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Major Differences between Mononuclear and Binuclear Manganese Carbonyl Cyanides and Isoelectronic Binary Chromium Carbonyls Arising from Basicity of the Cyanide Nitrogen Atom

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Supplementary Material

Tables S1-S5: Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (in parentheses) predicted by BP86 method for the optimized structures $Mn(CO)_5(CN)$, $Mn(CO)_4(CN)$, $Mn(CO)_3(CN)$, $Mn_2(CO)_8(CN)_2$, and $Mn_2(CO)_7(CN)_2$.

Table S6. The ν(CO) and ν(CN) frequencies of the mononuclear derivatives $Mn(CO)_n(CN)$ (n = 5, 4, 3) and the binuclear derivatives $Mn_2(CO)_n(CN)_2$ (n = 8, 7) with the BP86 method. Infrared intensities are given in parentheses in km/mol.

Table S7. Cartesian coordinates for the optimized structures $Mn(CO)_5(CN)$.

Table S8. Cartesian coordinates for the optimized structures $Mn(CO)_4(CN)$.

Table S9. Cartesian coordinates for the optimized structures $Mn(CO)_3(CN)$.

Table S10. Cartesian coordinates for the optimized structures $Mn_2(CO)_8(CN)_2$.

Table S11. Cartesian coordinates for the optimized structures $Mn_2(CO)_7(CN)_2$.

Table S12. Cartesian coordinates for all optimized structures by the M06-L method.

Tables S13-S17: Total energies (E in Hartree) by the B3LYP, the BP86, and the M06-L methods and relative energies (ΔE in kJ/mol) by the M06-L method for all structures.

Table S18. Single-point energies with the larger basis sets (M06-L/cc-pVTZ) for all of the structures.

Complete Gaussian 03 and Gaussian09 references (Reference 28)

Table S1. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (in parentheses, km/mol) predicted for the optimized structures of $Mn(CO)_5(CN)$ by BP86 method.

	frequencies (cm^{-1})
15-1	50(0), 66(1), 66(1), 84(0), 84(0), 94(0), 106(2), 106(2), 106(1), 321(0), 321(0), 366(0), 390(7), 415(0), 421(0), 443(6), 443(6), 468(14), 468(14), 475(0), 504(0), 542(0), 542(0), 546(0), 674(145), 674(145), 684(151), 2007(732), 2028(1240), 2028(1240), 2051(0), 2109(33), 2137(0)
15-2	56(0), 71(2), 71(2), 85(0), 85(0), 92(0), 103(1), 107(3), 107(3), 267(0), 267(0), 360(0), 382(9), 409(0), 413(0), 432(4), 432(4), 445(21), 445(21), 484(0), 510(0), 538(0), 547(2), 547(2), 667(126), 667(126), 680(152), 2000(718), 2030(1228), 2030(1228), 2054(0), 2063(91), 2113(51)

Table S2. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (in parentheses, km/mol) predicted for the optimized structures of $Mn(CO)_4(CN)$ by the BP86 method.

	frequencies (cm^{-1})
14-1	55(3), 72(0), 80(1), 85(0), 90(2), 104(2), 104(0), 271(1), 324(0), 361(0), 405(13), 415(1), 432(20), 437(4), 478(3), 489(17), 506(1), 541(9), 553(2), 625(35), 646(66), 685(62), 1984(846), 2005(465), 2012(1311), 2078(9), 2087(90)
14-2	46(5), 73(0), 81(2), 85(1), 85(0), 106(0), 106(3), 208(0), 288(0), 356(0), 404(1), 407(1), 418(25), 422(22), 471(22), 495(7), 505(9), 547(9), 556(0), 617(33), 637(57), 699(47), 1979(830), 1997(247), 2001(566), 2016(1281), 2089(55)
14-3	43(0), 72(0), 72(0), 92(0), 96(3), 96(3), 100(0), 334(3), 334(3), 363(0), 414(0), 422(0), 433(27), 433(27), 446(3), 483(9), 483(9), 505(0), 551(0), 639(85), 639(85), 664(47), 1992(1515), 1992(1515), 2029(0), 2083(41), 2117(3)

Table S3. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (in parentheses, km/mol) predicted for the optimized structures of $Mn(CO)_3(CN)$ by the BP86 method.

	frequencies (cm^{-1})
13-1	65(4), 68(4), 88(1), 93(1), 107(1), 268(4), 276(0), 395(0), 413(17), 444(4), 449(0), 498(9), 523(5), 533(6), 623(3), 628(25), 697(16), 1968(863), 1971(802), 2039(287), 2065(94)
13-2	63(4), 64(5), 93(1), 93(2), 107(1), 216(0), 221(0), 395(0), 417(0), 421(1), 444(20), 522(22), 523(8), 534(27), 629(9), 643(21), 714(5), 1963(534), 1968(884), 1969(824), 2039(259)
13-3	25(5), 81(1), 91(1), 93(1), 107(0), 172(0), 255(4), 395(0), 412(0), 431(8), 475(2), 520(23), 522(9), 523(17), 629(16), 636(23), 710(2), 1911(8), 1966(868), 1976(777), 2040(324)

Table S4. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (in parentheses,km/mol) predicted for the optimized structures of $Mn_2(CO)_8(CN)_2$ by the BP86 method.

