Supplementary Materials: Heterobimetallic Chromium Manganese Carbonyl Nitrosyls: Comparison with Isoelectronic Homometallic Binuclear Chromium Carbonyl Nitrosyls and Manganese Carbonyls

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Figure S1. The three optimized $CrMn(NO)(CO)_9$ structures at the B3LYP/DZP and BP86/DZP levels.

Figure S2. The 12 optimized $CrMn(NO)(CO)_8$ structures at the B3LYP/DZP and BP86/DZP levels.

Table S1: Relative energies and Cr-Mn distances for the optimized $CrMn(NO)(CO)_n$ (n = 9, 8) structures at the B3LYP/DZP, BP86/DZP and M06-L/cc-pVTZ levels.

Table S2-S3: The vibrational frequencies for the isomers of $CrMn(NO)(CO)_n$ (n = 9, 8) at the B3LYP/DZP, BP86/DZP and M06-L/cc-pVTZ levels.

Table S4-S5: The Cartesian coordinates of the optimized $CrMn(NO)(CO)_n$ (n = 9, 8) isomers at the B3LYP/DZP, BP86/DZP and M06-L/cc-pVTZ levels.

Complete Gaussian 03and Gaussian 09 references

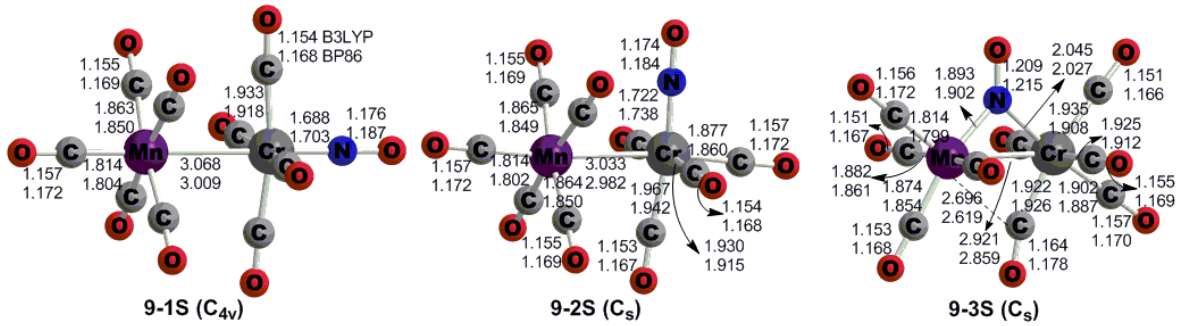

Figure S1. The three optimized $CrMn(NO)(CO)_9$ structures at the B3LYP/DZP and BP86/DZP levels.

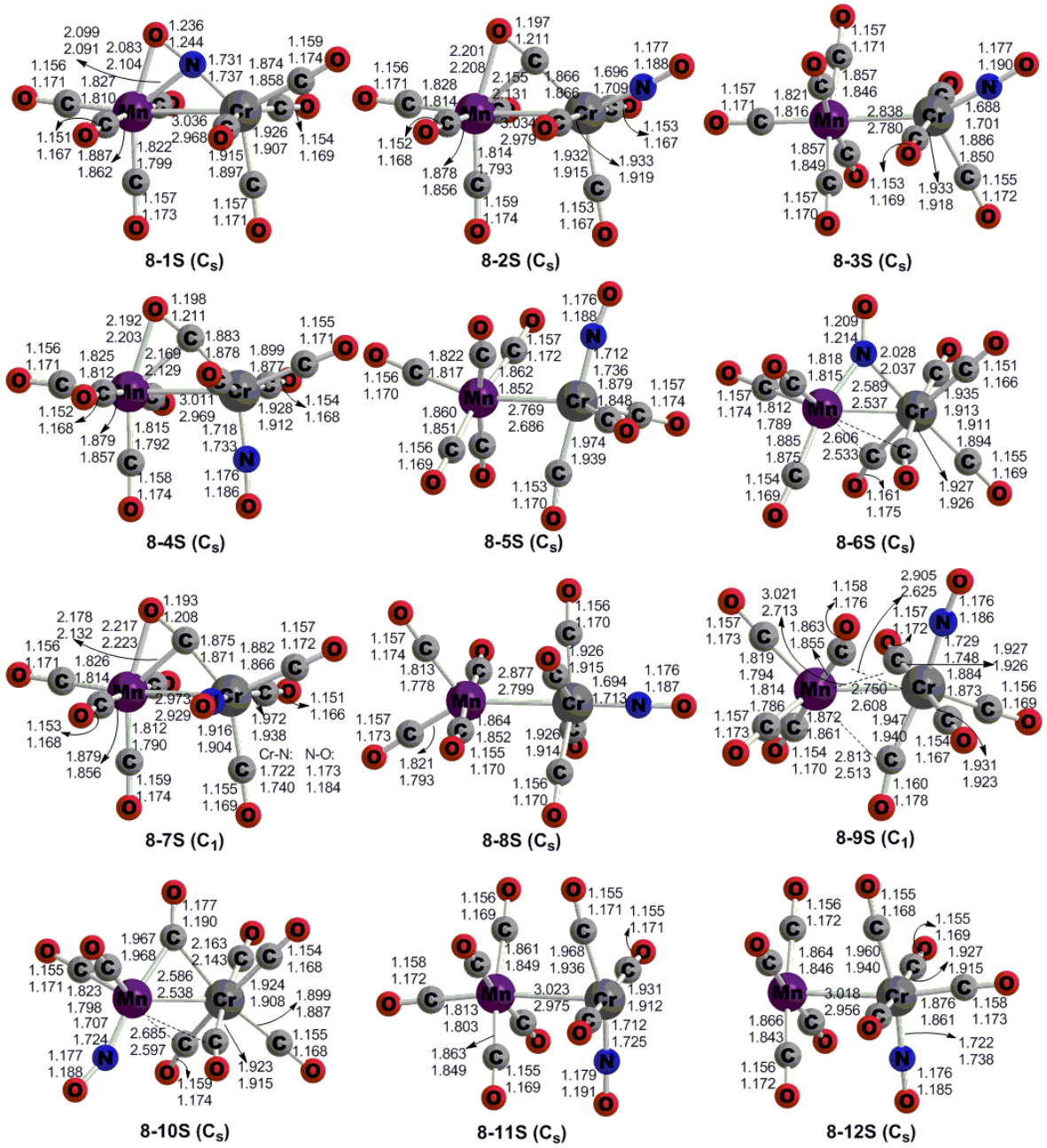

Figure S2. The 12 optimized $CrMn(NO)(CO)_8$ structures at the B3LYP/DZP and BP86/DZP levels.

Table S1. Relative energies (ΔE, in kcal/mol) and Cr-Mn distances (in Å) for the optimized $CrMn(NO)(CO)_n$ (n = 9, 8) structures at the B3LYP/DZP, BP86/DZP, and M06-L/cc-pVTZ levels.

Structure	State (Sym.)	B3LYP/DZP		BP86/DZP		M06-L/cc-pVTZ	
		ΔE	Cr-Mn	ΔE	Cr-Mn	ΔE	Cr-Mn
9-1S	$^1A_1$ (C_{4v})	0.0	3.068	0.0	3.009	0.0	2.987
9-2S	$^1A'$ (C_s)	4.7	3.033	5.0	2.982	5.8	2.961
9-3S	$^1A'$ (C_s)	11.8	2.921	13.9	2.859	20.2	2.871
8-1S	$^1A'$ (C_s)	0.0	3.036	0.0	2.968	0.0	2.937
8-2S	$^1A'$ (C_s)	5.6	3.034	1.1	2.979	1.1	2.938
8-3S	$^1A'$ (C_s)	9.5	2.838	5.1	2.780	3.5	2.845
8-4S	$^1A'$ (C_s)	7.8	3.011	3.4	2.969	3.6	2.925
8-5S	$^1A'$ (C_s)	10.2	2.769	5.3	2.686	6.4	2.689
8-6S	$^1A'$ (C_s)	8.9	2.589	5.4	2.537	6.5	2.531
8-7S	^1A (C_1)	12.1	2.973	7.1	2.929	7.4	2.879
8-8S	$^1A'$ (C_s)	14.2	2.877	11.3	2.799	8.2	2.876
8-9S	^1A (C_1)	16.5	2.750	11.4	2.608	11.4	2.629
8-10S	$^1A'$ (C_s)	19.2	2.586	8.3	2.538	11.5	2.531
8-11S	$^1A'$ (C_s)	26.5	3.023	24.4	2.975	17.8	2.956
8-12S	$^1A'$ (C_s)	30.5	3.018	28.6	2.956	21.6	2.951

Table S2. The vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol, given in parentheses) of the $CrMn(NO)(CO)_9$ isomers at the B3LYP/DZP, BP86/DZP and M06-L/cc-pVTZ levels of theory.

Isomers	B3LYP/DZP	BP86/DZP	M06-L/cc-pVTZ
9-1S	42 (0), 56 (0), 56 (0), 61 (0), 61 (0), 70 (0), 73 (0), 83 (0), 83 (0), 92 (0), 95 (1), 95 (1), 95 (0), 99 (0), 102 (0), 102 (0), 108 (0), 108 (0), 114 (4), 142 (0), 354 (0), 369 (20), 372 (0), 373 (0), 398 (1), 398 (1), 402 (13), 411 (0), 417 (1), 417 (1), 439 (0), 445 (12), 445 (12), 470 (16), 470 (16), 473 (0), 481 (0), 519 (0), 530 (137), 549 (3), 549 (3), 560 (0), 561 (0), 561 (0), 665 (115), 665 (115), 672 (72), 672 (72), 680 (393), 706 (52), 1854 (1348), 2050 (13), 2050 (13), 2060 (128), 2076 (0), 2077 (0),2085 (2505), 2085 (2505), 2088 (1434), 2165 (79)	44 (0), 53 (0), 53 (0), 58 (0), 58 (0), 64 (0), 71 (0), 80 (0), 80 (0), 89 (0), 92 (1), 92 (1), 94 (0), 97 (0), 99 (0), 99 (0), 104 (0), 104 (0), 111 (4), 142 (0), 357 (0), 374 (0), 385 (0), 386 (11), 389 (0), 389 (0), 411 (0), 411 (0), 424 (8), 427 (0), 438 (0), 456 (8), 456 (8), 463 (0), 482 (9), 482 (9), 493 (5), 507 (0), 522 (94), 537 (1), 537 (1), 544 (0), 549 (0), 549 (0), 659 (105), 659 (105), 663 (58), 663 (58), 677 (346), 686 (27), 1807 (984), 1966 (0), 1966 (0), 1983 (298), 1994 (0), 1999 (2182), 1999 (2182), 2002 (0), 2020 (819), 2082 (86)	58 (0), 58 (0), 72 (0), 72 (0), 80 (0), 80 (0), 80 (0), 83 (0), 83 (0), 94 (1), 94 (1), 105 (0), 106 (0), 106 (0), 110 (0), 113 (1), 113 (2), 114 (0), 114 (0), 154 (0), 367 (0), 372 (9), 377 (0), 387 (0), 398 (7), 410 (1), 410 (1), 411 (0), 429 (8), 429 (8), 438 (3), 438 (3), 453 (0), 453 (20), 453 (20), 480 (0), 481 (0), 522 (0), 532 (119), 555 (3), 555 (3), 559 (0), 567 (0), 567 (0), 661 (97), 661 (97), 672 (71), 672 (71), 679 (388), 698 (6), 1857 (1305), 2036 (4), 2036 (4), 2054 (247), 2068 (0), 2071 (0), 2078 (2312), 2078 (2312), 2091 (1008), 2163 (68)
9-2S	34 (0), 50 (0), 53 (0), 55 (0), 57 (0), 65 (0), 70 (0), 82 (0), 84 (0), 92 (0), 93 (0), 93 (0), 94 (0), 98 (0), 99 (0), 102 (0), 107 (0), 107 (0), 115 (3), 145 (0), 351 (0), 370 (0), 370 (28), 378 (0), 390 (0), 397 (8), 401 (10), 411 (0), 414 (0), 417 (1), 441 (20), 453 (6), 465 (13), 466 (18), 470 (3), 471 (0), 482 (0), 506 (2), 522 (4), 528 (5), 554 (7), 557 (1), 560 (6), 560 (0), 664 (87), 664 (190), 665 (539), 679 (80), 690 (75), 695 (21), 1844 (810), 2049 (6), 2051 (343), 2061 (620), 2065 (223), 2079 (30), 2082 (2512), 2082 (1789), 2091 (1657), 2162 (77)	32 (0), 45 (0), 46 (0), 50 (0), 53 (0), 60 (0), 64 (0), 78 (0), 80 (0), 88 (0), 89 (0), 89 (0), 91 (0), 94 (0), 96 (0), 101 (0), 103 (0), 103 (0), 112 (3), 146 (0), 351 (0), 373 (0), 376 (7), 389 (0), 395 (2), 403 (5), 408 (0), 415 (3), 424 (6), 430 (0), 452 (0), 454 (14), 458 (0), 470 (1), 479 (7), 480 (9), 495 (2), 496 (2), 509 (5), 518 (1), 542 (2), 545 (0), 546 (1), 549 (3), 663 (72), 663 (143), 664 (92), 669 (441), 676 (73), 690 (4), 1804 (641), 1965 (5), 1970 (550), 1977 (601), 1983 (146), 1996 (2193), 2000 (1133), 2001 (37), 2021 (1285), 2078 (70)	52 (0), 56 (0), 59 (0), 66 (0), 69 (0), 72 (0), 74 (0), 81 (0), 83 (0), 92 (1), 92 (1), 95 (0), 98 (0), 100 (0), 100 (0), 105 (0), 107 (1), 111 (0), 116 (2), 156 (0), 360 (0), 372 (18), 378 (1), 386 (0), 398 (6), 403 (0), 408 (3), 412 (0), 426 (15), 428 (3), 430 (0), 449 (16), 450 (22), 454 (6), 476 (0), 477 (0), 484 (0), 509 (1), 519 (3), 533 (3), 557 (6), 560 (1), 565 (2), 566 (6), 655 (148), 661 (79), 662 (108), 670 (459), 689 (63), 700 (8), 1847 (763), 2035 (2), 2042 (610), 2050 (863), 2056 (70), 2070 (9), 2075 (2342), 2082 (1063), 2093 (1495), 2159 (70)
9-3S	10 (0), 52 (0), 53 (0), 57 (0), 64 (0), 67 (0), 80 (0), 82 (0), 85 (0), 89 (1), 90 (0), 100 (1), 101 (1), 102 (0), 107 (1), 107 (0), 117 (0), 137 (1), 169 (3), 253 (4), 355 (2), 355 (0), 364 (0), 366 (17), 380 (1), 389 (4), 390 (0), 392 (6), 403 (0), 423 (26), 435 (27), 439 (60), 441 (3), 447 (2), 469 (2), 485 (11), 510 (1), 521 (1), 526 (0), 532 (1), 539 (10), 547 (0), 565 (3), 583 (38), 627 (2), 647 (162), 667 (187), 668 (153), 673 (263), 706 (264), 1631 (393), 1996 (525), 2043 (527), 2058 (779), 2069 (817), 2082 (616), 2091 (2174), 2092 (422), 2116 (1593), 2164 (24)	11 (0), 46 (0), 48 (0), 55 (0), 59 (0), 62 (0), 78 (0), 80 (0), 82 (0), 87 (1), 89 (0), 94 (0), 97 (1), 99 (1), 102 (0), 102 (1), 115 (0), 139 (0), 177 (1), 254 (9), 352 (2), 358 (0), 367 (0), 376 (8), 389 (0), 395 (3), 405 (5), 409 (0), 417 (2), 441 (11), 444 (14), 451 (24), 454 (8), 470 (11), 479 (5), 487 (2), 492 (2), 506 (1), 511 (0), 516 (1), 527 (8), 530 (0), 550 (2), 571 (99), 618 (2), 643 (176), 660 (161), 661 (224), 670 (115), 702 (290), 1595 (363), 1923 (371), 1961 (184), 1981 (230), 1983 (988), 1996 (2151), 1997 (740), 2003 (145), 2031 (1642), 2076 (11)	2i (0), 48 (0), 49 (0), 56 (0), 57 (0), 62 (0), 74 (0), 79 (0), 80 (0), 83 (1), 85 (0), 86 (0), 92 (1), 94 (1), 96 (0), 97 (1), 108 (0), 143 (1), 173 (1), 249 (9), 356 (3), 362 (0), 369 (22), 372 (0), 378 (1), 384 (3), 393 (10), 396 (1), 407 (4), 418 (20), 423 (59), 429 (19), 433 (12), 434 (0), 474 (2), 484 (9), 510 (0), 523 (1), 529 (0), 530 (0), 539 (0), 544 (14), 562 (3), 575 (61), 621 (1), 644 (232), 660 (222), 661 (164), 661 (90), 697 (242), 1645 (440), 1996 (391), 2034 (259), 2053 (320), 2056 (1200), 2075 (778), 2077 (2277), 2081 (179), 2109 (1704), 2158 (10)

