 |
| 16 | 16 | 0 | -0.196815 | -1.012188 | 2.382451 |

**Table S30**. The theoretical Cartesian coordinates (in Å) for the structure **5-3** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | 1.561822 | -0.052528 | -0.034194 |
| 2 | 25 | 0 | -1.124544 | -0.473782 | -0.154653 |
| 3 | 6 | 0 | 3.347468 | 0.446739 | 0.063905 |
| 4 | 6 | 0 | 0.998536 | 1.153481 | 1.188388 |
| 5 | 6 | 0 | -1.955549 | 1.157384 | -0.115706 |
| 6 | 6 | 0 | -2.449956 | -1.370247 | -1.011394 |
| 7 | 6 | 0 | -1.794512 | -0.968230 | 1.438812 |
| 8 | 6 | 0 | 1.170445 | 1.113280 | -1.352053 |
| 9 | 8 | 0 | 0.968891 | 1.837813 | -2.237929 |
| 10 | 8 | 0 | 0.714282 | 1.912013 | 2.020630 |
| 11 | 8 | 0 | 4.455089 | 0.765085 | 0.134722 |
| 12 | 8 | 0 | -3.269373 | -1.953810 | -1.584473 |
| 13 | 8 | 0 | -2.203104 | -1.267965 | 2.479886 |
| 14 | 6 | 0 | 0.339004 | -1.572506 | -0.131649 |
| 15 | 16 | 0 | 1.768425 | -2.352914 | -0.072508 |
| 16 | 16 | 0 | -2.655353 | 2.543742 | -0.068950 |

**Table S31**. The theoretical Cartesian coordinates (in Å) for the structure **5-4** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -1.079646 | -0.037151 | -0.099527 |
| 2 | 25 | 0 | 1.546343 | -0.159824 | -0.171061 |
| 3 | 6 | 0 | -1.365388 | -1.866537 | -0.180376 |
| 4 | 6 | 0 | -1.192898 | 1.819556 | 0.106330 |
| 5 | 6 | 0 | -2.903079 | 0.028286 | -0.051693 |
| 6 | 6 | 0 | -0.058531 | -0.024353 | -1.598639 |
| 7 | 6 | 0 | 0.051102 | -0.253359 | 1.274755 |
| 8 | 6 | 0 | 3.270492 | -0.769899 | -0.389506 |
| 9 | 6 | 0 | 2.128576 | 1.529666 | -0.119376 |
| 10 | 8 | 0 | -1.613993 | -2.994004 | -0.210276 |
| 11 | 8 | 0 | -1.324060 | 2.955355 | 0.249799 |
| 12 | 8 | 0 | 0.905123 | -0.158535 | -2.293847 |
| 13 | 8 | 0 | 2.491791 | 2.629377 | -0.055423 |
| 14 | 8 | 0 | 4.348703 | -1.167748 | -0.514356 |
| 15 | 16 | 0 | 1.349261 | -0.586473 | 2.180226 |
| 16 | 16 | 0 | -4.456110 | 0.088265 | 0.014057 |

**Table S32**. The theoretical Cartesian coordinates (in Å) for the structure **5-5** using the B3LYP/DZP method

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 25 | 0 | -0.919586 | -0.046563 | 0.027015 |
| 2 | 25 | 0 | 1.647069 | -0.190290 | -0.368356 |
| 3 | 6 | 0 | -1.157330 | -1.903324 | 0.108234 |
| 4 | 6 | 0 | -0.978961 | 1.833713 | 0.078431 |
| 5 | 6 | 0 | -2.716077 | 0.027710 | -0.210874 |
| 6 | 6 | 0 | -0.106648 | -0.109723 | -1.572061 |
| 7 | 6 | 0 | 0.849873 | -0.158823 | 1.197508 |
| 8 | 6 | 0 | 3.269475 | -1.006993 | -0.191292 |
| 9 | 6 | 0 | 2.436572 | 1.407276 | -0.169505 |
| 10 | 8 | 0 | -1.387853 | -3.032600 | 0.148627 |
| 11 | 8 | 0 | -1.082266 | 2.980429 | 0.096615 |
| 12 | 8 | 0 | 0.573211 | -0.219294 | -2.545899 |
| 13 | 8 | 0 | 2.920403 | 2.451889 | -0.030066 |
| 14 | 8 | 0 | 4.270399 | -1.557637 | 0.004367 |
| 15 | 16 | 0 | -0.137203 | -0.069086 | 2.464355 |
| 16 | 16 | 0 | -4.245274 | 0.094087 | -0.482997 |

## Complete Gaussian 03 reference (Reference 40)

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