	frequencies (cm^{-1})
28-1	29(0), 35(0), 47(0), 56(0), 65(0), 66(0), 68(1), 79(0), 84(0), 87(0), 88(0), 96(1), 101(0), 104(0), 109(0), 151(0), 159(6), 188(1), 245(11), 305(1), 326(2), 341(0), 345(0), 400(1), 402(48), 410(0), 410(0), 417(3), 421(0), 440(16), 445(27), 451(0), 451(0), 467(1), 469(1), 476(0), 486(5), 493(6), 493(5), 513(13), 537(1), 556(0), 559(9), 573(0), 633(30), 649(1), 653(174), 664(136), 684(109), 693(57), 1980(680), 1998(18), 1999(887), 2004(849), 2014(2322), 2014(458), 2056(792), 2074(13), 2088(35), 2111(8)
28-2	31(0), 35(0), 50(0), 54(0), 66(0), 66(0), 69(0), 77(0), 85(0), 86(0), 88(0), 97(1), 101(0), 103(0), 107(0), 145(0), 153(0), 189(1), 262(14), 287(0), 336(0), 343(0), 347(37), 360(0), 414(0), 415(0), 416(0), 418(0), 423(10), 428(0), 436(0), 437(28), 458(0), 460(9), 476(0), 481(3), 487(0), 491(31), 500(0), 500(8), 546(8), 550(0), 562(4), 562(0), 645(0), 648(0), 653(166), 656(169), 685(0), 686(148), 1986(0), 1987(1491), 1997(0), 2009(1405), 2013(0), 2013(2334), 2058(840), 2063(0), 2100(0), 2101(2)

Table S5. Harmonic vibrational frequencies (cm^{-1}) and corresponding infrared intensities (in parentheses, km/mol) predicted for the optimized structures of $Mn_2(CO)_7(CN)_2$ by the BP86 method.

	frequencies (cm^{-1})
27-1	21(0), 26(0), 48(0), 62(0), 66(0), 72(0), 80(0), 82(0), 90(0), 90(0), 99(0), 105(0), 106(0), 115(0), 167(10), 169(3), 252(11), 311(2), 315(2), 336(0), 340(0), 406(1), 407(68), 415(1), 420(1), 437(2), 445(10), 449(0), 456(0), 465(1), 470(1), 480(1), 491(3), 506(11), 514(13), 517(20), 532(5), 535(3), 555(0), 627(11), 640(6), 653(126), 659(110), 682(126), 709(17), 1961(624), 1963(711), 2003(839), 2012(1334), 2016(1306), 2034(671), 2055(3), 2057(269), 2107(0)
27-2	24(0), 30(0), 51(0), 62(0), 66(0), 69(0), 76(0), 84(0), 87(0), 90(0), 99(0), 102(0), 105(0), 115(1), 141(0), 176(2), 270(15), 289(1), 318(1), 337(0), 347(34), 374(1), 412(1), 415(1), 416(0), 425(6), 437(14), 438(11), 456(7), 458(3), 474(1), 476(1), 492(18), 496(5), 499(3), 533(11), 539(7), 545(8), 560(2), 620(24), 627(11), 648(94), 651(91), 682(89), 700(26), 1962(650), 1973(615), 1990(827), 2010(1375), 2013(747), 2015(1193), 2039(286), 2059(7), 2094(69)
27-3	30(0), 35(0), 53(0), 64(0), 66(1), 69(0), 79(0), 88(0), 89(0), 89(0), 101(0), 103(0), 108(0), 138(0), 165(5), 190(1), 249(9), 309(1), 316(0), 332(1), 335(1), 403(0), 409(25), 410(14), 411(0), 417(3), 445(36), 450(1), 453(1), 462(4), 465(1), 478(0), 484(6), 487(0), 497(6), 531(18), 536(3), 556(18), 572(0), 623(19), 624(2), 634(95), 651(67), 685(39), 690(77), 1971(562), 1980(213), 1983(1357), 2007(1142), 2009(567), 2012(1443), 2030(0), 2060(174), 2087(151)
27-4	32(0), 42(0), 49(0), 55(0), 58(0), 70(0), 70(0), 83(0), 85(0), 88(0), 95(1), 101(0), 102(0), 119(0), 144(0), 176(1), 306(27), 338(9), 340(1), 353(0), 357(7), 375(5), 411(1), 413(2), 414(13), 416(0), 423(12), 426(15), 438(24), 452(8), 468(3), 484(3), 494(7), 506(3), 508(1), 523(18), 542(2), 549(2), 560(2), 623(26), 629(32), 650(94), 655(76), 681(108), 682(42), 1953(721), 1974(589), 1975(332), 1986(706), 1997(1077), 2007(1825), 2021(134), 2059(170), 2089(99)

Table S6. The ν(CO) and ν(CN) frequencies of the mononuclear derivatives $Mn(CO)_n(CN)$ (n = 5, 4, 3) and the binuclear derivatives $Mn_2(CO)_n(CN)_2$ (n = 8, 7) with the BP86 method. Infrared intensities are given in parentheses in km/mol.

	Sym.	***ν*(CN)**	**ν(CO)**
15-1	C_{4v}	2137(0)	2007(732), 2028(1240), 2028(1240), 2051(0), 2109(33)
Expt.		2145	1930–1985 (unresolved), 2055, 2075sh
15-2	C_{4v}	2063(91)	2000(718), 2030(1228), 2030(1228), 2054(0), 2113(51)
14-1	C_s	2078(9)	1984(846), 2005(465), 2012(1311), 2087(90)
14-2	C_s	1997(247)	1979(830), 2001(566), 2016(1281), 2089(55)
14-3	C_{4v}	2117(3)	1992(1515), 1992(1515), 2029(0), 2083(41)
13-1	C_s	2065(94)	1968(863), 1971(802), 2039(287)
13-2	C_s	1968(884)	1963(534), 1969(824), 2039(259)
13-3	C_s	1911(8)	1966(868), 1976(777), 2040(324)
28-1	C_{2v}	2074(13), 2111(8)	1980(680), 1998(18), 1999(887), 2004(849), 2014(2322), 2014(458), 2056(792), 2088(35)
28-2	C_{2h}	2063(0), 2101(2)	1986(0), 1987(1491), 1997(0), 2009(1405), 2013(0), 2013(2334), 2058(840), 2100(0)
27-1	C_s	2055(3), 2107(0)	1961(624), 1963(711), 2003(839), 2012(1334), 2016(1306), 2034(671), 2057(269)
27-2	C_1	2039(286), 2059(7)	1962(650), 1973(615), 1990(827), 2010(1375), 2013(747), 2015(1193), 2094(69)
27-3	C_s	2030(0), 2060(174)	1971(562), 1980(213), 1983(1357), 2007(1142), 2009(567), 2012(1443), 2087(151)
27-4	C_s	1953(721),1997(1077)	1974(589), 1975(332), 1986(706), 2007(1825), 2021(134), 2059(170), 2089(99)

Table S7. Cartesian coordinates for the optimized structures $Mn(CO)_5(CN)$.