Table S3. The vibrational frequencies (in cm^{-1}) and infrared intensities (in km/mol, given in parentheses) of the $CrMn(NO)(CO)_8$ isomers at the B3LYP/DZP, BP86/DZP and M06-L/cc-pVTZ levels.

Isomer	B3LYP/DZP	BP86/DZP	M06-L/cc-pVTZ
8-1S	21 (0), 50 (0), 54 (0), 54 (0), 66 (0), 74 (0), 78 (0), 82 (0), 89 (0), 92 (0), 93 (0), 97 (0), 101 (1), 107 (0), 109 (0), 159 (1), 165 (0), 340 (8), 345 (1), 379 (10), 380 (1), 382 (0), 385 (1), 397 (0), 404 (8), 414 (18), 424 (30), 433 (1), 450 (1), 456 (15), 465 (3), 474 (7), 476 (15), 514 (43), 528 (0), 532 (9), 542 (0), 563 (1), 579 (2), 636 (50), 646 (44), 659 (330), 665 (104), 671 (23), 693 (82), 1527 (488), 2032 (657), 2053 (474), 2059 (402), 2067 (1072), 2083 (630), 2094 (2228), 2108 (1077), 2161 (91)	21 (0), 50 (0), 50 (0), 54 (0), 64 (0), 73 (0), 76 (0), 82 (0), 87 (0), 90 (0), 91 (0), 94 (0), 98 (1), 106 (0), 106 (0), 159 (0), 163 (0), 327 (1), 349 (1), 373 (9), 389 (0), 401 (0), 402 (0), 415 (0), 417 (5), 418 (0), 431 (0), 439 (2), 449 (34), 467 (2), 482 (0), 489 (10), 495 (3), 510 (33), 515 (0), 520 (30), 532 (1), 550 (2), 567 (3), 635 (53), 652 (49), 654 (81), 658 (264), 674 (82), 688 (56), 1511 (397), 1954 (517), 1970 (86), 1970 (346), 1984 (869), 1995 (2232), 1996 (393), 2027 (1112), 2073 (93)	19 (0), 49 (0), 60 (0), 61 (0), 66 (0), 74 (0), 78 (1), 87 (0), 88 (0), 89 (1), 95 (0), 98 (0), 100 (1), 102 (0), 103 (0), 158 (0), 171 (0), 326 (1), 358 (0), 377 (4), 381 (0), 388 (37), 397 (0), 399 (2), 405 (11), 408 (8), 424 (4), 446 (1), 447 (15), 455 (1), 471 (4), 477 (15), 483 (4), 527 (23), 532 (0), 538 (27), 548 (4), 570 (1), 581 (5), 637 (50), 650 (42), 659 (383), 664 (81), 676 (4), 688 (70), 1559 (478), 2024 (474), 2044 (580), 2047 (57), 2059 (983), 2073 (416), 2079 (2420), 2104 (1172), 2154 (75)
8-2S	22 (0), 47 (1), 50 (0), 68 (0), 72 (0), 76 (0), 78 (0), 85 (0), 90 (1), 94 (0), 99 (1), 106 (1), 107 (0), 108 (0), 115 (0), 155 (0), 158 (0), 276 (9), 353 (0), 373 (5), 387 (12), 392 (0), 393 (0), 403 (0), 406 (7), 415 (1), 423 (7), 434 (12), 440 (50), 451 (6), 464 (10), 481 (4), 492 (2), 518 (10), 529 (1), 531 (2), 553 (82), 558 (15), 582 (2), 635 (59), 646 (131), 671 (154), 671 (77), 691 (82), 705 (105), 1802 (509), 1851 (1313), 2044 (263), 2058 (2), 2074 (600), 2086 (685), 2091 (2556), 2102 (1102), 2157 (207)	18 (0), 45 (0), 50 (0), 66 (0), 68 (0), 72 (0), 78 (0), 82 (0), 87 (0), 91 (0), 96 (1), 101 (0), 102 (0), 105 (0), 110 (0), 153 (0), 157 (0), 276 (4), 351 (0), 381 (3), 388 (0), 390 (0), 401 (0), 412 (7), 419 (0), 419 (2), 425 (2), 433 (12), 452 (19), 470 (15), 475 (7), 489 (2), 496 (1), 509 (13), 514 (0), 521 (2), 541 (10), 543 (79), 569 (2), 630 (57), 653 (111), 654 (65), 676 (127), 677 (67), 684 (100), 1742 (406), 1803 (991), 1964 (204), 1966 (39), 1987 (463), 1999 (2207), 2000 (609), 2024 (845), 2070 (189)	18 (0), 44 (1), 56 (0), 66 (0), 67 (0), 75 (0), 81 (0), 81 (0), 89 (1), 90 (1), 95 (1), 99 (0), 101 (1), 121 (0), 125 (0), 150 (0), 164 (0), 269 (2), 362 (0), 375 (2), 388 (3), 393 (5), 404 (9), 410 (1), 416 (9), 417 (21), 431 (31), 438 (1), 442 (0), 448 (5), 468 (10), 485 (2), 491 (5), 527 (24), 529 (0), 536 (3), 560 (12), 565 (69), 586 (2), 634 (53), 651 (123), 670 (63), 673 (163), 686 (68), 690 (86), 1807 (509), 1853 (1268), 2034 (215), 2043 (33), 2063 (516), 2077 (681), 2081 (2382), 2099 (955), 2151 (175)
8-3S	15 (1), 16 (0), 26 (0), 69 (0), 69 (0), 71 (0), 76 (0), 82 (1), 87 (0), 90 (0), 91 (0), 94 (1), 103 (0), 108 (2), 108 (0), 109 (0), 114 (1), 150 (2), 351 (0), 365 (13), 374 (0), 374 (7), 390 (6), 409 (13), 411 (3), 414 (0), 416 (0), 434 (12), 460 (20), 470 (0), 475 (0), 477 (14), 485 (15), 514 (79), 535 (3), 540 (73), 553 (2), 561 (1), 564 (3), 629 (31), 638 (48), 667 (120), 669 (89), 688 (313), 702 (31), 1844 (1129), 2036 (68), 2049 (838), 2056 (441), 2061 (1), 2069 (708), 2078 (2502), 2091 (1605), 2153 (87)	9i (0), 12 (0), 17 (0), 63 (0), 63 (0), 68 (0), 75 (0), 79 (1), 86 (0), 86 (0), 88 (0), 90 (1), 99 (0), 104 (1), 105 (1), 107 (0), 111 (0), 153 (3), 352 (0), 375 (0), 378 (2), 383 (9), 389 (2), 407 (0), 408 (1), 424 (0), 426 (10), 458 (0), 464 (20), 467 (5), 481 (1), 485 (6), 492 (8), 512 (75), 532 (13), 533 (1), 535 (2), 545 (2), 547 (1), 623 (42), 630 (24), 659 (108), 664 (78), 681 (309), 684 (2), 1792 (856), 1951 (20), 1965 (91), 1978 (1476), 1985 (320), 1988 (1127), 1993 (1058), 2011 (1039), 2068 (145)	19 (0), 40 (0), 45 (0), 67 (0), 67 (0), 77 (0), 78 (0), 85 (0), 89 (1), 89 (2), 91 (1), 96 (0), 97 (0), 106 (1), 106 (0), 116 (0), 117 (0), 154 (2), 365 (0), 371 (7), 388 (0), 404 (9), 405 (8), 416 (0), 420 (1), 421 (10), 425 (1), 451 (7), 452 (4), 462 (19), 466 (18), 473 (0), 473 (0), 516 (62), 551 (27), 557 (0), 557 (7), 561 (2), 567 (2), 645 (57), 647 (30), 661 (106), 664 (69), 682 (354), 699 (3), 1846 (1283), 2023 (9), 2033 (148), 2052 (252), 2058 (1604), 2059 (129), 2072 (2281), 2084 (1100), 2150 (120)

