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Mononuclear and Binuclear Manganese Carbonyl Hydrides: The Preference for Bridging Hydrogens over Bridging Carbonyls

Xian Mei Liu,[a] Qian-shu Li,*[a,b] Yaoming Xie,[c]
R. Bruce King,*[a,c] and Henry F. Schaefer III[c]

[a] Center for Computational Quantum Chemistry, South China Normal University, Guangzhou 510631, P. R. China
[b]Institute of Chemical Physics, Beijing Institute of Technology, Beijing 100081, P. R. China
[c]Department of Chemistry and Center for Computational Chemistry, University of Georgia, Athens, Georgia 30602, USA

Supporting Information

Tables S1 to S5: Harmonic vibrational frequencies and infrared intensities for $HMn(CO)_n$ (n = 5, 4, 3).

Tables S6 to S12: Harmonic vibrational frequencies and infrared intensities for $H_2Mn_2(CO)_n$ (n = 9, 8, 7, 6).

Tables S13 to S20: Atomic coordinates of the optimized structures $HMn(CO)_n$ (n = 5, 4, 3).

Tables S21 to S35: Atomic coordinates of the optimized structures $H_2Mn_2(CO)_n$ (n = 9, 8, 7, 6).

Complete Gaussian 03 reference (Reference 40)

Table S1. Harmonic vibrational frequencies(in cm^{-1}) and Infrared Intensities (in Parentheses in km/mol) for **15-1.**

–	**15-1**	
–	B3LYP	BP86
b_2	44(0)	33(0)
e	79(0)	75(0)
e	79(0)	75(0)
b_1	98(0)	94(0)
e	103(0)	99(0)
e	103(0)	99(0)
a_1	111(0)	106(0)
e	353(2)	349(0)
e	353(2)	349(0)
a_2	371(0)	375(0)
a_1	406(0)	478(0)
b_2	417(0)	440(0)
a_1	459(5)	476(2)
e	467(26)	483(12)
e	467(26)	483(12)
b_2	507(0)	491(0)
e	550(1)	537(0)
e	550(1)	537(0)
b_1	574(0)	560(0)
e	634(64)	611(23)
e	634(64)	611(23)
a_1	685(149)	685(132)
e	771(138)	752(180)
e	771(138)	752(180)
a_1	1846(17)	1839(0)
a_1	2077(892)	1998(779)
e	2085(1557)	2001(1397)
e	2085(1558)	2001(1397)
b_2	2101(0)	2022(0)
a_1	2173(6)	2093(2)

Table S2. Harmonic vibrational frequencies(in cm^{-1}) and Infrared Intensities (in Parentheses in km/mol) for **14-1** and **14-2.**

_	**14-1**		_	**14-2**	
_	B3LYP	BP86	_	B3LYP	BP86
a'	69(0)	65(0)	b_2	30(0)	22(0)
a"	81(0)	79(0)	e	90(1)	84(1)
a'	91(0)	87(0)	e	90(1)	84(1)
a"	100(1)	98(1)	b_1	95(0)	93(0)
a'	102(0)	99(0)	a_1	111(0)	105(0)
a'	314(10)	311(7)	e	342(4)	336(1)
a"	354(5)	349(2)	e	342(4)	336(1)
a"	358(0)	363(0)	a_2	367(0)	371(0)
a'	408(2)	428(0)	a_1	415(1)	439(0)
a'	449(7)	468(3)	b_2	417(0)	440(0)
a"	451(39)	467(20)	e	464(56)	481(29)
a'	480(6)	512(0)	e	464(56)	481(29)
a'	532(4)	521(3)	b_2	503(0)	497(0)
a"	554(11)	541(8)	b_1	578(0)	564(0)
a'	570(28)	574(17)	e	633(77)	621(52)
a'	621(80)	624(63)	e	633(77)	621(52)
a"	625(36)	607(9)	a_1	669(58)	670(46)
a'	703(57)	713(61)	e	808(15)	801(45)
a"	756(47)	722(73)	e	808(15)	801(45)
a'	1835(47)	1828(15)	a_1	1924(63)	1968(21)
a'	2054(942)	1966(787)	e	2053(1957)	1964(1690)
a'	2068(751)	1978(1448)	e	2053(1957)	1964(1690)
a"	2069(1674)	1983(661)	b_2	2079(0)	1998(0)
a'	2147(28)	2060(22)	a_1	2152(3)	2066(2)