	B3LYP				BP86			
15-1	Mn	0.000000	0.000000	0.091945	Mn	0.000000	0.000000	0.088214
	C	0.000000	1.878091	-0.037060	C	0.000000	1.856081	-0.037180
	C	0.000000	0.000000	1.948745	C	0.000000	0.000000	1.928160
	C	1.878091	0.000000	-0.037060	C	1.856081	0.000000	-0.037180
	C	0.000000	0.000000	-1.913260	C	0.000000	0.000000	-1.904775
	C	0.000000	-1.878091	-0.037060	C	0.000000	-1.856081	-0.037180
	C	-1.878091	0.000000	-0.037060	C	-1.856081	0.000000	-0.037180
	O	3.019901	0.000000	-0.151140	O	3.013301	0.000000	-0.143356
	O	0.000000	-3.019901	-0.151140	O	0.000000	-3.013301	-0.143356
	O	0.000000	3.019901	-0.151140	O	0.000000	3.013301	-0.143356
	O	-3.019901	0.000000	-0.151140	O	-3.013301	0.000000	-0.143356
	O	0.000000	0.000000	3.102004	O	0.000000	0.000000	3.096285
	N	0.000000	0.000000	-3.085944	N	0.000000	0.000000	-3.090890

	B3LYP				BP86			
15-2	Mn	0.000000	0.000000	0.070381	Mn	0.000000	0.000000	0.055534
	C	0.000000	1.889234	-0.043632	C	0.000000	1.864895	-0.041525
	C	0.000000	0.000000	1.915910	C	0.000000	0.000000	1.879897
	C	1.889234	0.000000	-0.043632	C	1.864895	0.000000	-0.041525
	C	0.000000	-1.889234	-0.043632	C	0.000000	-1.864895	-0.041525
	C	-1.889234	0.000000	-0.043632	C	-1.864895	0.000000	-0.041525
	O	3.031382	0.000000	-0.142470	O	3.024039	0.000000	-0.112674
	O	0.000000	-3.031382	-0.142470	O	0.000000	-3.024039	-0.112674
	O	0.000000	3.031382	-0.142470	O	0.000000	3.024039	-0.112674
	O	-3.031382	0.000000	-0.142470	O	-3.024039	0.000000	-0.112674
	O	0.000000	0.000000	3.070287	O	0.000000	0.000000	3.049659
	N	0.000000	0.000000	-1.932355	N	0.000000	0.000000	-1.945650
	C	0.000000	0.000000	-3.114100	C	0.000000	0.000000	-3.140546

Table S8. Cartesian coordinates for the optimized structures $Mn(CO)_4(CN)$.

	B3LYP				BP86			
14-1	Mn	-0.262966	0.026611	0.000000	Mn	-0.254573	0.089545	0.000000
	C	-0.293986	-0.103324	1.880817	C	1.479774	-0.279926	0.000000
	C	1.543701	0.117114	0.000000	C	0.049051	1.902437	0.000000
	C	-0.466270	1.874257	0.000000	C	-1.015464	-1.701276	0.000000
	C	-0.293986	-0.103324	-1.880817	C	-0.295679	-0.030790	1.855721
	C	-0.500916	-1.928354	0.000000	O	2.617831	-0.556375	0.000000
	N	-0.758815	-3.075938	0.000000	O	0.223905	3.059009	0.000000
	O	-0.293986	-0.215950	-3.022954	O	-0.295679	-0.139014	3.013846
	O	2.697645	0.129291	0.000000	C	-0.295679	-0.030790	-1.855721
	O	-0.293986	-0.215950	3.022954	O	-0.295679	-0.139014	-3.013846
	O	-0.615349	3.018620	0.000000	N	-1.595818	-2.741914	0.000000

	B3LYP				BP86			
14-2	Mn	0.197603	0.057422	0.000000	Mn	0.174380	0.119981	0.000000
	C	0.663786	-1.724333	0.000000	C	0.224000	0.096999	1.868746
	C	0.223857	0.143425	1.895379	C	0.224000	0.096999	-1.868746
	C	0.753459	3.117307	0.000000	C	-1.068507	1.443805	0.000000
	C	-1.572339	-0.320878	0.000000	O	0.224000	0.068515	3.030593
	C	0.223857	0.143425	-1.895379	O	0.224000	0.068515	-3.030593
	N	0.480221	1.960734	0.000000	O	-1.830186	2.333707	0.000000
	O	-2.713037	-0.499466	0.000000	O	-1.890822	-1.983647	0.000000
	O	0.223857	0.206100	-3.040095	C	-1.094453	-1.124136	0.000000
	O	1.008158	-2.827030	0.000000	N	1.938439	-0.607332	0.000000
	O	0.223857	0.206100	3.040095	C	3.090876	-0.954490	0.000000

	B3LYP				BP86			
14-3	Mn	0.000000	0.000000	0.441574	Mn	0.000000	0.000000	0.437904
	C	0.000000	1.880196	0.362146	C	0.000000	0.000000	-1.486828
	C	-1.880196	0.000000	0.362146	C	1.854505	0.000000	0.358520
	C	1.880196	0.000000	0.362146	C	0.000000	1.854505	0.358520
	C	0.000000	-1.880196	0.362146	C	-1.854505	0.000000	0.358520
	C	0.000000	0.000000	-1.515282	C	0.000000	-1.854505	0.358520
	O	0.000000	3.024652	0.255764	N	0.000000	0.000000	-2.675326
	O	-3.024652	0.000000	0.255764	O	0.000000	3.014746	0.253005
	O	0.000000	-3.024652	0.255764	O	3.014746	0.000000	0.253005
	O	3.024652	0.000000	0.255764	O	-3.014746	0.000000	0.253005
	N	0.000000	0.000000	-2.689084	O	0.000000	-3.014746	0.253005

Table S9. Cartesian coordinates for the optimized structures $Mn(CO)_3(CN)$.