8-4S	21 (0), 46 (0), 53 (0), 65 (0), 71 (0), 75 (0), 85 (0), 87 (0), 93 (0), 94 (0), 95 (0), 100 (0), 103 (0), 107 (0), 109 (0), 155 (0), 155 (0), 281 (16), 358 (0), 378 (3), 384 (0), 390 (2), 395 (2), 398 (0), 408 (6), 415 (2), 434 (4), 441 (52), 446 (8), 459 (3), 472 (4), 479 (1), 481 (7), 510 (10), 528 (4), 536 (6), 540 (12), 557 (3), 581 (4), 635 (52), 643 (114), 669 (262), 675 (84), 685 (147), 699 (64), 1799 (707), 1845 (487), 2056 (807), 2056 (66), 2066 (834), 2078 (169), 2089 (2535), 2103 (1513), 2154 (44)	10 (0), 45 (0), 52 (0), 59 (0), 69 (0), 70 (0), 82 (0), 83 (0), 87 (0), 91 (0), 91 (0), 94 (0), 98 (0), 105 (0), 105 (0), 151 (0), 155 (1), 281 (7), 352 (0), 387 (0), 388 (1), 398 (0), 400 (0), 410 (1), 418 (0), 419 (1), 441 (1), 455 (26), 461 (3), 464 (12), 478 (8), 488 (4), 497 (2), 502 (4), 509 (3), 526 (0), 530 (16), 547 (0), 569 (4), 631 (50), 652 (85), 658 (71), 668 (350), 677 (16), 683 (61), 1739 (499), 1801 (430), 1966 (2), 1971 (701), 1978 (700), 1990 (107), 1995 (2296), 2026 (1184), 2067 (44)	16 (0), 45 (0), 54 (0), 60 (0), 68 (0), 68 (0), 83 (0), 84 (0), 86 (0), 89 (0), 93 (0), 95 (0), 97 (0), 100 (1), 103 (0), 148 (0), 163 (0), 273 (6), 364 (0), 378 (1), 386 (2), 398 (2), 401 (15), 405 (4), 413 (11), 413 (1), 428 (24), 435 (14), 440 (4), 458 (5), 476 (3), 488 (1), 495 (6), 514 (6), 524 (2), 541 (9), 544 (5), 566 (3), 582 (6), 635 (46), 648 (121), 670 (270), 674 (68), 678 (50), 685 (112), 1806 (681), 1849 (419), 2042 (4), 2043 (768), 2054 (909), 2066 (88), 2077 (2461), 2102 (1306), 2148 (18)
8-5S	20 (0), 25 (0), 39 (0), 63 (1), 68 (0), 70 (0), 74 (1), 75 (0), 85 (0), 90 (0), 93 (0), 96 (0), 99 (1), 104 (1), 108 (0), 109 (0), 119 (1), 154 (1), 348 (0), 365 (24), 373 (0), 376 (0), 403 (4), 407 (10), 409 (0), 418 (0), 432 (8), 437 (9), 452 (17), 467 (1), 472 (7), 476 (7), 478 (13), 505 (7), 517 (28), 551 (1), 557 (3), 563 (4), 581 (16), 629 (4), 654 (167), 664 (120), 667 (64), 675 (378), 694 (35), 1837 (851), 2043 (101), 2050 (382), 2060 (2086), 2062 (566), 2068 (172), 2077 (850), 2087 (2299), 2150 (155)	19 (0), 23 (0), 36 (1), 57 (1), 65 (0), 68 (1), 71 (0), 75 (1), 84 (0), 88 (0), 90 (1), 95 (0), 96 (0), 102 (1), 106 (0), 112 (1), 126 (1), 160 (2), 355 (0), 374 (0), 376 (14), 382 (0), 397 (3), 401 (0), 423 (0), 424 (7), 439 (5), 446 (3), 471 (5), 472 (2), 476 (1), 484 (5), 486 (7), 511 (30), 511 (7), 534 (1), 534 (5), 545 (4), 569 (31), 613 (7), 636 (53), 653 (103), 653 (77), 667 (373), 690 (14), 1785 (718), 1953 (250), 1962 (19), 1972 (1451), 1976 (992), 1993 (409), 1995 (309), 2004 (1818), 2065 (238)	18 (0), 24 (0), 37 (0), 60 (1), 70 (0), 70 (0), 74 (1), 78 (0), 86 (0), 89 (0), 90 (1), 96 (1), 97 (1), 100 (0), 105 (0), 114 (1), 124 (1), 165 (2), 365 (0), 372 (19), 387 (0), 398 (0), 402 (7), 409 (1), 410 (0), 421 (1), 445 (6), 451 (4), 455 (22), 460 (16), 461 (0), 462 (10), 469 (5), 517 (6), 526 (27), 549 (2), 553 (2), 560 (10), 581 (31), 638 (3), 639 (75), 654 (109), 655 (77), 673 (376), 701 (6), 1841 (831), 2028 (69), 2039 (530), 2044 (1674), 2053 (430), 2064 (443), 2071 (658), 2083 (2101), 2146 (201)
8-6S	27 (0), 41 (0), 48 (0), 65 (0), 72 (0), 78 (0), 82 (0), 82 (0), 86 (0), 94 (0), 95 (1), 98 (0), 109 (1), 110 (0), 122 (0), 134 (1), 191 (0), 249 (1), 346 (0), 361 (0), 367 (1), 380 (15), 382 (3), 390 (1), 401 (11), 412 (18), 412 (2), 431 (18), 449 (19), 451 (14), 462 (6), 483 (11), 500 (2), 502 (6), 523 (0), 525 (16), 531 (0), 538 (3), 583 (5), 610 (4), 623 (72), 652 (154), 660 (56), 664 (315), 712 (244), 1645 (459), 2021 (703), 2026 (349), 2057 (1103), 2063 (585), 2075 (1624), 2094 (650), 2101 (2019), 2152 (85)	24 (0), 44 (0), 47 (0), 60 (0), 67 (0), 77 (0), 80 (0), 80 (0), 84 (0), 91 (0), 94 (0), 97 (0), 107 (0), 107 (0), 121 (0), 135 (0), 201 (0), 244 (2), 344 (0), 359 (1), 361 (0), 381 (0), 394 (7), 401 (2), 409 (5), 422 (10), 423 (1), 442 (5), 448 (5), 462 (8), 475 (4), 483 (4), 489 (1), 499 (3), 500 (0), 517 (6), 526 (4), 529 (9), 584 (8), 596 (10), 617 (52), 638 (122), 651 (290), 658 (91), 704 (179), 1618 (415), 1942 (476), 1944 (228), 1966 (1020), 1975 (643), 1995 (1175), 2002 (566), 2013 (1844), 2063 (133)	32 (0), 46 (0), 48 (0), 61 (0), 66 (0), 74 (0), 75 (0), 77 (0), 82 (0), 89 (1), 91 (0), 93 (1), 101 (0), 103 (1), 135 (0), 144 (0), 203 (0), 248 (1), 353 (0), 367 (2), 369 (0), 375 (23), 385 (4), 390 (7), 392 (1), 409 (11), 428 (9), 430 (13), 441 (17), 445 (2), 472 (6), 485 (9), 498 (7), 499 (4), 519 (0), 526 (14), 535 (1), 539 (3), 585 (6), 606 (8), 622 (83), 641 (134), 652 (280), 657 (70), 705 (197), 1661 (515), 2011 (575), 2013 (276), 2043 (1058), 2053 (546), 2069 (1513), 2084 (664), 2094 (2036), 2147 (109)

8-7S	24 (0), 42 (0), 50 (0), 63 (0), 67 (0), 78 (0), 81 (0), 87 (0), 89 (0), 94 (0), 96 (0), 102 (1), 107 (0), 108 (0), 109 (0), 156 (0), 159 (0), 260 (5), 351 (1), 372 (12), 382 (0), 392 (4), 394 (0), 400 (3), 404 (4), 417 (4), 423 (1), 434 (17), 446 (21), 461 (13), 465 (15), 478 (10), 484 (10), 497 (4), 524 (15), 530 (1), 537 (18), 551 (16), 579 (5), 636 (53), 642 (131), 667 (208), 670 (76), 690 (145), 704 (72), 1823 (528), 1860 (812), 2041 (70), 2061 (1388), 2066 (535), 2075 (989), 2087 (965), 2100 (1746), 2151 (202)	23 (0), 40 (0), 50 (0), 58 (0), 62 (0), 76 (0), 79 (0), 81 (0), 86 (0), 89 (0), 91 (0), 96 (0), 101 (1), 105 (0), 106 (0), 152 (0), 160 (0), 265 (2), 348 (1), 381 (0), 387 (0), 397 (1), 404 (5), 411 (3), 419 (1), 420 (2), 423 (1), 433 (11), 465 (14), 471 (17), 473 (13), 487 (8), 490 (6), 496 (2), 508 (11), 518 (2), 527 (12), 542 (10), 566 (5), 632 (49), 649 (70), 651 (111), 672 (215), 679 (97), 690 (61), 1756 (402), 1810 (673), 1960 (128), 1974 (621), 1978 (1193), 1987 (651), 1999 (734), 2019 (1427), 2064 (180)	21 (0), 41 (0), 52 (0), 62 (0), 71 (0), 75 (0), 81 (0), 86 (0), 88 (0), 91 (1), 93 (0), 101 (0), 104 (0), 107 (0), 114 (0), 148 (0), 169 (0), 250 (1), 359 (1), 377 (8), 389 (3), 391 (1), 400 (1), 406 (17), 413 (3), 417 (8), 427 (1), 432 (8), 448 (3), 457 (13), 471 (14), 482 (16), 487 (2), 506 (7), 523 (5), 536 (4), 547 (22), 551 (10), 581 (11), 636 (56), 644 (65), 646 (134), 669 (196), 690 (121), 700 (57), 1828 (529), 1864 (749), 2031 (142), 2050 (792), 2054 (1267), 2062 (584), 2081 (918), 2096 (1521), 2146 (212)
8-8S	13 (1), 15 (0), 29 (0), 65 (0), 66 (0), 72 (0), 77 (1), 82 (0), 84 (1), 88 (1), 89 (0), 95 (1), 96 (0), 100 (0), 106 (0), 109 (0), 114 (3), 147 (2), 356 (0), 368 (0), 373 (0), 375 (20), 382 (0), 394 (0), 405 (11), 408 (1), 415 (3), 433 (0), 453 (11), 457 (8), 459 (19), 474 (9), 485 (27), 521 (51), 528 (114), 542 (2), 549 (1), 554 (3), 560 (27), 592 (34), 632 (60), 669 (129), 674 (100), 678 (83), 703 (138), 1853 (1391), 2035 (1), 2049 (72), 2057 (91), 2061 (7), 2063 (2219), 2074 (2560), 2085 (1169), 2150 (107)	3i (0), 14 (1), 15 (0), 57 (0), 59 (0), 72 (0), 75 (0), 78 (1), 81 (1), 87 (1), 89 (0), 90 (0), 95 (0), 96 (0), 106 (0), 109 (0), 112 (3), 152 (2), 358 (0), 370 (0), 378 (0), 386 (0), 389 (14), 392 (1), 394 (0), 414 (1), 421 (7), 433 (0), 461 (7), 467 (9), 488 (4), 495 (19), 501 (8), 506 (27), 513 (66), 523 (2), 536 (1), 542 (1), 552 (35), 599 (25), 630 (55), 655 (111), 664 (64), 676 (143), 682 (64), 1805 (1093), 1949 (11), 1960 (67), 1972 (260), 1977 (1830), 1981 (89), 1988 (2072), 2010 (785), 2063 (60)	26 (0), 42 (0), 47 (0), 64 (0), 71 (0), 74 (0), 80 (0), 81 (0), 88 (1), 90 (1), 92 (2), 92 (0), 103 (0), 105 (0), 108 (1), 115 (0), 115 (0), 151 (2), 368 (0), 375 (9), 377 (0), 386 (0), 398 (5), 405 (0), 417 (3), 426 (0), 426 (15), 440 (7), 444 (0), 445 (15), 457 (25), 475 (2), 489 (5), 523 (87), 526 (4), 540 (22), 552 (2), 558 (5), 573 (3), 619 (74), 633 (43), 665 (186), 675 (75), 675 (59), 692 (84), 1853 (1418), 2020 (1), 2031 (69), 2046 (584), 2052 (210), 2058 (1550), 2069 (2163), 2080 (1008), 2146 (90)
8-9S	20 (0), 27 (0), 36 (0), 63 (0), 70 (0), 73 (0), 80 (0), 87 (1), 88 (0), 89 (0), 90 (0), 97 (1), 99 (1), 101 (0), 108 (0), 117 (0), 132 (4), 156 (2), 360 (0), 373 (8), 376 (11), 378 (2), 383 (6), 391 (7), 395 (3), 412 (9), 419 (3), 444 (9), 446 (20), 458 (5), 471 (14), 476 (11), 484 (10), 514 (9), 516 (0), 531 (7), 549 (15), 552 (128), 553 (0), 595 (40), 631 (48), 668 (217), 673 (73), 687 (112), 691 (96), 1840 (951), 2026 (156), 2041 (348), 2050 (442), 2059 (1269), 2066 (278), 2071 (2083), 2091 (1979), 2147 (80)	27 (0), 40 (0), 41 (0), 56 (0), 68 (0), 75 (0), 80 (0), 83 (0), 85 (0), 86 (0), 91 (1), 94 (1), 97 (0), 101 (0), 104 (0), 127 (0), 148 (5), 174 (0), 350 (2), 361 (0), 371 (1), 388 (22), 388 (1), 393 (1), 408 (0), 415 (5), 425 (6), 431 (3), 446 (5), 462 (5), 474 (6), 488 (4), 498 (3), 500 (1), 513 (14), 517 (6), 530 (25), 534 (86), 543 (1), 602 (34), 624 (36), 641 (64), 657 (118), 664 (234), 688 (2), 1796 (753), 1925 (208), 1941 (620), 1959 (97), 1970 (1165), 1978 (566), 1992 (1192), 2012 (1718), 2056 (51)	29 (0), 39 (0), 42 (0), 57 (0), 71 (0), 74 (0), 79 (0), 82 (0), 83 (1), 85 (0), 87 (1), 94 (1), 95 (0), 98 (0), 112 (0), 127 (0), 146 (4), 175 (1), 368 (1), 374 (7), 374 (3), 384 (15), 390 (2), 399 (0), 410 (13), 421 (3), 425 (6), 431 (9), 434 (13), 459 (9), 467 (6), 478 (10), 490 (9), 513 (9), 518 (2), 525 (1), 544 (25), 552 (124), 557 (1), 606 (36), 630 (39), 642 (69), 669 (282), 677 (62), 691 (8), 1842 (941), 2010 (172), 2021 (541), 2030 (284), 2047 (1206), 2057 (465), 2068 (1592), 2089 (1939), 2141 (61)