Table S3. Harmonic vibrational frequencies(in cm^{-1}) and Infrared Intensities (in Parentheses in km/mol) for **14-3T.**

	14-3T	
	B3LYP	BP86
a_1	46(0)	51(0)
b_2	54(2)	13i(3)
a_2	68(0)	71(0)
b_1	91(0)	88(0)
a_1	96(0)	91(0)
b_1	209(4)	280(1)
b_1	302(1)	385(0)
a_1	334(9)	382(4)
a_2	335(0)	344(0)
b_2	346(0)	355(1)
a_1	370(0)	402(1)
b_2	386(37)	333(17)
b_1	408(10)	453(1)
a_1	438(3)	463(2)
a_2	498(0)	503(0)
b_2	537(61)	562(44)
a_1	591(73)	586(61)
b_1	592(59)	608(69)
b_2	670(1)	603(0)
a_1	1801(112)	1835(39)
b_2	2051(1930)	1968(1544)
a_1	2071(515)	1974(495)
b_1	2088(1032)	1985(872)
a_1	2145(46)	2046(51)

Table S4. Harmonic vibrational frequencies(in cm^{-1}) and Infrared Intensities (in Parentheses in km/mol) for **13-1 and 13-2.**

	13-1			**13-2**	
	B3LYP	BP86		B3LYP	BP86
a"	82(0)	78(0)	a'	73(1)	70(1)
a'	91(0)	91(0)	a'	91(0)	91(1)
a'	105(1)	105(1)	a"	96(1)	96(1)
a"	305(12)	289(6)	a'	337(18)	344(3)
a'	318(35)	325(30)	a"	347(8)	352(11)
a"	379(2)	397(2)	a"	360(0)	366(0)
a'	438(11)	458(9)	a'	428(1)	455(1)
a'	476(14)	501(1)	a"	463(76)	482(38)
a"	497(22)	524(4)	a'	488(9)	525(0)
a"	526(10)	541(11)	a'	577(16)	579(10)
a'	584(67)	589(46)	a'	604(49)	612(28)
a'	626(34)	645(28)	a"	626(27)	622(20)
a"	706(13)	709(17)	a'	713(17)	760(16)
a'	732(47)	745(60)	a"	798(1)	777(12)
a'	1841(139)	1823(57)	a'	1923(104)	1933(645)
a"	2037(1046)	1943(861)	a'	2023(816)	1973(28)
a'	2042(1161)	1950(959)	a"	2033(2059)	1937(1684)
a'	2112(275)	2021(208)	a'	2119(26)	2027(23)

Table S5. Harmonic vibrational frequencies(in cm^{-1}) and Infrared Intensities (in Parentheses in km/mol) for **13-3T** and **13-4.**

	13-3T			**13-4**	
	B3LYP	BP86		B3LYP	BP86
b_2	43(0)	10(0)	b_2	80(0)	79(0)
b_1	81(3)	59(7)	a_1	82(0)	75(0)
a_1	92(0)	88(0)	b_1	93(1)	90(1)
b_1	228(26)	184(21)	b_1	255(9)	252(3)
a_2	320(0)	315(0)	a_2	321(0)	315(0)
b_2	326(11)	316(5)	b_2	349(8)	345(3)
b_1	366(19)	317(7)	a_1	412(0)	430(0)
a_1	375(5)	397(2)	a_1	461(9)	480(2)
a_1	431(3)	451(2)	b_2	462(56)	474(32)
b_2	457(53)	454(2)	b_1	551(15)	566(8)
b_2	487(55)	474(56)	b_2	575(48)	563(26)
b_1	561(7)	558(3)	a_1	599(75)	586(49)
a_1	599(90)	592(75)	b_1	662(2)	686(5)
b_2	742(36)	708(52)	b_2	752(39)	713(56)
a_1	1802(51)	1804(13)	a_1	1798(60)	1797(8)
b_2	2026(2267)	1945(1854)	a_1	2047(1028)	1960(891)
a_1	2071(686)	1989(632)	b_2	2052(1840)	1957(1625)
a_1	2141(176)	2050(102)	a_1	2131(18)	2039(5)