	B3LYP				BP86			
13-1	Mn	-0.049862	-0.458564	0.000000	Mn	-0.045512	-0.478179	0.000000
	C	-1.972473	-0.769340	0.000000	C	-0.001505	0.772591	1.242618
	C	0.017793	0.801330	1.290986	C	-1.938006	-0.796828	0.000000
	C	0.017793	0.801330	-1.290986	C	-0.001505	0.772591	-1.242618
	C	1.794482	-0.712793	0.000000	C	1.784190	-0.652553	0.000000
	O	0.017793	1.610319	2.114330	O	2.949835	-0.768460	0.000000
	O	2.935107	-0.892027	0.000000	O	-0.001505	1.609083	-2.064502
	N	-3.094937	-1.126850	0.000000	N	-3.070831	-1.173997	0.000000
	O	0.017793	1.610319	-2.114330	O	-0.001505	1.609083	2.064502

	B3LYP				BP86			
13-2	Mn	-0.101516	-0.384848	0.000000	Mn	-0.102434	-0.397510	0.000000
	C	-0.029247	0.871718	1.293501	C	-0.048798	0.850789	1.247081
	C	-0.029247	0.871718	-1.293501	C	-0.048798	0.850789	-1.247081
	C	1.726926	-0.586653	0.000000	C	1.704093	-0.502643	0.000000
	O	2.868045	-0.770129	0.000000	O	2.871117	-0.622284	0.000000
	O	-0.029247	1.673768	-2.124021	O	-0.048798	1.680929	-2.075912
	O	-0.029247	1.673768	2.124021	O	-0.048798	1.680929	2.075912
	N	-1.835432	-1.090329	0.000000	N	-1.795475	-1.152955	0.000000
	C	-2.850181	-1.717743	0.000000	C	-2.782994	-1.850297	0.000000

	B3LYP				BP86			
13-3	Mn	0.320067	0.247573	0.000000	Mn	0.326151	0.270661	0.000000
	C	-1.500588	0.420154	0.000000	C	-1.463533	0.358132	0.000000
	C	0.271886	-1.013554	1.306396	C	0.289621	-0.984229	1.261394
	C	0.271886	-1.013554	-1.306396	C	0.289621	-0.984229	-1.261394
	C	1.627456	1.708331	0.000000	C	1.567575	1.742553	0.000000
	O	0.271886	-1.779232	-2.171220	O	0.289621	-1.776614	-2.126484
	O	0.271886	-1.779232	2.171220	O	0.289621	-1.776614	2.126484
	O	-2.642816	0.574910	0.000000	O	-2.630125	0.451718	0.000000
	N	0.680979	2.438692	0.000000	N	0.593368	2.464600	0.000000

Table S10. Cartesian coordinates for the optimized structures $Mn_2(CO)_8(CN)_2$.

	B3LYP				BP86			
28-1	Mn	-0.000004	2.181062	0.000000	Mn	-0.000008	2.177843	0.000000
	Mn	0.000003	-2.162106	0.000000	Mn	-0.000008	-2.141743	0.000000
	C	-0.000008	2.117436	1.875278	C	-0.000001	2.143321	1.855305
	C	1.371325	3.425821	0.000000	C	1.362535	3.408522	0.000000
	C	-1.371339	3.425819	0.000000	C	-1.362527	3.408555	0.000000
	C	-0.000008	2.117436	-1.875278	C	-0.000001	2.143321	-1.855305
	C	-0.000002	-2.088307	1.889816	C	-0.000004	-2.116709	1.864426
	C	1.337854	-3.414132	0.000000	C	1.303616	-3.387259	0.000000
	C	1.337832	-3.414148	0.000000	C	-1.303615	-3.387269	0.000000
	C	-0.000002	-2.088307	-1.889816	C	-0.000004	-2.116709	-1.864426
	O	-2.237267	4.188026	0.000000	O	-2.238654	4.180926	0.000000
	O	-0.000002	2.067453	3.024207	O	0.000007	2.130389	3.019707
	O	-0.000002	-2.040633	3.037150	O	-0.000006	-2.133501	3.028040
	O	2.237257	4.188025	0.000000	O	2.238676	4.180878	0.000000
	O	-2.185064	-4.198350	0.000000	O	-2.143059	-4.203408	0.000000
	O	-0.000002	-2.040633	-3.037150	O	-0.000006	-2.133501	-3.028040
	O	-0.000002	2.067453	-3.024207	O	0.000007	2.130389	-3.019707
	O	2.185107	-4.198311	0.000000	O	2.143070	-4.203386	0.000000
	C	1.204867	0.571284	0.000000	C	1.162352	0.581149	0.000000
	N	1.451151	-0.577373	0.000000	N	1.441986	-0.574372	0.000000
	C	-1.204878	0.571280	0.000000	C	-1.162401	0.581160	0.000000
	N	-1.451155	-0.577378	0.000000	N	-1.441928	-0.574384	0.000000

	B3LYP				BP86			
28-1	Mn	0.020105	2.174010	0.000000	Mn	1.967595	-0.886074	0.000000
	C	0.008775	2.098311	1.881655	C	1.936425	-0.846209	1.858688
	C	1.388931	3.432411	0.000000	C	2.584406	-2.619774	0.000000
	C	-1.318666	3.418525	0.000000	C	3.621601	-0.168395	0.000000
	C	0.008775	2.098311	-1.881655	C	1.936425	-0.846209	-1.858688
	O	2.239924	4.209545	0.000000	O	2.988885	-3.714840	0.000000
	O	-2.173639	4.195917	0.000000	O	4.695354	0.299452	0.000000
	O	-0.008775	2.042253	-3.029384	O	1.936425	-0.809833	-3.022287
	O	-0.008775	2.042253	3.029384	O	1.936425	-0.809833	3.022287
	Mn	-0.020105	-2.174010	0.000000	Mn	-1.967595	0.886074	0.000000
	C	-1.388931	-3.432411	0.000000	C	-2.584406	2.619774	0.000000
	C	-0.008775	-2.098311	1.881655	C	-1.936425	0.846209	1.858688
	C	1.318666	-3.418525	0.000000	C	-3.621601	0.168395	0.000000
	C	-0.008775	-2.098311	-1.881655	C	-1.936425	0.846209	-1.858688
	O	0.008775	-2.042253	3.029384	O	-1.936425	0.809833	3.022287
	O	2.173639	-4.195917	0.000000	O	-4.695354	-0.299452	0.000000
	O	0.008775	-2.042253	-3.029384	O	-1.936425	0.809833	-3.022287
	O	-2.239924	-4.209545	0.000000	O	-2.988885	3.714840	0.000000
	C	-1.211197	0.572306	0.000000	C	0.996369	0.841302	0.000000
	N	-1.456879	-0.576316	0.000000	N	0.051744	1.563477	0.000000
	C	1.211197	-0.572306	0.000000	C	-0.996369	-0.841302	0.000000
	N	1.456879	0.576316	0.000000	N	-0.051744	-1.563477	0.000000