8-10S	24 (0), 36 (0), 50 (0), 67 (0), 75 (0), 76 (0), 79 (0), 82 (0), 87 (0), 91 (1), 94 (1), 98 (1), 108 (0), 112 (1), 113 (2), 124 (2), 183 (1), 221 (10), 336 (5), 366 (0), 371 (12), 377 (0), 381 (1), 392 (14), 392 (2), 407 (4), 429 (4), 440 (34), 455 (5), 456 (22), 462 (8), 471 (27), 485 (4), 508 (72), 512 (2), 527 (0), 528 (5), 544 (23), 561 (13), 612 (5), 621 (60), 652 (138), 657 (287), 664 (240), 691 (16), 1830 (1226), 1921 (253), 2032 (865), 2038 (1090), 2072 (911), 2073 (510), 2077 (1057), 2095 (1931), 2146 (199)	22 (0), 38 (0), 48 (0), 61 (0), 71 (0), 77 (0), 78 (0), 82 (0), 85 (0), 85 (0), 93 (1), 96 (0), 106 (0), 110 (1), 113 (0), 128 (1), 192 (0), 224 (5), 342 (3), 364 (0), 372 (7), 377 (0), 389 (0), 404 (4), 405 (1), 420 (2), 428 (0), 451 (7), 453 (5), 470 (6), 470 (19), 482 (1), 489 (9), 501 (40), 502 (3), 506 (0), 515 (10), 530 (25), 571 (16), 590 (8), 607 (60), 642 (115), 650 (241), 657 (196), 687 (17), 1775 (897), 1853 (230), 1950 (558), 1957 (879), 1977 (959), 1993 (545), 1995 (691), 2011 (1662), 2060 (273)	29 (0), 41 (0), 51 (0), 62 (0), 72 (0), 75 (0), 77 (0), 79 (0), 82 (0), 84 (1), 89 (1), 94 (1), 102 (1), 102 (1), 125 (0), 135 (1), 198 (0), 222 (5), 353 (6), 372 (2), 375 (8), 382 (0), 385 (10), 393 (1), 393 (7), 425 (9), 430 (26), 432 (11), 450 (13), 455 (10), 468 (0), 480 (13), 488 (9), 508 (1), 516 (57), 525 (0), 526 (8), 541 (17), 576 (11), 599 (16), 619 (71), 643 (128), 647 (155), 658 (268), 692 (38), 1837 (1110), 1926 (248), 2018 (682), 2026 (1009), 2057 (911), 2070 (842), 2070 (688), 2089 (1937), 2142 (230)
8-11S	34 (0), 49 (0), 52 (0), 56 (0), 62 (0), 70 (0), 72 (0), 86 (1), 86 (1), 90 (0), 92 (0), 95 (1), 100 (0), 105 (0), 106 (0), 107 (0), 118 (3), 158 (0), 348 (0), 352 (24), 363 (0), 372 (0), 373 (11), 394 (8), 404 (7), 411 (0), 417 (1), 421 (1), 430 (50), 467 (12), 469 (13), 470 (4), 481 (0), 484 (2), 510 (5), 529 (8), 558 (1), 559 (1), 562 (1), 641 (181), 653 (171), 666 (61), 667 (96), 673 (71), 684 (135), 1826 (868), 2034 (237), 2042 (43), 2059 (416), 2071 (1829), 2071 (1891), 2074 (843), 2082 (1061), 2154 (129)	33 (0), 41 (0), 46 (0), 51 (0), 62 (0), 62 (0), 70 (0), 81 (1), 81 (1), 87 (0), 88 (0), 92 (0), 99 (0), 102 (0), 105 (0), 107 (0), 115 (3), 155 (0), 345 (0), 345 (11), 349 (0), 374 (0), 393 (3), 401 (7), 405 (0), 419 (5), 424 (3), 431 (0), 442 (34), 458 (0), 477 (6), 481 (9), 483 (2), 495 (1), 502 (3), 515 (6), 545 (1), 546 (1), 546 (0), 638 (70), 646 (190), 657 (15), 663 (104), 665 (91), 682 (131), 1779 (661), 1939 (557), 1955 (17), 1979 (384), 1987 (1996), 1987 (1448), 1999 (0), 2004 (827), 2071 (133)	52 (0), 60 (1), 60 (0), 66 (0), 69 (0), 73 (0), 75 (0), 85 (1), 85 (1), 93 (0), 95 (0), 97 (0), 101 (0), 105 (0), 106 (0), 111 (0), 117 (2), 171 (0), 358 (0), 359 (20), 382 (6), 384 (0), 386 (0), 399 (3), 400 (5), 413 (0), 425 (33), 429 (8), 434 (1), 451 (14), 453 (21), 478 (0), 483 (0), 494 (0), 513 (3), 530 (4), 560 (0), 565 (1), 566 (2), 638 (33), 656 (322), 662 (70), 663 (90), 674 (41), 692 (64), 1830 (835), 2015 (237), 2039 (163), 2050 (455), 2063 (2302), 2067 (113), 2069 (1116), 2078 (1197), 2151 (120)
8-12S	35 (0), 49 (0), 52 (0), 55 (0), 63 (0), 66 (0), 66 (0), 85 (0), 88 (0), 92 (0), 92 (0), 93 (1), 94 (1), 96 (0), 100 (0), 102 (0), 111 (2), 159 (0), 352 (0), 366 (0), 370 (17), 378 (9), 379 (0), 386 (11), 398 (16), 402 (0), 405 (0), 412 (2), 443 (11), 453 (16), 457 (46), 457 (22), 468 (3), 479 (0), 509 (2), 522 (0), 528 (9), 556 (13), 566 (0), 633 (43), 634 (47), 644 (325), 680 (91), 690 (115), 691 (73), 1835 (748), 2035 (59), 2040 (272), 2051 (787), 2068 (1776), 2070 (353), 2072 (2383), 2081 (1001), 2153 (68)	33 (0), 44 (0), 45 (0), 48 (0), 56 (0), 62 (0), 64 (0), 81 (0), 82 (0), 87 (0), 87 (1), 89 (0), 89 (1), 93 (0), 96 (0), 99 (0), 107 (1), 155 (0), 350 (0), 359 (2), 365 (0), 370 (0), 382 (9), 395 (0), 396 (0), 413 (5), 423 (10), 427 (0), 449 (2), 451 (12), 471 (26), 471 (1), 472 (21), 482 (0), 494 (1), 510 (4), 515 (2), 545 (6), 555 (0), 636 (54), 637 (46), 640 (207), 664 (59), 674 (64), 680 (102), 1800 (579), 1941 (318), 1947 (933), 1969 (556), 1985 (2029), 1986 (106), 1989 (882), 2012 (712), 2065 (66)	58 (0), 58 (0), 62 (0), 70 (0), 71 (0), 74 (0), 77 (0), 85 (1), 86 (1), 95 (0), 96 (0), 100 (0), 101 (0), 103 (0), 105 (0), 107 (0), 111 (1), 172 (0), 359 (0), 372 (15), 378 (0), 381 (0), 394 (0), 396 (3), 403 (12), 414 (0), 421 (2), 427 (9), 427 (2), 444 (33), 445 (46), 455 (5), 475 (1), 493 (0), 510 (1), 520 (4), 533 (2), 559 (12), 566 (0), 636 (35), 637 (41), 653 (263), 662 (144), 690 (59), 697 (45), 1842 (690), 2015 (240), 2024 (948), 2043 (628), 2057 (0), 2065 (2327), 2071 (1136), 2082 (620), 2149 (92)

Table S4. The Cartesian coordinates of the optimized $CrMn(NO)(CO)_9$ isomers at the B3LYP/DZP, BP86/DZP and M06-L/cc-pVTZ levels.