Table S6. Harmonic vibrational frequencies(in cm^{-1}) and Infrared Intensities (in Parentheses in km/mol) for **29-1** and **29-2 .**

_	**29-1**		_	**29-2**	
_	B3LYP	BP86	_	B3LYP	BP86
a"	36(0)	36(0)	a	16(0)	14(0)
a"	53(0)	50(0)	a	22(0)	29(0)
a'	54(0)	51(0)	a	37(0)	40(0)
a'	60(0)	53(0)	a	52(1)	54(0)
a"	63(0)	60(0)	a	64(0)	62(0)
a"	69(0)	60(0)	a	72(0)	73(0)
a'	80(0)	73(0)	a	73(0)	76(0)
a'	86(0)	81(0)	a	77(1)	81(0)
a"	87(0)	83(0)	a	82(0)	84(0)
a'	96(0)	93(0)	a	85(0)	86(1)
a'	98(0)	94(0)	a	87(0)	90(2)
a"	98(0)	95(0)	a	96(0)	94(0)
a'	104(1)	100(1)	a	101(0)	101(0)
a"	105(1)	102(1)	a	103(0)	104(0)
a'	108(0)	104(0)	a	107(1)	107(1)
a"	108(0)	104(0)	a	110(1)	115(1)
a'	116(2)	113(2)	a	112(1)	116(7)
a'	150(0)	153(0)	a	131(0)	142(1)
a"	343(1)	346(1)	a	299(1)	297(2)
a'	368(12)	363(19)	a	357(3)	348(3)
a"	371(0)	373(0)	a	360(1)	367(0)
a"	397(0)	396(0)	a	369(12)	392(12)
a"	413(0)	410(0)	a	387(1)	408(6)
a'	399(24)	416(6)	a	396(0)	417(1)
a'	406(1)	424(6)	a	410(4)	421(0)
a'	419(1)	427(0)	a	413(1)	427(2)
a"	417(0)	431(0)	a	421(1)	437(1)
a"	452(13)	459(4)	a	440(20)	462(10)
a'	459(9)	460(12)	a	443(25)	469(16)
a"	468(19)	461(2)	a	452(2)	478(1)
a"	472(0)	480(10)	a	469(4)	482(1)
a'	470(18)	481(9)	a	478(22)	486(4)
a'	476(2)	487(3)	a	486(5)	492(9)
a"	487(5)	492(7)	a	510(0)	498(2)
a'	480(4)	493(1)	a	534(0)	509(3)
a'	491(0)	506(1)	a	548(3)	538(3)
a'	555(1)	542(0)	a	550(3)	543(1)
a'	560(0)	545(0)	a	557(0)	546(4)
a"	558(0)	547(0)	a	562(6)	548(1)

a'	572(5)	564(6)	a	592(0)	572(8)
a"	580(1)	573(1)	a	603(30)	579(3)
a"	610(7)	599(3)	a	629(41	607(16)
a'	659(332)	662(124)	a	646(52)	653(163)
a'	664(423)	664(176)	a	658(217)	660(103)
a"	666(67)	664(64)	a	672(156)	674(109)
a'	668(129)	670(427)	a	680(130)	678(224)
a"	682(136)	680(125)	a	738(46)	712(109)
a'	694(3)	696(8)	a	758(127)	749(155)
a'	1031(33)	1091(31)	a	773(80)	997(93)
a'	1658(50)	1709(54)	a	1784(533)	1491(67)
a"	2044(3)	1962(13)	a	1824(74)	1823(1)
a'	2048(153)	1970(211)	a	2039(767)	1963(600)
a'	2056(656)	1978(834)	a	2041(914)	1970(490)
a'	2065(59)	1987(46)	a	2052(678)	1980(454)
a'	2073(1617)	1993(1306)	a	2092(865)	2003(485)
a"	2073(368)	1994(1826)	a	2114(1365)	2013(1367)
a"	2081(2167)	2002(374)	a	2116(1530)	2020(1560)
a'	2090(2130)	2027(1271)	a	2124(225)	2036(13)
a'	2162(43)	2081(38)	a	2132(69)	2042(650)
a'	3210(159)	2847(114)	a	2192(42)	2100(84)