Table S11. Cartesian coordinates for the optimized structures $Mn_2(CO)_7(CN)_2$.

	B3LYP				BP86			
27-1	Mn	0.188981	2.251343	0.000000	Mn	0.182838	2.231897	0.000000
	C	0.067888	-0.445129	1.199252	C	0.063702	-0.454357	1.158141
	C	-0.003525	-3.301054	1.373286	C	0.009841	-3.277206	1.366601
	C	1.906509	-2.045390	0.000000	C	1.881162	-2.069335	0.000000
	C	-0.003525	-3.301054	-1.373286	C	-0.009841	-3.277206	-1.366601
	C	-1.844750	-1.944894	0.000000	C	-1.830296	-1.966425	0.000000
	C	0.067888	-0.445129	-1.199252	C	0.063702	-0.454357	-1.158141
	C	-1.516935	2.817876	0.000000	C	-1.459119	2.861831	0.000000
	C	0.628367	3.435955	1.323885	C	0.619084	3.410253	1.283109
	O	3.056261	-2.025501	0.000000	O	3.045237	-2.085165	0.000000
	O	-0.024395	-4.062121	2.239331	O	-0.032303	-4.046435	2.244324
	O	-0.024395	-4.062121	-2.239331	O	-0.032303	-4.046435	-2.244324
	O	-2.991458	-1.867810	0.000000	O	-2.993025	-1.922712	0.000000
	O	-2.628067	3.139534	0.000000	O	-2.565891	3.256598	0.000000
	Mn	0.030780	-2.056458	0.000000	Mn	0.025870	-2.048440	0.000000
	C	0.628367	3.435955	-1.323885	C	0.619084	3.410253	-1.283109
	O	0.913824	4.183599	-2.157277	O	0.912698	4.193812	-2.105112
	O	0.913824	4.183599	2.157277	O	0.912698	4.193812	2.105112
	N	0.085679	0.712259	-1.407539	N	0.084257	0.711793	-1.398293
	N	0.085679	0.712259	1.407539	N	0.084257	0.711793	1.398293

	B3LYP				BP86			
27-2	Mn	-2.267906	-0.205462	0.040675	Mn	-2.245578	-0.199995	0.057351
	Mn	2.041073	-0.032395	0.018044	Mn	2.017399	-0.028937	0.012505
	C	0.425919	-0.040947	1.219671	C	0.432466	-0.052769	1.180784
	C	3.267566	0.062765	1.371542	C	3.230246	0.061755	1.345738
	C	2.038120	-1.913291	0.093533	C	2.057972	-1.886252	0.087143
	C	3.316803	-0.033245	-1.337594	C	3.287174	-0.012739	-1.324162
	C	1.898428	1.846595	-0.042973	C	1.901786	1.828470	-0.021533
	C	-3.529525	-0.409734	1.391830	C	-3.521275	-0.362368	1.372015
	C	-3.399462	-0.806099	-1.256681	C	-3.352193	-0.830308	-1.204942
	C	-2.760760	1.498176	-0.252786	C	-2.776590	1.439677	-0.305927
	O	2.024025	-3.061067	0.149097	O	2.091766	-3.047871	0.151697
	O	4.032648	0.122565	2.235035	O	4.014238	0.120678	2.213204
	O	4.102210	-0.034257	-2.180202	O	4.097761	-0.002083	-2.162905
	O	-3.033053	2.607366	-0.438068	O	-3.099343	2.544109	-0.542929
	O	-4.102514	-1.204120	-2.084617	O	-4.069209	-1.261807	-2.027889
	O	-4.323431	-0.533444	2.219285	O	-4.362612	-0.457766	2.178385
	N	-0.731967	-0.060924	1.429749	N	-0.730897	-0.084082	1.442597
	O	1.803452	2.990954	-0.070117	O	1.842514	2.990303	-0.024658
	C	-0.677961	-0.157976	-1.188498	C	-0.686304	-0.155199	-1.133697
	N	0.470449	-0.144074	-1.443968	N	0.465733	-0.136320	-1.442331

	B3LYP				BP86			
27-3	Mn	-0.037805	-2.024393	0.000000	Mn	-0.037314	-1.994445	0.000000
	Mn	-0.250473	2.293949	0.000000	Mn	-0.263680	2.289083	0.000000
	C	0.021349	-3.275995	1.338722	C	0.033909	-3.237674	1.307550
	C	1.848388	-1.864180	0.000000	C	1.824775	-1.869292	0.000000
	C	0.021349	-3.275995	-1.338722	C	0.033909	-3.237674	-1.307550
	C	-0.137897	0.703612	1.199572	C	-0.152727	0.719261	1.153218
	C	-0.137897	0.703612	-1.199572	C	-0.152727	0.719261	-1.153218
	C	-0.586865	3.502868	-1.361067	C	-0.575378	3.492080	-1.346890
	C	-0.586865	3.502868	1.361067	C	-0.575378	3.492080	1.346890
	C	1.504926	2.683063	0.000000	C	1.455325	2.678901	0.000000
	C	-1.927198	-2.041299	0.000000	C	-1.898965	-2.080740	0.000000
	O	-0.797109	4.248082	2.217535	O	-0.767334	4.256342	2.211642
	O	-0.797109	4.248082	-2.217535	O	-0.767334	4.256342	-2.211642
	O	0.057911	-4.058773	2.186122	O	0.080212	-4.049231	2.149382
	O	0.057911	-4.058773	-2.186122	O	0.080212	-4.049231	-2.149382
	O	-3.075703	-2.045389	0.000000	O	-3.059861	-2.161480	0.000000
	O	2.992054	-1.766236	0.000000	O	2.986896	-1.823148	0.000000
	N	-0.110944	-0.446496	1.447061	N	-0.121580	-0.439479	1.434475
	O	2.642598	2.893092	0.000000	O	2.606023	2.911603	0.000000
	N	-0.110944	-0.446496	-1.447061	N	-0.121580	-0.439479	-1.434475