$CrMn(NO)(CO)_9$ (**9-1S**) C_{4v} B3LYP/DZP	$CrMn(NO)(CO)_9$ (**9-1S**) C_{4v} BP86/DZP	$CrMn(NO)(CO)_9$ (**9-1S**) C_{4v} M06-L/cc-pVTZ
0 1	0 1	0 1
Mn,0.,0.,-0.1474083073	Mn,0.,0.,-0.1130319761	Mn,0.,0.,-1.4587656793
Cr,0.,0.,2.9208267606	Cr,0.,0.,2.8962385343	Cr,0.,0.,1.5279510536
C,1.8588965619,0.,-0.0209380371	C,1.8470071287,0.,-0.0073403624	C,0.,1.8566227758,-1.3100901331
C,0.,-1.8588965619,-0.0209380371	C,0.,-1.8470071287,-0.0073403624	C,1.8566227758,0.,-1.3100901331
C,-1.8588965619,0.,-0.0209380371	C,-1.8470071287,0.,-0.0073403624	C,0.,-1.8566227758,-1.3100901331
C,0.,1.8588965619,-0.0209380371	C,0.,1.8470071287,-0.0073403624	C,-1.8566227758,0.,-1.3100901331
C,0.,0.,-1.9615935936	C,0.,0.,-1.9165469035	C,0.,0.,-3.2691291041
C,1.3593318099,-1.3593318099,2.7160372295	C,1.3495451243,-1.3495451243,2.7012079964	C,1.3582962296,1.3582962296,1.2887357674
C,-1.3593318099,-1.3593318099,2.7160372295	C,-1.3495451243,-1.3495451243,2.7012079964	C,1.3582962296,-1.3582962296,1.2887357674
C,-1.3593318099,1.3593318099,2.7160372295	C,-1.3495451243,1.3495451243,2.7012079964	C,-1.3582962296,-1.3582962296,1.2887357674
C,1.3593318099,1.3593318099,2.7160372295	C,1.3495451243,1.3495451243,2.7012079964	C,-1.3582962296,1.3582962296,1.2887357674
N,0.,0.,4.6086469707	N,0.,0.,4.5993590388	N,0.,0.,3.2218048155
O,3.013403745,0.,0.0148823525	O,3.0160160718,0.,-0.0036458353	O,0.,2.9995628711,-1.241986275
O,0.,-3.013403745,0.0148823525	O,0.,-3.0160160718,-0.0036458353	O,2.9995628711,0.,-1.241986275
O,-3.013403745,0.,0.0148823525	O,-3.0160160718,0.,-0.0036458353	O,0.,-2.9995628711,-1.241986275
O,0.,3.013403745,0.0148823525	O,0.,3.0160160718,-0.0036458353	O,-2.9995628711,0.,-1.241986275
O,0.,0.,-3.118431845	O,0.,0.,-3.0881593344	O,0.,0.,-4.4160656704
O,2.1737116422,-2.1737116422,2.6509155254	O,2.1745903598,-2.1745903598,2.6510863447	O,2.1628104116,2.1628104116,1.1735353317
O,-2.1737116422,-2.1737116422,2.6509155254	O,-2.1745903598,-2.1745903598,2.6510863447	O,2.1628104116,-2.1628104116,1.1735353317
O,-2.1737116422,2.1737116422,2.6509155254	O,-2.1745903598,2.1745903598,2.6510863447	O,-2.1628104116,-2.1628104116,1.1735353317
O,2.1737116422,2.1737116422,2.6509155254	O,2.1745903598,2.1745903598,2.6510863447	O,-2.1628104116,2.1628104116,1.1735353317
O,0.,0.,5.7843717416	O,0.,0.,5.7867375151	O,0.,0.,4.3813888596
$CrMn(NO)(CO)_9$ (**9-2S**) C_s B3LYP/DZP	$CrMn(NO)(CO)_9$ (**9-2S**) C_s BP86/DZP	$CrMn(NO)(CO)_9$ (**9-2S**) C_s M06-L/cc-pVTZ
0 1	0 1	0 1
Mn,0.0079924064,-1.5258468644,0.	Mn,-0.0214948327,-1.5069085998,0.	Mn,0.0014393387,-1.4953265934,0.
Cr,0.0517177615,1.5067332941,0.	Cr,0.0891211131,1.4730548048,0.	Cr,0.0679929606,1.4645672551,0.
C,1.318367789,-1.304590413,1.308440148	C,1.275934367,-1.2876155975,1.298777555	C,1.309553426,-1.2482150495,1.3026120801
C,-1.3069913937,-1.4666918359,1.3201122688	C,-1.3254642679,-1.4786559615,1.3123648772	C,-1.3073657372,-1.3991207888,1.3209633987
C,-1.3069913937,-1.4666918359,-1.3201122688	C,-1.3254642679,-1.4786559615,-1.3123648772	C,-1.3073657372,-1.3991207888,-1.3209633987
C,1.318367789,-1.304590413,-1.308440148	C,1.275934367,-1.2876155975,-1.298777555	C,1.309553426,-1.2482150495,-1.3026120801
C,0.1194272637,-3.3359768661,0.	C,0.1117283104,-3.3042100068,0.	C,0.1057532902,-3.3015867981,0.
C,-0.0597968419,1.4468007877,1.925358112	C,-0.0420270058,1.4519898368,1.9099331086	C,-0.0538636692,1.3578393234,1.925082509
C,-1.8959042546,1.2320923535,0.	C,-1.8327516976,1.1941224243,0.	C,-1.8849350665,1.1800503172,0.
C,-0.0597968419,1.4468007877,-1.925358112	C,-0.0420270058,1.4519898368,-1.9099331086	C,-0.0538636692,1.3578393234,-1.925082509
O,2.1377763124,-1.2033441728,2.1155997208	O,2.1064456444,-1.2086610106,2.1183391528	C,-0.092535843,3.3283513014,0.
O,-2.1191550402,-1.4569244655,2.140880597	O,-2.1449334114,-1.5047007639,2.1455362909	N,1.7960853497,1.3904832613,0.
O,-2.1191550402,-1.4569244655,-2.140880597	O,-2.1449334114,-1.5047007639,-2.1455362909	O,2.1213661457,-1.1102716644,2.0986131135
O,2.1377763124,-1.2033441728,-2.1155997208	O,2.1064456444,-1.2086610106,-2.1183391528	O,-2.1070351564,-1.3419452873,2.1384682845
O,0.1916313446,-4.4906564694,0.	O,0.2019238724,-4.4726614502,0.	O,-2.1070351564,-1.3419452873,-2.1384682845
O,-0.1260415052,1.4356181096,3.0775067481	O,-0.1339239179,1.4908443339,3.0739723078	O,2.1213661457,-1.1102716644,-2.0986131135
O,-3.0432752473,1.1163319388,0.	O,-2.9968005255,1.1072642487,0.	O,0.1727404409,-4.4468599757,0.
O,-0.1260415052,1.4356181096,-3.0775067481	O,-0.1339239179,1.4908443339,-3.0739723078	O,-0.1334312283,1.2918876267,3.0642352059
O,2.9432750941,1.3385274119,0.	O,3.0111628195,1.4109669482,0.	O,-3.0185230209,1.0427170071,0.
O,-0.1315972515,4.5343099201,0.	O,-0.1633863757,4.494614775,0.	O,-0.1334312283,1.2918876267,-3.0642352059
C,-0.0936437161,3.3777403252,0.	C,-0.0893477293,3.324844142,0.	O,2.9513091357,1.3325127136,0.
N,1.7710622032,1.4059914277,0.	N,1.8267937045,1.4220097402,0.	O,-0.1480413875,4.4743546398,0.
$CrMn(NO)(CO)_9$ (**9-3S**) C_s B3LYP/DZP	$CrMn(NO)(CO)_9$ (**9-3S**) C_s BP86/DZP	$CrMn(NO)(CO)_9$ (**9-3S**) C_s M06-L/cc-pVTZ
0 1	0 1	0 1
Mn,0.3150786642,1.4765355783,0.	Mn,0.3080402702,1.4368193153,0.	Mn,0.3285687457,1.4399754514,0.
Cr,-0.2614525904,-1.3866014967,0.	Cr,-0.2338286219,-1.3699940068,0.	Cr,-0.2440066741,-1.3734494032,0.
C,-1.7848165381,-0.2147479195,0.	C,-1.7503448677,-0.181936879,0.	C,-1.7686176864,-0.1927332395,0.
C,-1.1020292361,2.7024452904,0.	C,-1.1062275548,2.6356314458,0.	C,-1.1103773409,2.6299715309,0.
C,1.6720352981,2.6802435001,0.	C,1.6447294168,2.6404888478,0.	C,1.6585777131,2.6599174176,0.
C,0.3304719309,1.5703852858,1.8793011825	C,0.3182959746,1.5841740946,1.8547103835	C,0.3275818948,1.5387848217,1.8746261772
C,0.3304719309,1.5703852858,-1.8793011825	C,0.3182959746,1.5841740946,-1.8547103835	C,0.3275818948,1.5387848217,-1.8746261772
C,-1.5857760228,-2.7514696712,0.	C,-1.5696020032,-2.7023350698,0.	C,-1.5830678246,-2.7107794347,0.
C,-0.2509352974,-1.4567481974,1.9232225936	C,-0.22966767,-1.4577805357,1.9103783646	C,-0.2477018871,-1.4157416588,1.9252991447
O,-2.8620136974,0.2275561908,0.	O,-2.8552171575,0.2264832799,0.	C,-0.2477018871,-1.4157416588,-1.9252991447
O,2.5245887701,-0.3563776959,0.	O,2.5702489807,-0.3570252317,0.	C,1.0226211908,-2.8289798404,0.
O,-1.9586318445,3.4741929515,0.	O,-1.9675418308,3.4248583453,0.	N,1.400632514,-0.1342016071,0.
O,2.5574310059,3.4233299456,0.	O,2.5229098762,3.4159862425,0.	O,-2.8377389444,0.2414184446,0.
O,0.358675283,1.7146137753,3.0210776129	O,0.3426404497,1.7871496244,3.0038136359	O,2.5647352515,-0.3699342566,0.
O,0.358675283,1.7146137753,-3.0210776129	O,0.3426404497,1.7871496244,-3.0038136359	O,-1.9736869166,3.3798001362,0.
O,-2.3964990747,-3.5764291999,0.	O,-2.403707142,-3.5228024821,0.	O,2.5169003036,3.4210846656,0.
O,1.7814764614,-3.6999057887,0.	O,1.7240881486,-3.7394919252,0.	O,0.338852576,1.6813393999,3.0074924694
O,-0.2604125204,-1.567252162,3.0730680118	O,-0.2455174549,-1.5945633149,3.0711012569	O,0.338852576,1.6813393999,-3.0074924694
O,-0.2604125204,-1.567252162,-3.0730680118	O,-0.2455174549,-1.5945633149,-3.0711012569	O,-2.4036534589,-3.5108247593,0.
C,-0.2509352974,-1.4567481974,-1.9232225936	C,-0.22966767,-1.4577805357,-1.9103783646	O,1.7636933919,-3.6966208828,0.
C,1.0274789129,-2.8298517985,0.	C,0.9919422209,-2.8316217054,0.	O,-0.2746852175,-1.493719675,3.0668512414
N,1.3402042414,-0.1149587251,0.	N,1.3756807991,-0.1370613451,0.	O,-0.2746852175,-1.493719675,-3.0668512414

Table S5. The Cartesian coordinates of the optimized $CrMn(NO)(CO)_8$ isomers at the B3LYP/DZP, BP86/DZP and M06-L/cc-pVTZ levels.

$CrMn(NO)(CO)_8$ (**8-1S**) C_s B3LYP/DZP
0 1
Mn,-0.1354984392,0.,-0.1772288059
Cr,0.0699197426,0.,2.8517458711
C,1.6799795751,0.,-0.3314683826
C,-0.1103146053,1.8871156354,-0.1917030323
C,-0.1103146053,-1.8871156354,-0.1917030323
C,-0.4834979321,0.,-1.970436014
C,1.9793239067,0.,2.9947551015
C,0.2241162135,1.9030729455,3.1050227083
C,0.2241162135,-1.9030729455,3.1050227083
C,-0.5949235573,0.,4.6034128655
N,-1.1734076926,0.,1.6476370737
O,2.8323707413,0.,-0.438470311
O,-0.0548568947,3.0341923168,-0.2610975574
O,-0.0548568947,-3.0341923168,-0.2610975574
O,-0.7267262581,0.,-3.1001492256
O,3.1364049292,0.,2.998833469
O,0.3191551733,3.0337433936,3.3165354954
O,0.3191551733,-3.0337433936,3.3165354954
O,-1.0907853331,0.,5.6512461467
O,-2.0079244109,0.,0.7353750501

$CrMn(NO)(CO)_8$ (**8-1S**) C_s BP86/DZP
0 1
Mn,-0.1543240444,0.,-0.1499745322
Cr,0.0393596075,0.,2.8121777946
C,1.6384530816,0.,-0.3009302911
C,-0.0830386022,1.8602253177,-0.1870766146
C,-0.0830386022,-1.8602253177,-0.1870766146
C,-0.4875227697,0.,-1.928578998
C,1.933698262,0.,2.9115239814
C,0.2343036214,1.8700782894,3.1322206961
C,0.2343036214,-1.8700782894,3.1322206961
C,-0.6082696266,0.,4.5536328915
N,-1.2405477608,0.,1.6371834369
O,2.8035256791,0.,-0.4358564782
O,0.0274647279,3.0168394436,-0.2920216584
O,0.0274647279,-3.0168394436,-0.2920216584
O,-0.7133542547,0.,-3.0773724388
O,3.1047449744,0.,2.9185507594
O,0.3637993844,2.9985058251,3.4086553219
O,0.3637993844,-2.9985058251,3.4086553219
O,-1.0863661841,0.,5.625596716
O,-2.0734362297,0.,0.7136562609

$CrMn(NO)(CO)_8$ (**8-1S**) C_s M06-L/cc-pVTZ
0 1
Mn,-0.1487440341,0.,-0.1374582445
Cr,0.0017517376,0.,2.7952793648
C,1.654609835,0.,-0.2440264658
C,-0.091527849,1.8795575593,-0.1160710636
C,-0.091527849,-1.8795575593,-0.1160710636
C,-0.4308782368,0.,-1.9325001559
C,1.9102692855,0.,2.8438427038
C,0.1953766087,1.9006163231,3.0452676021
C,0.1953766087,-1.9006163231,3.0452676021
C,-0.5529442933,0.,4.5837998417
N,-1.2957298507,0.,1.643417775
O,2.7997951562,0.,-0.3313969072
O,0.0060020086,3.0164366922,-0.1443217588
O,0.0060020086,-3.0164366922,-0.1443217588
O,-0.6046959621,0.,-3.065641235
O,3.0566230999,0.,2.8081869852
O,0.3317615122,3.0173301519,3.2505515997
O,0.3317615122,-3.0173301519,3.2505515997
O,-0.9575491614,0.,5.6590071046
O,-2.0744301729,0.,0.7090115131

$CrMn(NO)(CO)_8$ (**8-2S**) C_s B3LYP/DZP
0 1
Mn,-0.2017493698,1.4743026727,0.
Cr,-0.1489333945,-1.5596962419,0.
C,1.609310354,1.5699788409,0.
C,-0.1609001316,1.5081919737,1.8769583034
C,-0.1609001316,1.5081919737,-1.8769583034
C,-0.5297375008,3.2721546251,0.
C,1.7780058149,-1.7056425531,0.
C,-0.1074964388,-1.5431193878,1.9324638983
C,-0.1074964388,-1.5431193878,-1.9324638983
O,2.7656447879,1.6448586944,0.
O,-0.091484701,1.6154729914,3.0223326823
O,-0.091484701,1.6154729914,-3.0223326823
O,-0.7407219817,4.4083190955,0.
O,2.9268535466,-1.8039817526,0.
O,-0.0934859019,-1.6037846513,3.0837108614
O,-0.0934859019,-1.6037846513,-3.0837108614
O,-1.23240291,-4.2188402228,0.
O,-2.2487950267,0.6652366296,0.
N,-0.742971687,-3.1485370071,0.
C,-1.4847093469,-0.2565882062,0.

$CrMn(NO)(CO)_8$ (**8-2S**) C_s BP86/DZP
0 1
Mn,-0.2359664917,1.4413848034,0.
Cr,-0.1428238803,-1.5364359808,0.
C,1.555422873,1.5072188328,0.
C,-0.1651765921,1.5204472075,1.8534179467
C,-0.1651765921,1.5204472075,-1.8534179467
C,-0.5419475495,3.2289953735,0.
C,1.7625042823,-1.7255064288,0.
C,-0.0807121097,-1.5115734815,1.9173576437
C,-0.0807121097,-1.5115734815,-1.9173576437
O,2.7265363747,1.5929571667,0.
O,-0.0582515834,1.6808916548,3.0055747739
O,-0.0582515834,1.6808916548,-3.0055747739
O,-0.729816166,4.38455715,0.
O,2.9227823531,-1.8543897409,0.
O,-0.0455883453,-1.5747919687,3.082268322
O,-0.0455883453,-1.5747919687,-3.082268322
O,-1.2263820088,-4.2217033837,0.
O,-2.2980629989,0.6525935683,0.
N,-0.7397985347,-3.1377163011,0.
C,-1.5099126065,-0.2665050843,0.