Table S7. Harmonic vibrational frequencies(in cm^{-1}) and Infrared Intensities (in Parentheses in km/mol) for **28-1 .**

–	**28-1**	
–	B3LYP	BP86
a_u	19(0)	18(0)
b_{1u}	37(0)	32(0)
b_{2g}	49(0)	44(0)
b_{3u}	69(0)	66(0)
b_{1g}	78(0)	74(0)
a_g	79(0)	79(0)
b_{2u}	88(1)	81(1)
a_u	90(0)	88(0)
b_{3g}	91(0)	88(0)
b_{1u}	93(0)	88(0)
b_{3u}	109(0)	107(0)
b_{1g}	117(0)	113(0)
b_{2g}	122(0)	117(0)
a_g	127(0)	118(0)
b_{2u}	128(0)	120(0)
a_g	196(0)	193(0)
b_{3g}	358(0)	359(0)
b_{2u}	379(0)	353(1)

b_{3u}	390(0)	418(3)
a_g	399(0)	424(0)
a_u	405(0)	407(0)
b_{1g}	411(0)	418(0)
b_{1u}	429(4)	426(3)
b_{2g}	449(0)	448(0)
b_{2u}	453(82)	471(41)
b_{3u}	454(4)	481(4)
a_g	463(0)	488(0)
b_{1g}	471(0)	491(0)
b_{2g}	472(0)	491(0)
b_{1u}	473(30)	496(11)
b_{3u}	547(2)	541(0)
a_g	565(0)	558(0)
a_u	580(0)	570(0)
b_{3g}	581(0)	569(0)
b_{1u}	631(128)	633(104)
b_{2u}	632(50)	613(1)
b_{1g}	643(0)	643(0)
b_{2g}	646(0)	652(0)
b_{3u}	678(337)	684(273)
b_{3g}	685(0)	586(0)
a_g	695(0)	698(0)
b_{2u}	731(151)	664(192)
b_{1u}	1250(4)	1240(6)
b_{2g}	1270(0)	1274(0)
b_{3u}	1327(1523)	1326(950)
a_g	1338(0)	1317(0)
b_{1g}	2058(0)	1967(0)
b_{2g}	2060(0)	1977(0)
b_{1u}	2064(1958)	1980(1683)
b_{3u}	2073(813)	1989(627)
a_g	2084(0)	1999(0)
b_{2u}	2091(2515)	2000(2226)
b_{3u}	2133(721)	2054(666)
a_g	2166(0)	2082(0)

Table S8. Harmonic vibrational frequencies(in cm^{-1}) and Infrared Intensities (in Parentheses in km/mol) for **27-1 , 27-2** and **27-5.**