	B3LYP				BP86			
27-4	Mn	0.062229	1.793553	0.000000	Mn	0.062853	1.737108	0.000000
	Mn	-0.380380	-2.273345	0.000000	Mn	-0.399041	-2.204005	0.000000
	C	1.517276	2.957578	0.000000	C	1.491767	2.903272	0.000000
	C	0.056574	1.722747	1.882283	C	0.052054	1.702221	1.859633
	C	-1.181819	3.130019	0.000000	C	-1.163101	3.057570	0.000000
	C	1.025210	-0.956848	0.000000	C	0.960605	-0.935057	0.000000
	C	-0.353429	-2.286323	-1.884617	C	-0.338266	-2.261693	-1.856560
	C	0.629028	-3.783540	0.000000	C	0.614377	-3.685593	0.000000
	C	-0.353429	-2.286323	1.884617	C	-0.338266	-2.261693	1.856560
	C	0.056574	1.722747	-1.882283	C	0.052054	1.702221	-1.859633
	O	-0.287171	-2.309189	-3.033360	O	-0.230052	-2.343164	-3.015572
	O	-0.287171	-2.309189	3.033360	O	-0.230052	-2.343164	3.015572
	O	1.272366	-4.747727	0.000000	O	1.268535	-4.661613	0.000000
	O	2.420232	3.672433	0.000000	O	2.389478	3.647693	0.000000
	O	-1.975985	3.969817	0.000000	O	-1.958952	3.917437	0.000000
	O	0.044923	1.673552	-3.030341	O	0.031736	1.702003	-3.023658
	O	0.044923	1.673552	3.030341	O	0.031736	1.702003	3.023658
	N	1.471824	0.135747	0.000000	N	1.529362	0.123428	0.000000
	N	-1.819573	-0.742151	0.000000	N	-1.861283	-0.752333	0.000000
	C	-1.307472	0.322214	0.000000	C	-1.279768	0.296285	0.000000

Table S12. Cartesian coordinates for all optimized structures by the M06-L method.

15-1				15-2			
Mn	0.00000000	0.00000000	0.09614400	Mn	0.00000000	0.00000000	0.07086500
C	0.00000000	1.87346200	-0.03684100	C	0.00000000	1.88438300	-0.04237500
C	0.00000000	0.00000000	1.94627800	C	0.00000000	0.00000000	1.90517800
C	1.87346200	0.00000000	-0.03684100	C	1.88438300	0.00000000	-0.04237500
C	0.00000000	0.00000000	-1.91316300	C	0.00000000	-1.88438300	-0.04237500
C	0.00000000	-1.87346200	-0.03684100	C	-1.88438300	0.00000000	-0.04237500
C	-1.87346200	0.00000000	-0.03684100	O	3.02991000	0.00000000	-0.13353700
O	3.01760100	0.00000000	-0.15337000	O	0.00000000	-3.02991000	-0.13353700
O	0.00000000	-3.01760100	-0.15337000	O	0.00000000	3.02991000	-0.13353700
O	0.00000000	3.01760100	-0.15337000	O	-3.02991000	0.00000000	-0.13353700
O	-3.01760100	0.00000000	-0.15337000	O	0.00000000	0.00000000	3.06310400
O	0.00000000	0.00000000	3.10263600	N	0.00000000	0.00000000	-1.94599900
N	0.00000000	0.00000000	-3.09019400	C	0.00000000	0.00000000	-3.13255700

14-1				14-2			
Mn	-0.26961900	0.10910800	0.00000000	Mn	-0.22346900	0.09886700	0.00000000
C	-0.31343700	-0.01478100	1.87561300	C	0.54257300	1.76291400	0.00000000
C	1.46985100	-0.31441900	0.00000000	C	-0.27173700	0.04369400	1.89052700
C	0.07881800	1.92691400	0.00000000	C	-2.44707300	-2.09308700	0.00000000
C	-0.31343700	-0.01478100	-1.87561300	C	1.37609300	-0.70580000	0.00000000
C	-1.00356600	-1.72069300	0.00000000	C	-0.27173700	0.04369400	-1.89052700
N	-1.54359700	-2.77002700	0.00000000	N	-1.54065400	-1.31890000	0.00000000
O	-0.31343700	-0.13023800	-3.02032400	O	2.39308200	-1.25991300	0.00000000
O	2.58715600	-0.61753900	0.00000000	O	-0.27173700	-0.00553200	-3.03886800
O	-0.31343700	-0.13023800	3.02032400	O	1.00071500	2.82749300	0.00000000
O	0.29425300	3.06414700	0.00000000	O	-0.27173700	-0.00553200	3.03886800