$CrMn(NO)(CO)_8$ (**8-2S**) C_s M06-L/cc-pVTZ
0 1
Mn,-0.2233700612,1.420972993,0.
Cr,-0.1754849979,-1.51703807,0.
C,1.5760961129,1.4515176772,0.
C,-0.170020588,1.4595298498,1.8707777265
C,-0.170020588,1.4595298498,-1.8707777265
C,-0.490300782,3.2224523101,0.
C,1.7507192554,-1.6323002217,0.
C,-0.113771477,-1.463417041,1.933106342
C,-0.113771477,-1.463417041,-1.933106342
C,-1.5745462439,-0.2631389861,0.
N,-0.696684174,-3.1376057398,0.
O,2.7253562995,1.4926195906,0.
O,-0.0798029087,1.5692069411,3.0050526961
O,-0.0798029087,1.5692069411,-3.0050526961
O,-0.6411919442,4.3587454243,0.
O,2.8915990362,-1.699643985,0.
O,-0.0781030448,-1.4924658237,3.0747527942
O,-0.0781030448,-1.4924658237,-3.0747527942
O,-1.1144256757,-4.2203207976,0.
O,-2.3012387684,0.6743446274,0.

$CrMn(NO)(CO)_8$ (**8-3S**) C_s B3LYP/DZP
0 1
Mn,-0.0065644303,1.406659846,0.
Cr,-0.119383732,-1.4286096695,0.
C,-1.3339973423,1.3094898268,1.2950663902
C,1.310490889,1.2078011434,1.294330945
C,1.310490889,1.2078011434,-1.294330945
C,-1.3339973423,1.3094898268,-1.2950663902
C,0.0624062202,3.226679076,0.
C,-0.1043248529,-1.27174166,1.9264329332
C,1.4593462364,-2.4600755841,0.
C,-0.1043248529,-1.27174166,-1.9264329332
N,-1.1093250896,-2.7960230996,0.
O,-2.1722934594,1.2893857037,2.0927505132
O,2.1452085963,1.1253752437,2.0916955774
O,2.1452085963,1.1253752437,-2.0916955774
O,-2.1722934594,1.2893857037,-2.0927505132
O,0.106640748,4.3827026461,0.
O,-0.1075429094,-1.2767464547,3.0798320335
O,2.4370362075,-3.075044466,0.
O,-0.1075429094,-1.2767464547,-3.0798320335
O,-1.8750152474,-3.6905058356,0.

$CrMn(NO)(CO)_8$ (**8-3S**) C_s BP86/DZP
0 1
Mn,0.0032937804,1.3667659678,0.
Cr,-0.2304068001,-1.4034214919,0.
C,-1.3169149435,1.3236017355,1.2898857842
C,1.309945776,1.1453983268,1.2893360638
C,1.309945776,1.1453983268,-1.2893360638
C,-1.3169149435,1.3236017355,-1.2898857842
C,0.1206482131,3.1785623176,0.
C,-0.1856715959,-1.2595162856,1.9118783173
C,1.4032165769,-2.271348833,0.
C,-0.1856715959,-1.2595162856,-1.9118783173
N,-1.079154175,-2.877482189,0.
O,-2.1662727384,1.3538169006,2.095821737
O,2.1543216958,1.0639043819,2.0955657154
O,2.1543216958,1.0639043819,-2.0955657154
O,-2.1662727384,1.3538169006,-2.095821737
O,0.1954561694,4.347077226,0.
O,-0.146371454,-1.2903247108,3.0795503772
O,2.4461214735,-2.8056834952,0.
O,-0.146371454,-1.2903247108,-3.0795503772
O,-1.726211509,-3.8763696516,0.

$CrMn(NO)(CO)_8$ (**8-3S**) C_s M06-L/cc-pVTZ
0 1
Mn,0.0291266254,1.3559854345,0.
Cr,-0.4574405482,-1.4472000675,0.
C,-1.2933663393,1.3926185204,1.2988359042
C,1.306261707,0.9753705055,1.2993190755
C,1.306261707,0.9753705055,-1.2993190755
C,-1.2933663393,1.3926185204,-1.2988359042
C,0.3041915721,3.1535530348,0.
C,-0.4297106013,-1.2690440501,1.9281573208
C,1.362658439,-1.8361510875,0.
C,-0.4297106013,-1.2690440501,-1.9281573208
N,-0.9266155954,-3.0727092211,0.
O,-2.1156983115,1.4420710577,2.0979320729
O,2.1020103342,0.756274898,2.0943749889
O,2.1020103342,0.756274898,-2.0943749889
O,-2.1156983115,1.4420710577,-2.0979320729
O,0.4745762134,4.2875521505,0.
O,-0.3808836783,-1.2245604465,3.0700200717
O,2.4887314064,-2.0551245321,0.
O,-0.3808836783,-1.2245604465,-3.0700200717
O,-1.218489301,-4.1976685127,0.

$CrMn(NO)(CO)_8$ (**8-4S**) C_s B3LYP/DZP
0 1
Mn,-0.2142352413,1.4911169936,0.
Cr,-0.0697182265,-1.5161042023,0.
C,1.598460432,1.5845214804,0.
C,-0.1680783318,1.509124659,1.878601758
C,-0.1680783318,1.509124659,-1.878601758
C,-0.5443361445,3.2864970355,0.
C,-0.2094216678,-1.606180809,1.9204315871
O,2.7547370187,1.640944783,0.
O,-0.0909577125,1.5915740952,3.0251802553
O,-0.0909577125,1.5915740952,-3.0251802553
O,-0.7571281544,4.4226491534,0.
O,2.8212679413,-1.5569924742,0.
O,-0.3055621939,-1.7187768793,3.0645302964
O,-0.3055621939,-1.7187768793,-3.0645302964
O,-0.976405051,-4.4322679267,0.
O,-2.2409908025,0.6557281496,0.
C,-1.4809948046,-0.2699426055,0.
C,-0.6447192616,-3.3254648978,0.
N,1.6463307653,-1.5978596081,0.
C,-0.2094216678,-1.606180809,-1.9204315871

$CrMn(NO)(CO)_8$ (**8-4S**) C_s BP86/DZP
0 1
Mn,-0.2393674669,1.4750286856,0.
Cr,-0.0468552471,-1.4876177518,0.
C,1.5509501238,1.5434691363,0.
C,-0.1602648789,1.5250635146,1.8546441603
C,-0.1602648789,1.5250635146,-1.8546441603
C,-0.5476332621,3.2607763889,0.
C,-0.2345369878,-1.6173320468,1.8980382093
O,2.7226362964,1.6145277291,0.
O,-0.0413831129,1.6451033781,3.0102712328
O,-0.0413831129,1.6451033781,-3.0102712328
O,-0.7364792083,4.416515315,0.
O,2.869116583,-1.5590026553,0.
O,-0.3793880609,-1.7738644077,3.0464752224
O,-0.3793880609,-1.7738644077,-3.0464752224
O,-0.9340479521,-4.4032192864,0.
O,-2.2779855951,0.6392350476,0.
C,-1.4698664212,-0.2628365602,0.
C,-0.598520739,-3.2815722659,0.
N,1.6833426641,-1.5789118392,0.
C,-0.2345369878,-1.6173320468,-1.8980382093

$CrMn(NO)(CO)_8$ (**8-4S**) C_s M06-L/cc-pVTZ
0 1
Mn,-0.2371986004,1.4596874976,0.
Cr,-0.0667328687,-1.4599719933,0.
C,1.5614615813,1.494042813,0.
C,-0.1736947175,1.4584807228,1.8721923733
C,-0.1736947175,1.4584807228,-1.8721923733
C,-0.5149397675,3.2579432967,0.
C,-0.2286744515,-1.5487452611,1.9203690968
C,-1.5350383941,-0.263470941,0.
C,-0.5747266075,-3.2830690837,0.
C,-0.2286744515,-1.5487452611,-1.9203690968
N,1.6577507249,-1.5150942665,0.
O,2.7108502644,1.5181729127,0.
O,-0.0709598559,1.5147147641,3.0090717849
O,-0.0709598559,1.5147147641,-3.0090717849
O,-0.6743994843,4.3934453266,0.
O,2.8152268925,-1.4713347017,0.
O,-0.3498291972,-1.6534589653,3.0522497003
O,-0.3498291972,-1.6534589653,-3.0522497003
O,-0.8647393406,-4.391410831,0.
O,-2.2870941448,0.6540515468,0.

$CrMn(NO)(CO)_8$ (**8-5S**) C_s B3LYP/DZP
0 1
Mn,-0.0000433883,-0.0000452503,0.0004728014
Cr,-0.0000512187,-0.000053421,2.7692123668
C,1.8279119619,0.0008361616,0.3529602912
C,0.0423294603,-1.858184658,-0.0626877517
C,-1.858322005,-0.0357957741,-0.0626877489
C,-0.0759802489,1.8263323478,0.352960294
C,0.2100443481,0.2190647172,-1.7960572369
C,0.8113653423,-1.1007595498,4.0575074981
C,-1.3510549898,-1.4090761161,2.4777201644
O,2.973962849,-0.0059665092,0.5106602325
O,0.0747549247,-3.0118995928,-0.1293266518
O,-3.012380402,-0.0518823539,-0.1293266473
O,-0.1309382383,2.9710849547,0.5106602369
O,0.3495245495,0.3645349045,-2.9347918991
O,1.3518170603,-1.7789827663,4.8235655745
O,-2.1475239332,-2.2397494577,2.4104832475
O,1.9775633884,2.0624899432,3.1699921701
O,-1.8342196197,1.2758633932,4.8235655791
C,-1.1338837431,0.7643905708,4.0575075009
N,1.1782070165,1.2288051724,2.9484779845

$CrMn(NO)(CO)_8$ (**8-5S**) C_s BP86/DZP
0 1
Mn,-1.3635655703,0.063522377,-0.000003058
Cr,1.3130474127,-0.1589031847,0.0000054444
C,-0.9492488435,-1.1547995207,1.3324593692
C,-1.5517774968,1.3770526183,1.2900170911
C,-1.5518132967,1.375921091,-1.2911694241
C,-0.9493995272,-1.1559992205,-1.3314139075
C,-3.1215270125,-0.397137696,0.0002711292
C,2.5960699675,0.1210760788,1.3008552547
C,0.9932917262,1.7537616216,-0.0007664725
O,-0.8023998104,-1.9174642126,2.2103486259
O,-1.7146729031,2.2062015282,2.0977367038
O,-1.7147189652,2.2043669207,-2.0996085251
O,-0.8026430484,-1.9194505396,-2.208633973
O,-4.2473688047,-0.7152839201,0.0004677693
O,3.3940376886,0.284516828,2.1458473415
O,0.9756921638,2.9236906618,-0.0012475277
O,1.9148988512,-3.0139690885,0.0010828313
O,3.3942652946,0.282883467,-2.1459566922
C,2.596200626,0.1200908727,-1.3009310172
N,1.5797734795,-1.8741112827,0.00066233

$CrMn(NO)(CO)_8$ (**8-5S**) C_s M06-L/cc-pVTZ
0 1
Mn,-1.3842338829,-0.1218241561,0.
Cr,1.300107797,0.0283855158,0.
C,-0.8080351623,-1.2988341579,1.3224686472
C,-1.650250546,1.1821458531,1.3001559445
C,-1.650250546,1.1821458531,-1.3001559445
C,-0.8080351623,-1.2988341579,-1.3224686472
C,-3.1020501308,-0.7378287038,0.
C,2.5579973111,0.4247073393,1.3159152828
C,0.7790508212,1.9300938879,0.
C,2.5579973111,0.4247073393,-1.3159152828
N,1.7108834154,-1.6444357511,0.
O,-0.5260662202,-2.0358528329,2.1568923267
O,-1.8257795623,1.9920602298,2.0905162453
O,-1.8257795623,1.9920602298,-2.0905162453
O,-0.5260662202,-2.0358528329,-2.1568923267
O,-4.1743915352,-1.1410117105,0.
O,3.3229835198,0.6470295926,2.1425854359
O,0.5795023601,3.0560475868,0.
O,2.0842566844,-2.7417784508,0.
O,3.3229835198,0.6470295926,-2.1425854359

$CrMn(NO)(CO)_8$ (**8-6S**) C_s B3LYP/DZP
0 1
C,-1.128118973,-0.4803785818,1.3941591601
C,-1.128118973,-0.4803785818,-1.3941591601
N,1.4454128151,0.1780393189,0.
Mn,0.0698580046,1.366559166,0.
Cr,-0.0233633132,-1.2208081908,0.
C,0.7031787085,2.4892222041,-1.2738010154
C,0.7031787085,2.4892222041,1.2738010154
C,-1.6463626464,2.1471594721,0.
C,1.0379799416,-2.1308862135,-1.3384364727
C,1.0379799416,-2.1308862135,1.3384364727
C,-1.2818412118,-2.6583772417,0.
O,-1.8463825398,-0.2449349558,2.2749339777
O,-1.8463825398,-0.2449349558,-2.2749339777
O,2.6518445708,0.1044606545,0.
O,1.122876237,3.1772872866,-2.1039333324
O,1.122876237,3.1772872866,2.1039333324
O,-2.6644315377,2.6911729223,0.
O,1.6857929846,-2.6678662342,-2.1239330313
O,1.6857929846,-2.6678662342,2.1239330313
O,-2.0483455569,-3.5219857814,0.