_	**27-1**			**27-2**			**27-5**	
_	B3LYP	BP86	_	B3LYP	BP86	_	B3LYP	BP86
a"	28(0)	20(0)	a"	54i(0)	71i(0)	a"	23(0)	19(0)
a'	32(1)	30(0)	a"	30(0)	14(0)	a'	43(0)	37(0)
a"	42(0)	39(0)	a'	45(0)	41(0)	a'	49(0)	47(0)
a"	70(0)	66(0)	a"	58(0)	48(0)	a'	70(0)	67(0)
a'	72(0)	69(0)	a'	72(0)	69(0)	a"	75(0)	70(0)
a'	82(0)	82(0)	a'	76(0)	73(1)	a"	87(1)	82(0)
a'	87(0)	88(0)	a'	83(0)	81(0)	a"	90(0)	87(0)
a"	87(0)	85(0)	a"	86(0)	84(0)	a'	90(0)	86(0)
a"	93(0)	92(0)	a"	89(0)	89(0)	a'	98(0)	95(0)
a'	100(1)	102(0)	a'	94(0)	92(0)	a"	108(0)	103(0)
a'	111(0)	113(0)	a"	100(0)	98(0)	a'	120(0)	112(0)
a'	124(1)	148(0)	a'	111(0)	109(0)	a"	121(0)	115(0)
a"	131(0)	131(0)	a'	132(0)	130(0)	a'	124(0)	122(0)
a'	203(4)	211(0)	a'	202(5)	208(4)	a'	205(0)	201(0)
a"	356(0)	355(0)	a"	310(1)	311(0)	a"	333(0)	325(0)
a'	358(0)	352(7)	a"	355(0)	351(0)	a"	371(0)	354(0)
a'	401(3)	417(1)	a"	382(0)	395(0)	a'	384(9)	416(6)
a"	411(0)	418(0)	a'	407(6)	429(4)	a"	392(9)	394(2)
a"	428(2)	424(2)	a"	427(1)	429(0)	a'	397(0)	423(0)
a'	435(1)	447(0)	a'	432(2)	432(1)	a"	407(2)	412(0)
a'	446(11)	461(20)	a'	445(4)	456(0)	a'	437(5)	431(4)
a"	450(0)	458(0)	a'	449(3)	468(1)	a"	443(107)	461(62)
a'	454(18)	467(2)	a'	461(1)	489(4)	a'	459(3)	476(3)
a'	469(16)	497(9)	a"	467(33)	478(14)	a"	466(0)	484(0)
a"	472(25)	487(2)	a'	473(26)	496(2)	a'	467(11)	485(2)
a"	501(20)	518(19)	a'	502(21)	525(14)	a'	474(2)	494(3)
a'	503(17)	511(8)	a"	503(13)	531(6)	a'	481(11)	509(1)
a'	537(2)	528(10)	a'	547(3)	534(16)	a'	556(0)	548(0)
a"	566(0)	547(0)	a"	563(0)	549(0)	a"	580(0)	568(0)
a"	604(49)	571(0)	a"	613(49)	594(14)	a'	605(39)	614(30)
a'	616(76)	612(52)	a'	619(64)	619(64)	a"	617(21)	586(3)
a'	632(6)	639(13)	a"	620(3)	619(1)	a'	629(64)	633(50)
a"	637(0)	629(63)	a'	639(44)	642(25)	a"	638(18)	606(4)
a'	656(239)	650(196)	a'	667(237)	664(201)	a'	644(57)	648(29)
a"	678(38)	651(17)	a"	675(7)	633(16)	a"	685(19)	641(13)
a'	686(1)	692(4)	a'	688(3)	696(2)	a'	685(138)	688(105)
a'	754(77)	718(72)	a"	732(92)	702(113)	a"	742(83)	668(116)
a"	1252(6)	1177(8)	a'	1301(60)	1264(6)	a'	1216(18)	1110(86)
a'	1306(470)	1221(158)	a'	1358(305)	1299(92)	a'	1231(478)	1201(155)

a"	1487(0)	1497(2)	a'	1454(2)	1464(3)	a'	1316(504)	1327(220)
a'	1513(31)	1520(4)	a'	1491(66)	1483(6)	a'	1391(378)	1499(242)
a'	2044(309)	1958(203)	a"	2044(296)	1954(333)	a"	2036(339)	1934(508)
a"	2051(773)	1962(663)	a'	2053(737)	1961(693)	a'	2043(780)	1954(576)
a'	2064(1366)	1972(1189)	a'	2072(1104)	1989(894)	a'	2059(1080)	1976(884)
a"	2075(1115)	1992(964)	a"	2078(1969)	1995(1617)	a'	2076(329)	1990(1898)
a'	2096(1186)	2012(791)	a'	2084(510)	2005(357)	a"	2082(2439)	1993(274)
a'	2108(847)	2022(922)	a'	2104(1142)	2018(1044)	a'	2117(566)	2025(552)
a'	2157(133)	2071(201)	a'	2154(68)	2068(135)	a	2157(52)	2072(95)

Table S9. Harmonic vibrational frequencies(in cm^{-1}) and Infrared Intensities (in Parentheses in km/mol) for **27-3T** and **27-4T.**