14-3				13-1			
Mn	0.00000000	0.00000000	0.45705100	Mn	-0.04009700	-0.48893200	0.00000000
C	0.00000000	1.87165500	0.36183600	C	-1.96591200	-0.77794800	0.00000000
C	-1.87165500	0.00000000	0.36183600	C	0.00086900	0.77251500	1.25952900
C	1.87165500	0.00000000	0.36183600	C	0.00086900	0.77251500	-1.25952900
C	0.00000000	-1.87165500	0.36183600	C	1.80188200	-0.66710900	0.00000000
C	0.00000000	0.00000000	-1.48973200	O	0.00086900	1.60284100	2.06761400
O	0.00000000	3.01715600	0.23460800	O	2.95553100	-0.77410500	0.00000000
O	-3.01715600	0.00000000	0.23460800	N	-3.09742500	-1.11845100	0.00000000
O	0.00000000	-3.01715600	0.23460800	O	0.00086900	1.60284100	-2.06761400
O	3.01715600	0.00000000	0.23460800				
N	0.00000000	0.00000000	-2.66848700				

13-2				13-3			
Mn	-0.08888600	-0.41503400	0.00000000	Mn	0.32723900	0.27344000	0.00000000
C	-0.05071000	0.84304900	1.26287100	C	-1.48019100	0.36048000	0.00000000
C	-0.05071000	0.84304900	-1.26287100	C	0.29890000	-0.98908500	1.27466500
C	1.73354200	-0.52067400	0.00000000	C	0.29890000	-0.98908500	-1.27466500
O	2.88898300	-0.62361400	0.00000000	C	1.55862700	1.75627600	0.00000000
O	-0.05071000	1.66801100	-2.07687200	O	0.29890000	-1.77583200	-2.12683600
O	-0.05071000	1.66801100	2.07687200	O	0.29890000	-1.77583200	2.12683600
N	-1.83705800	-1.10450300	0.00000000	O	-2.63379700	0.44770700	0.00000000
C	-2.83528000	-1.76407100	0.00000000	N	0.57851400	2.45201800	0.00000000

28-1				28-2			
Mn	0.00020000	2.18104800	0.00000000	Mn	0.02662400	2.16343800	0.00000000
Mn	-0.00020000	-2.15364400	0.00000000	C	0.01147800	2.06042600	1.87703200
C	0.00019900	2.08252100	1.87041000	C	1.37092700	3.43894300	0.00000000
C	1.35913100	3.43043600	0.00000000	C	-1.29735700	3.40075600	0.00000000
C	-1.35850800	3.43068100	0.00000000	C	0.01147800	2.06042600	-1.87703200
C	0.00019900	2.08252100	-1.87041000	O	2.20032700	4.24326100	0.00000000
C	-0.00019400	-2.05466000	1.88520800	O	-2.14508600	4.19143700	0.00000000
C	1.31021100	-3.41012000	0.00000000	O	-0.01147800	1.96749200	-3.02481200
C	-1.31083400	-3.40988700	0.00000000	O	-0.01147800	1.96749200	3.02481200
C	-0.00019400	-2.05466000	-1.88520800	Mn	-0.02662400	-2.16343800	0.00000000
O	-2.21630500	4.20617000	0.00000000	C	-1.37092700	-3.43894300	0.00000000
O	0.00020100	1.98496400	3.01877800	C	-0.01147800	-2.06042600	1.87703200
O	-0.00019400	-1.97183600	3.03306000	C	1.29735700	-3.40075600	0.00000000
O	2.21706700	4.20577200	0.00000000	C	-0.01147800	-2.06042600	-1.87703200
O	-2.13974700	-4.21897400	0.00000000	O	0.01147800	-1.96749200	3.02481200
O	-0.00019400	-1.97183600	-3.03306000	O	2.14508600	-4.19143700	0.00000000
O	0.00020100	1.98496400	-3.01877800	O	0.01147800	-1.96749200	-3.02481200
O	2.13898500	-4.21935000	0.00000000	O	-2.20032700	-4.24326100	0.00000000
C	1.19108200	0.56897700	0.00000000	C	-1.19231700	0.56213200	0.00000000
N	1.46318200	-0.57828500	0.00000000	N	-1.49140800	-0.57865900	0.00000000
C	-1.19098000	0.56919600	0.00000000	C	1.19231700	-0.56213200	0.00000000
N	-1.46329100	-0.57801600	0.00000000	N	1.49140800	0.57865900	0.00000000

27-1				27-2			
Mn	0.24146800	2.25659800	0.00000000	Mn	-2.26958300	-0.27973700	0.02772600
C	0.12335600	-0.44688300	1.18487500	Mn	2.03319500	-0.03663900	0.01276100
C	-0.04970200	-3.30569900	1.36363900	C	0.41799100	-0.16830300	1.19928200
C	1.90293700	-2.11670200	0.00000000	C	3.24555400	0.09314100	1.35511400
C	-0.04970200	-3.30569900	-1.36363900	C	2.14338800	-1.91168000	0.03732800
C	-1.83413400	-1.87182700	0.00000000	C	3.31626600	0.08207400	-1.32071000
C	0.12335600	-0.44688300	-1.18487500	C	1.76293700	1.82601300	0.01083700
C	-1.47224400	2.73051100	0.00000000	C	-3.56228000	-0.46003200	1.33919900
C	0.58870600	3.47006700	1.29868700	C	-3.43620700	-0.66819600	-1.29618100
O	3.05513600	-2.13676400	0.00000000	C	-2.62314600	1.45515600	-0.14266200
O	-0.09991700	-4.07546500	2.22458200	O	2.20293100	-3.06153400	0.06581500
O	-0.09991700	-4.07546500	-2.22458200	O	4.01822600	0.17578900	2.21487400
O	-2.97807500	-1.73822300	0.00000000	O	4.12238600	0.15634700	-2.14437700
O	-2.59658500	3.01809400	0.00000000	O	-2.82132700	2.59340500	-0.25449400
Mn	0.03145300	-2.06297300	0.00000000	O	-4.18549000	-0.91700000	-2.14703900

C	0.58870600	3.47006700	-1.29868700	O	-4.39583300	-0.55624600	2.13552500
O	0.80767400	4.26310700	-2.11596800	N	-0.73476400	-0.24612200	1.44328100
O	0.80767400	4.26310700	2.11596800	O	1.57749500	2.96200100	0.02228800
N	0.17724300	0.71075300	-1.40625200	C	-0.66833500	-0.22921400	-1.17791200
N	0.17724300	0.71075300	1.40625200	N	0.47556500	-0.18622600	-1.46880700