$CrMn(NO)(CO)_8$ (**8-6S**) C_s BP86/DZP
0 1
C,-1.0889030228,-0.4461916293,1.3873343591
C,-1.0889030228,-0.4461916293,-1.3873343591
N,1.4878268507,0.1883571784,0.
Mn,0.0736889411,1.3259576965,0.
Cr,0.0073512244,-1.2105116315,0.
C,0.6681095106,2.4815053995,-1.2301194323
C,0.6681095106,2.4815053995,1.2301194323
C,-1.6470010514,2.0701624775,0.
C,1.0358661842,-2.1579719339,-1.3054051227
C,1.0358661842,-2.1579719339,1.3054051227
C,-1.2925531437,-2.5875752856,0.
O,-1.8093588451,-0.2249918572,2.2885677897
O,-1.8093588451,-0.2249918572,-2.2885677897
O,2.7011811137,0.1380579039,0.
O,1.0722591856,3.21992477,-2.0477799902
O,1.0722591856,3.21992477,2.0477799902
O,-2.6738698746,2.6292198038,0.
O,1.6734450612,-2.7496841046,-2.0820102452
O,1.6734450612,-2.7496841046,2.0820102452
O,-2.106001023,-3.4264367409,0.

$CrMn(NO)(CO)_8$ (**8-6S**) C_s M06-L/cc-pVTZ
0 1
Mn,0.0793893004,1.3104866287,0.
Cr,0.0120302739,-1.2195330823,0.
C,0.6688201771,2.469487423,-1.2466479571
C,0.6688201771,2.469487423,1.2466479571
C,-1.6650388259,2.0371756319,0.
C,1.052406985,-2.1628452313,-1.3314941789
C,1.052406985,-2.1628452313,1.3314941789
C,-1.3202627653,-2.5818183372,0.
C,-1.0799029124,-0.4244604211,1.3838602225
C,-1.0799029124,-0.4244604211,-1.3838602225
N,1.5013712683,0.1744132159,0.
O,-1.7933438372,-0.1755651948,2.2528765204
O,-1.7933438372,-0.1755651948,-2.2528765204
O,2.6888073557,0.1184311839,0.
O,1.0600856345,3.1925755886,-2.0482196404
O,1.0600856345,3.1925755886,2.0482196404
O,-2.68819189,2.5489139884,0.
O,1.6844121098,-2.7165190432,-2.1031474841
O,1.6844121098,-2.7165190432,2.1031474841
O,-2.1391387119,-3.3809408217,0.

$CrMn(NO)(CO)_8$ (**8-7S**) C_1 B3LYP/DZP
0 1
Mn,1.4904506185,-0.0211518505,-0.210528487
Cr,-1.4819223619,-0.051396441,-0.1407578196
C,1.5890388972,0.0458178282,1.597770732
C,1.6146117089,1.8494107708,-0.2430425915
C,1.3366710047,-1.8900216391,-0.0899986887
C,3.2834772644,-0.1634280384,-0.5235047151
C,-1.691566347,0.023442076,1.7627198868
C,-1.4556460362,1.9172671768,-0.0269049763
O,1.6623584144,0.0913476679,2.7531914631
O,1.7571801493,2.9935856693,-0.2202652858
O,1.2975153327,-3.0359942311,0.0285554897
O,4.4183169617,-0.2582874465,-0.7220292008
O,-1.7810763093,0.0464632413,2.914214005
O,-1.5066264051,3.0643456128,0.0525339352
O,-1.9242389605,-2.9101200411,-0.1128694259
O,-4.2698851099,0.3052540305,-1.2927527336
O,0.6987518745,-0.0293812425,-2.281373565
C,-0.2348407947,0.0125333378,-1.5390914321
C,-3.2151147518,0.1964403527,-0.8301301202
N,-1.6969094406,-1.7595732104,-0.1380476397

$CrMn(NO)(CO)_8$ (**8-7S**) C_1 BP86/DZP
0 1
Mn,1.4745819434,-0.0180971991,-0.2354155463
Cr,-1.4524915176,-0.0642357033,-0.1346301065
C,1.5506876697,0.052084209,1.5513761552
C,1.6204238293,1.832164643,-0.2334724232
C,1.3607909764,-1.8643328644,-0.0799621545
C,3.2598334074,-0.1519456688,-0.5268638793
C,-1.6370451712,0.0235080639,1.7581351074
C,-1.4797948731,1.8709180928,-0.0299215797
O,1.641206158,0.09954468,2.7212320346
O,1.7961140496,2.9856030054,-0.169051646
O,1.3600896098,-3.021535222,0.0820980788
O,4.4135796059,-0.2436641959,-0.7044587252
O,-1.7365402172,0.0665488126,2.9221627453
O,-1.5791184609,3.0306205353,0.0425762985
O,-2.0474806231,-2.9237474663,-0.1343735241
O,-4.2374554294,0.3493587248,-1.2753693077
O,0.7040066816,-0.0283748736,-2.3203355806
C,-0.2142339403,0.0049461436,-1.5361812131
C,-3.1684630995,0.2077732034,-0.816634905
N,-1.7381448896,-1.7805832969,-0.1432209979

$CrMn(NO)(CO)_8$ (**8-7S**) C_1 M06-L/cc-pVTZ
0 1
Mn,1.4460671539,0.0189920924,-0.2229161411
Cr,-1.4304913191,-0.0991678508,-0.1759422138
C,1.4988043973,0.1883610967,1.5653327467
C,1.5832489495,1.8805582088,-0.3454663519
C,1.2266924686,-1.8258340187,0.0125654722
C,3.2392960541,-0.1662781642,-0.4738171678
C,-1.5813783723,-0.1278557766,1.7348688351
C,-1.3421386055,1.8572204533,0.0490779737
C,-0.2228271791,-0.006762172,-1.6223472879
C,-3.1820805221,0.2249397917,-0.7770084424
N,-1.6851060495,-1.8091714413,-0.2520027631
O,1.5461340345,0.3041699315,2.7084630003
O,1.7231700436,3.0154126729,-0.36635301
O,1.1392896805,-2.9491532284,0.2127282427
O,4.3705507674,-0.2910298006,-0.6126676993
O,-1.6371145023,-0.1656464253,2.8775713863
O,-1.350139438,2.9876724805,0.2014124518
O,-1.9273982223,-2.9393064759,-0.2749618892
O,-4.2461645295,0.3919540219,-1.1703196192
O,0.7221281901,-0.0625293959,-2.330530523

$CrMn(NO)(CO)_8$ (**8-8S**) C_s B3LYP/DZP
0 1
Mn,0.1021693185,-1.4076954356,0.
Cr,0.014633694,1.4680451583,0.
C,0.1001189643,-1.2967924484,1.8609149213
C,-1.3945860961,-2.4312746955,0.
C,0.1001189643,-1.2967924484,-1.8609149213
C,1.1557097612,-2.8927588519,0.
C,-1.3510362423,1.1802323712,1.3277755098
C,-1.3510362423,1.1802323712,-1.3277755098
C,1.3899738362,1.2904744752,-1.3362184514
C,1.3899738362,1.2904744752,1.3362184514
N,-0.0465130598,3.1613386105,0.
O,0.0920836957,-1.3302624517,3.0157309484
O,-2.3828039153,-3.0327058146,0.
O,0.0920836957,-1.3302624517,-3.0157309484
O,1.8652502433,-3.8062773315,0.
O,-2.1901356965,1.0682272124,2.1145656358
O,-2.1901356965,1.0682272124,-2.1145656358
O,2.2278812031,1.2435325694,-2.1312102066
O,2.2278812031,1.2435325694,2.1312102066
O,-0.0899264284,4.3362337267,0.

$CrMn(NO)(CO)_8$ (**8-8S**) C_s BP86/DZP
0 1
Mn,0.1015423177,-1.3585842525,0.
Cr,0.0132326705,1.4385691185,0.
C,0.0885047947,-1.2649480428,1.8496264463
C,-1.334007226,-2.408368713,0.
C,0.0885047947,-1.2649480428,-1.8496264463
C,1.1259946363,-2.8306222193,0.
C,-1.3490970425,1.1639616221,1.3173010678
C,-1.3490970425,1.1639616221,-1.3173010678
C,1.3804927366,1.2569615512,-1.3264936477
C,1.3804927366,1.2569615512,1.3264936477
N,-0.0347320547,3.1506541308,0.
O,0.0688714239,-1.3365204205,3.0172757816
O,-2.310067753,-3.0608233015,0.
O,0.0688714239,-1.3365204205,-3.0172757816
O,1.8320080156,-3.7679183633,0.
O,-2.2047081685,1.0661670449,2.1086411894
O,-2.2047081685,1.0661670449,-2.1086411894
O,2.2333629486,1.2155201623,-2.1264853403
O,2.2333629486,1.2155201623,2.1264853403
O,-0.067606226,4.3369121907,0.

$CrMn(NO)(CO)_8$ (**8-8S**) C_s M06-L/cc-pVTZ
0 1
Mn,0.4145809903,-1.4042421445,0.
Cr,-0.0308935275,1.4369431068,0.
C,0.3899076287,-1.2854469219,1.8622548552
C,-1.3115740859,-1.8635671733,0.
C,0.3899076287,-1.2854469219,-1.8622548552
C,0.9656574617,-3.1319945581,0.
C,-1.3502416096,0.968972452,1.3331809303
C,-1.3502416096,0.968972452,-1.3331809303
C,1.3496491816,1.3587105324,-1.3390847172
C,1.3496491816,1.3587105324,1.3390847172
N,-0.2559157136,3.1217835965,0.
O,0.3407630395,-1.2787005922,3.0064847763
O,-2.4302286527,-2.1264724887,0.
O,0.3407630395,-1.2787005922,-3.0064847763
O,1.2856531829,-4.2344463918,0.
O,-2.1455780871,0.7089183106,2.1144667311
O,-2.1455780871,0.7089183106,-2.1144667311
O,2.1790300989,1.3426761589,-2.1307388414
O,2.1790300989,1.3426761589,2.1307388414
O,-0.402074064,4.2723664497,0.

$CrMn(NO)(CO)_8$ (**8-9S**) C_1 B3LYP/DZP
0 1
Mn,1.3749062567,-0.0396859715,-0.0428632764
Cr,-1.3741402024,0.0402469929,-0.0760622534
C,1.708789468,1.7990482235,0.0606701959
C,2.4864285197,-0.3831383398,1.3487150893
C,0.8518344401,-1.8231535455,-0.172905852
C,2.7276721944,-0.2858594631,-1.233944229
C,-0.9278046371,1.4002659114,-1.3658029143
C,-0.7329152334,1.1580420107,1.3839742434
C,-1.7126157472,-1.2407552077,1.328335125
O,2.0007887312,2.9139512746,0.1190422587
O,3.1503242475,-0.5993562203,2.2709661815
O,0.6823073181,-2.9651254564,-0.25893373
O,3.5540758587,-0.4442887335,-2.0275057126
O,-0.7236919853,2.2166419443,-2.159881179
O,-0.4718176519,1.8009232696,2.3135997829
O,-1.9348654944,-2.0064931936,2.1629141642
O,-1.7900258767,-2.0610051575,-2.0360719708
O,-4.1977948739,1.1580152191,0.0552196064
C,-3.1176961602,0.7469304967,0.0312616842
N,-1.6072985612,-1.1868438037,-1.2715631719

$CrMn(NO)(CO)_8$ **8-9S**) C_1 BP86/DZP
0 1
Mn,1.2933160117,0.0964758637,0.0040106349
Cr,-1.3059128733,-0.103156848,-0.0856903145
C,1.6838049806,1.9072579683,0.1809517672
C,2.4796412457,-0.3121598895,1.2744552302
C,0.7903290229,-1.6804899283,-0.1745928493
C,2.5743857409,-0.1053077212,-1.2361418844
C,-0.7532445848,1.1901185999,-1.4008693863
C,-0.6224816437,0.988339812,1.3646913199
C,-1.8383218922,-1.2853109782,1.3342683869
O,2.0525550994,3.0123519553,0.2835518171
O,3.2276039764,-0.5875673796,2.1356556071
O,0.7508269434,-2.8519612033,-0.2736567736
O,3.3844875453,-0.2461641006,-2.072658254
O,-0.5544854122,1.9807993825,-2.2426019693
O,-0.4586547677,1.6127719689,2.3499076878
O,-2.1893509781,-1.9939516658,2.1919249136
O,-2.0041905759,-2.2702711842,-1.9293269387
O,-3.9545013797,1.3916251912,-0.0158228237
C,-2.9334529227,0.8217939327,-0.0242371616
N,-1.6758929252,-1.3668335254,-1.234654967