27-3				27-4			
Mn	-0.04111800	-2.01376400	0.00000000	Mn	-1.68683400	0.05115400	0.00000000
Mn	-0.31459300	2.29842500	0.00000000	Mn	2.15570900	-0.38760700	0.00000000
C	0.10178900	-3.26046400	1.31419800	C	-2.89555400	1.46283400	0.00000000
C	1.82521000	-1.71474500	0.00000000	C	-1.59463800	0.04670900	1.87825000
C	0.10178900	-3.26046400	-1.31419800	C	-2.99242300	-1.19993200	0.00000000
C	-0.24396800	0.70056000	1.18273800	C	0.87172200	1.00964200	0.00000000
C	-0.24396800	0.70056000	-1.18273800	C	2.15362800	-0.33094900	-1.87826000
C	-0.55363800	3.52922600	-1.35127700	C	3.61892800	0.66320500	0.00000000
C	-0.55363800	3.52922600	1.35127700	C	2.15362800	-0.33094900	1.87826000
C	1.44407200	2.56989700	0.00000000	C	-1.59463800	0.04670900	-1.87825000
C	-1.92020600	-2.16049300	0.00000000	O	2.15362800	-0.22146700	-3.02683400
O	-0.68762200	4.30160000	2.20327100	O	2.15362800	-0.22146700	3.02683400
O	-0.68762200	4.30160000	-2.20327100	O	4.56324600	1.34125900	0.00000000
O	0.19273600	-4.06118700	2.14580600	O	-3.65002800	2.33594100	0.00000000
O	0.19273600	-4.06118700	-2.14580600	O	-3.83153500	-2.00027100	0.00000000
O -	3.06750400	-2.25394700	0.00000000	O	-1.51616500	0.03161000	-3.02721700
O	2.95846700	-1.51762800	0.00000000	O	-1.51616500	0.03161000	3.02721700
N	-0.20218500	-0.44818700	1.45431000	N	-0.12969500	1.65397400	0.00000000
O	2.59614700	2.71053400	0.00000000	N	0.76826400	-1.97195800	0.00000000
N	-0.20218500	-0.44818700	-1.45431000	C	-0.22810800	-1.32402100	0.00000000

Table S13. Total energies (*E* in Hartree) by the B3LYP, the BP86, and the M06-L methods and relative energies (Δ*E* in kJ/mol) by the M06-L method for the two $Mn(CO)_5(CN)$ structures.

		15-1 (C_{4v})	**15-2** (C_{4v})
B3LYP	*E*	-1810.71458	-1810.69529
BP86	*E*	-1810.94465	-1810.92075
M06-L	*E*	-1810.61782	-1810.59763
M06-L	*ΔE*	0.0	53.0

Table S14. Total energies (*E* in Hartree) by the B3LYP, the BP86, and the M06-L methods and relative energies (Δ*E* in kJ/mol) by the M06-L method for the two $Mn(CO)_4(CN)$ structures.

		14-1 (C_s)	**14-2** (C_s)	**14-3** (C_{4v})
B3LYP	*E*	-1697.33010	-1697.31967	-1697.31482
BP86	*E*	-1697.55165	-1697.53738	-1697.53476
M06-L	*E*	-1697.23855	-1697.22578	-1697.22376
M06-L	*ΔE*	0.0	33.5	38.8

Table S15. Total energies (*E* in Hartree) by the B3LYP, the BP86, and the M06-L methods and relative energies (Δ*E* in kJ/mol) by the M06-L method for the two $Mn(CO)_3(CN)$ structures.

		13-1 (C_s)	**13-2** (C_s)	**13-3** (C_s)
B3LYP	*E*	-1583.94665	-1583.94642	-1583.93707
BP86	*E*	-1584.15983	-1584.15680	-1584.14955
M06-L	*E*	-1583.86141	-1583.85794	-1583.85258
M06-L	*ΔE*	0.0	9.1	23.2

Table S16. Total energies (*E* in Hartree) by the B3LYP, the BP86, and the M06-L methods and relative energies (Δ*E* in kJ/mol) by the M06-L method for the two $Mn_2(CO)_8(CN)_2$ structures.

		28-1 (C_{2v})	**28-2** (C_{2h})
B3LYP	*E*	-3394.74554	-3394.74305
BP86	*E*	-3395.19111	-3395.18767
M06-L	*E*	-3394.57606	-3394.57329
M06-L	*ΔE*	0.0	7.3

Table S17. Total energies (*E* in Hartree) by the B3LYP, the BP86, and the M06-L methods and relative energies (Δ*E* in kJ/mol) by the M06-L method for the two $Mn_2(CO)_7(CN)_2$ structures.

		27-1 (C_s)	**27-2** (C_1)	**27-3** (C_s)	**27-4** (C_s)
B3LYP	*E*	-3281.37093	-3281.36503	-3281.36343	-3281.35362
BP86	*E*	-3281.80987	-3281.80211	-3281.80043	-3281.79101
M06-L	*E*	-3281.20535	-3281.19923	-3281.19834	-3281.19154
	ΔE	0.0	16.1	18.4	36.3

Table S18. Single-point energies with the larger basis sets (M06-L/cc-pVTZ) for all of the structures.

	Sym.	*E*	*ΔE*
15-1	C_{4v}	-1810.74416	0.0
15-2	C_{4v}	-1810.72277	56.2
14-1	C_s	-1697.34941	0.0
14-2	C_s	-1697.33603	35.1
14-3	C_{4v}	-1697.33461	38.9
13-1	C_s	-1583.95716	0.0
13-2	C_s	-1583.95359	9.4
13-3	C_s	-1583.94746	25.5
28-1	C_{2v}	-3394.79367	0.0
28-2	C_{2h}	-3394.79084	7.4
27-1	C_s	-3281.40867	0.0
27-2	C_1	-3281.40190	17.8
27-3	C_s	-3281.40040	21.7
27-4	C_s	-3281.39277	41.8

Complete Gaussian 03 and Gaussian09 references (Reference 28)

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