$CrMn(NO)(CO)_8$ (**8-9S**) C_1 M06-L/cc-pVTZ
0 1
Mn,1.2889263914,0.061373504,-0.0022602529
Cr,-1.3355232886,-0.0632031601,-0.0824672883
C,1.6513907554,1.8957000023,0.1565863026
C,2.4809827046,-0.3314893139,1.2853646628
C,0.7763925507,-1.7220663462,-0.1595019744
C,2.5744289709,-0.1432632612,-1.2509097928
C,-0.7244036416,1.2285466018,-1.3865644028
C,-0.6719617128,1.0382684792,1.3875189899
C,-1.7748316355,-1.3065244717,1.3399662933
C,-2.9932431149,0.8346115053,-0.0344054713
N,-1.6699003387,-1.3229454726,-1.2358655652
O,1.9680685718,2.99138904,0.2466379326
O,3.213274611,-0.5867982354,2.1319737698
O,0.666347739,-2.8643998971,-0.2487504878
O,3.3679951101,-0.2818545057,-2.0686552891
O,-0.4575996823,2.0039778122,-2.1910548611
O,-0.4489771393,1.6553014422,2.3347647856
O,-2.029590871,-2.0487877641,2.1699728888
O,-1.9329668142,-2.2144076357,-1.9268923747
O,-4.0023301659,1.3749456767,-0.0362828651

CrMn(NO)(CO)$_8$ (**8-10S**) C_s B3LYP/DZP
0 1
C,0.440086688,0.3878929149,1.8575439154
C,1.8287235634,0.3878929149,-0.5476457061
C,-1.3517874914,-0.0765534899,-0.7804548721
Mn,-0.101937747,-1.4127303009,-0.0588537857
Cr,0.1905968175,1.1510870055,0.1100411239
C,-0.241485688,-2.3474069659,-1.6177503729
C,-1.5217557639,-2.3474069659,0.599742446
N,1.1547959425,-2.3118651214,0.6667217482
C,-0.0354534654,2.07514439,-1.5618866567
C,-1.3703602553,2.07514439,0.7502397267
C,1.2602606804,2.5931286516,0.7276118431
O,0.6147730903,0.0832211958,2.9624476049
O,2.8729414284,0.0832211958,-0.9488146886
O,-2.3595679956,0.0972580439,-1.3622972174
O,-0.3045914926,-2.9223127715,-2.6170662359
O,-2.41874159,-2.9223127715,1.0447491476
O,1.8022300389,-3.2205560174,1.0405179981
O,-0.1778170011,2.6522092532,-2.5505471005
O,-2.2977470831,2.6522092532,1.1212795101
O,1.9212504926,3.4598616315,1.1092344891

CrMn(NO)(CO)$_8$ (**8-10S**) C_s BP86/DZP
0 1
C,0.3925648356,0.3599174287,1.8273352197
C,1.7788011392,0.3599174287,-0.5736964896
C,-1.3582838881,-0.0740163671,-0.7842055685
Mn,-0.0796848513,-1.3748621896,-0.0460060703
Cr,0.1665857898,1.1475184237,0.0961783506
C,-0.2276704535,-2.3282305008,-1.5633876434
C,-1.4677686419,-2.3282305008,0.5845254253
N,1.1922001237,-2.2768217012,0.6883170624
C,-0.0610419874,2.1045849596,-1.5384664629
C,-1.3628720335,2.1045849596,0.7163693197
C,1.2814468712,2.5268061737,0.739843696
O,0.553650523,0.05835115,2.9504429892
O,2.8319838426,0.05835115,-0.9957460768
O,-2.3812638725,0.0707290248,-1.3748233378
O,-0.3122422425,-2.9417635274,-2.5574589102
O,-2.3709455066,-2.9417635274,1.0083197409
O,1.8471980759,-3.1935640707,1.0664803063
O,-0.2143710314,2.7195039839,-2.5190324624
O,-2.2887316211,2.7195039839,1.0738654722
O,1.9840179683,3.367620669,1.1454733081

CrMn(NO)(CO)$_8$ (**8-10S**) C_s M06-L/cc-pVTZ
0 1
Mn,0.0470161799,-1.3226200284,0.
Cr,0.0597949576,1.2079553972,0.
C,1.205110216,0.5114830947,1.3814107653
C,1.205110216,0.5114830947,-1.3814107653
C,-1.575450905,-0.2094929475,0.
C,-0.7355799632,-2.3679659159,-1.2534996815
C,-0.7355799632,-2.3679659159,1.2534996815
C,-1.0766673168,2.0292344103,-1.3198072919
C,-1.0766673168,2.0292344103,1.3198072919
C,1.203256751,2.7234381501,0.
N,1.610732724,-2.0255744392,0.
O,1.9224579761,0.2579540919,2.2445065176
O,1.9224579761,0.2579540919,-2.2445065176
O,-2.7413075497,-0.1740527548,0.
O,-1.2346278937,-3.0177365001,-2.0545626324
O,-1.2346278937,-3.0177365001,2.0545626324
O,2.476511715,-2.7970847051,0.
O,-1.7683573467,2.5296384296,-2.0795355658
O,-1.7683573467,2.5296384296,2.0795355658
O,1.9126270558,3.6209060045,0.

CrMn(NO)(CO)$_8$ (**8-11S**) C_s B3LYP/DZP
0 1
Mn,-0.0924314184,1.2048724967,0.
Cr,0.1253802823,-1.8101822351,0.
C,-1.3653969749,0.834727144,1.3091065064
C,1.2138140445,1.2814117326,1.3229780821
C,1.2138140445,1.2814117326,-1.3229780821
C,-1.3653969749,0.834727144,-1.3091065064
C,-0.4032758172,2.990609706,0.
C,0.2147618365,-1.8296928468,1.9284422752
C,2.0178626122,-1.2718351437,0.
C,0.2147618365,-1.8296928468,-1.9284422752
O,-2.1635948142,0.6422449501,2.1219531701
O,2.0169742437,1.349836124,2.1511261597
O,2.0169742437,1.349836124,-2.1511261597
O,-2.1635948142,0.6422449501,-2.1219531701
O,-0.6027506225,4.1309977912,0.
O,0.2583603621,-1.8437361868,3.0826776584
O,3.1388611917,-0.992216647,0.
O,0.2583603621,-1.8437361868,-3.0826776584
O,-2.7652084465,-1.8541394068,0.
N,-1.5859790999,-1.8683909076,0.

CrMn(NO)(CO)$_8$ (**8-11S**) C_s BP86/DZP
0 1
Mn,-0.0593848194,1.1832119494,0.
Cr,0.0828435627,-1.7882617468,0.
C,-1.3135354524,0.8143646492,1.30812885
C,1.2304829388,1.3128867462,1.3181365243
C,1.2304829388,1.3128867462,-1.3181365243
C,-1.3135354524,0.8143646492,-1.30812885
C,-0.4049934537,2.9522724778,0.
C,0.2079996901,-1.8751149228,1.9056038056
C,1.9297628125,-1.2087624425,0.
C,0.2079996901,-1.8751149228,-1.9056038056
O,-2.1167388093,0.6437949085,2.1408300621
O,2.0327544363,1.4361464232,2.1596873297
O,2.0327544363,1.4361464232,-2.1596873297
O,-2.1167388093,0.6437949085,-2.1408300621
O,-0.6352065764,4.1018718246,0.
O,0.2955538168,-1.9651228597,3.0698964377
O,3.0706178586,-0.9436931192,0.
O,0.2955538168,-1.9651228597,-3.0698964377
O,-2.8324702567,-1.8026730165,0.
N,-1.6420383736,-1.8321484798,0.

CrMn(NO)(CO)$_8$ (**8-11S**) C_s M06-L/cc-pVTZ
0 1
Mn,-0.0956711722,1.1640184375,0.
Cr,0.1178742612,-1.7841162929,0.
C,-1.3662477432,0.7775352464,1.3043606341
C,1.2058221659,1.200887731,1.3280863328
C,1.2058221659,1.200887731,-1.3280863328
C,-1.3662477432,0.7775352464,-1.3043606341
C,-0.389602138,2.9484859991,0.
C,0.2152815065,-1.7070235847,1.9211468402
C,2.0218984904,-1.2546905858,0.
C,0.2152815065,-1.7070235847,-1.9211468402
N,-1.5981758664,-1.8492658211,0.
O,-2.154304053,0.5543726005,2.1052729768
O,1.9977788273,1.2215167092,2.155682387
O,1.9977788273,1.2215167092,-2.155682387
O,-2.154304053,0.5543726005,-2.1052729768
O,-0.5762927162,4.0811584816,0.
O,0.2705656386,-1.6110947852,3.0622479602
O,3.1240059306,-0.948835109,0.
O,0.2705656386,-1.6110947852,-3.0622479602
O,-2.7604892004,-1.8340191012,0.

CrMn(NO)(CO)$_8$ (**8-12S**) C_s B3LYP/DZP
0 1
Mn,0.1388250044,-1.8133396039,0.
Cr,-0.0117603915,1.20058445,0.
C,1.4369376003,-1.5325228399,1.3101644327
C,-1.17291055,-1.8874812469,1.3227259055
C,-1.17291055,-1.8874812469,-1.3227259055
C,1.4369376003,-1.5325228399,-1.3101644327
C,-0.1207328064,1.1337667588,1.9225468794
C,-1.9192875406,0.7514082623,0.
C,-0.1207328064,1.1337667588,-1.9225468794
O,2.2460029985,-1.3624445672,2.1176575969
O,-1.9837176531,-1.9260063879,2.1455293814
O,-1.9837176531,-1.9260063879,-2.1455293814
O,2.2460029985,-1.3624445672,-2.1176575969
O,-0.1889706496,1.114398697,3.0754457078
O,-3.0528231797,0.5303121928,0.
O,-0.1889706496,1.114398697,-3.0754457078
O,2.8860660933,1.2009229003,0.
O,-0.425068455,4.2053340996,0.
C,-0.2997985082,3.0541001466,0.
N,1.7100640468,1.2040339712,0.

CrMn(NO)(CO)$_8$ (**8-12S**) C_s BP86/DZP
0 1
Mn,0.084300561,-1.7867087549,0.
Cr,0.0461177261,1.1689681112,0.
C,1.3663062683,-1.5100706183,1.2947680758
C,-1.2055211109,-1.9136271563,1.3148996831
C,-1.2055211109,-1.9136271563,-1.3148996831
C,1.3663062683,-1.5100706183,-1.2947680758
C,-0.0822042284,1.1480400592,1.9102613373
C,-1.836112918,0.6977421337,0.
C,-0.0822042284,1.1480400592,-1.9102613373
O,2.1915288441,-1.363064759,2.1141704272
O,-2.0168795261,-2.0039480458,2.1552457063
O,-2.0168795261,-2.0039480458,-2.1552457063
O,2.1915288441,-1.363064759,-2.1141704272
O,-0.1774189711,1.1863573379,3.0742857361
O,-2.9881525819,0.5036129636,0.
O,-0.1774189711,1.1863573379,-3.0742857361
O,2.9648732158,1.3303638011,0.
O,-0.4593453911,4.159630358,0.
C,-0.2861681661,2.9998261987,0.
N,1.782053424,1.2538095456,0.

CrMn(NO)(CO)$_8$ (**8-12S**) C_s M06-L/cc-pVTZ
0 1
Mn,0.1302748324,-1.7984450261,0.
Cr,0.0063635464,1.1498671568,0.
C,1.4181242872,-1.4775730475,1.2990777768
C,-1.1749321431,-1.8145800671,1.3211064448
C,-1.1749321431,-1.8145800671,-1.3211064448
C,1.4181242872,-1.4775730475,-1.2990777768
C,-0.1089531251,1.0309222348,1.9235146643
C,-1.9154530624,0.7099894725,0.
C,-0.1089531251,1.0309222348,-1.9235146643
C,-0.2922913336,2.9957909828,0.
N,1.7346496285,1.1967233,0.
O,2.2144345939,-1.2510075828,2.0939074114
O,-1.9766577939,-1.7788449701,2.1412345299
O,-1.9766577939,-1.7788449701,-2.1412345299
O,2.2144345939,-1.2510075828,-2.0939074114
O,-0.1861069627,0.9548807585,3.0626070645
O,-3.0348238157,0.4812854199,0.
O,-0.1861069627,0.9548807585,-3.0626070645
O,2.8920670136,1.2170292817,0.
O,-0.4325460741,4.1352550443,0.

Complete Gaussian 03 reference

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A. Gaussian 03, Revision D.01; Gaussian, Inc., Wallingford CT, **2004**.

Complete Gaussian 09 reference

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Hratchian, X. L., H. P. ; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Cioslowski, J. V. O., J.; J., D., Gaussian 09, Revision D. 01; Gaussian, Inc. Wallingford, CT, **2013**.