	27-3T			**27-4T**	
	B3LYP	BP86		B3LYP	BP86
a"	19(0)	18(0)	a_2	16(0)	9(0)
a'	42(0)	38(0)	b_1	25(0)	28(0)
a"	47(0)	36(0)	b_1	43(0)	39(0)
a'	51(0)	56(0)	b_2	60(2)	54(1)
a"	69(1)	69(0)	a_1	71(0)	69(0)
a'	70(0)	71(0)	b_2	78(0)	74(0)
a'	76(0)	74(0)	a_2	91(0)	88(0)
a'	77(0)	75(0)	b_1	93(1)	88(0)
a"	86(0)	84(0)	a_1	101(0)	98(0)
a"	93(1)	88(1)	b_2	103(0)	96(0)
a'	101(0)	99(0)	b_1	118(1)	116(1)
a"	106(0)	102(0)	b_2	126(0)	118(0)
a'	122(0)	120(0)	a_1	129(0)	121(0)
a'	197(4)	198(5)	a_1	187(9)	188(5)
a"	297(2)	310(0)	b_1	329(1)	338(1)
a"	335(0)	325(1)	a_2	337(0)	335(0)
a"	344(2)	354(0)	b_2	367(0)	347(0)
a'	344(13)	401(7)	a_1	389(4)	417(2)
a'	370(4)	406(4)	a_2	392(0)	389(0)
a"	374(12)	388(0)	b_2	399(11)	404(3)
a"	399(10)	437(17)	a_1	402(3)	426(1)
a'	406(3)	426(4)	a_1	409(15)	444(8)
a'	409(6)	428(1)	b_2	442(86)	456(41)
a'	446(0)	447(1)	b_1	444(3)	438(2)
a'	455(4)	476(0)	a_1	464(3)	483(1)
a"	459(32)	470(14)	b_2	469(18)	489(7)
a'	474(22)	490(4)	b_1	477(16)	492(6)
a'	486(14)	520(22)	b_2	532(12)	535(20)
a'	534(25)	539(5)	a_1	548(3)	539(2)
a'	553(1)	555(24)	b_1	583(14)	587(14)
a"	568(1)	553(0)	a_2	585(0)	567(0)
a"	570(6)	577(3)	a_1	628(75)	630(65)
a"	616(14)	584(7)	b_2	632(20)	612(0)
a'	639(69)	639(56)	b_1	643(85)	645(63)
a"	644(18)	607(0)	a_2	683(0)	593(0)
a'	674(191)	671(149)	a_1	687(174)	687(130)
a"	720(98)	674(111)	b_2	725(106)	662(120)
a'	1247(95)	1244(27)	b_1	1038(4)	1093(1)
a'	1328(475)	1294(273)	a_1	1150(433)	1158(281)

a'	1381(8)	1379(8)	b_1	1380(8)	1359(1)
a'	1435(286)	1415(60)	a_1	1418(1028)	1399(587)
a'	2038(775)	1953(545)	b_2	2029(266)	1941(289)
a"	2062(225)	1964(167)	b_1	2053(1052)	1974(900)
a'	2063(1046)	1981(883)	a_1	2066(703)	1982(794)
a'	2077(498)	1991(1960)	b_2	2074(2740)	1985(2228)
a"	2087(2204)	1998(420)	a_1	2080(158)	1991(0)
a'	2115(915)	2012(928)	a_1	2120(1042)	2033(900)
a'	2154(18)	2067(116)	a_1	2157(1)	2070(32)

Table S10. Harmonic vibrational frequencies(in cm^{-1}) and Infrared Intensities (in Parentheses in km/mol) for **26-1** and **26-2 .**

_	**26-1**		_	**26-2**	
_	B3LYP	BP86	_	B3LYP	BP86
a'	11(3)	34(0)	b_u	3(2)	27i(3)
a"	36(0)	34(2)	a_u	35(0)	35(0)
a"	50(0)	44(0)	a_u	50(0)	46(0)
a'	79(0)	77(0)	a_g	79(0)	77(0)
a"	79(0)	78(0)	b_g	80(0)	78(0)
a'	81(0)	81(0)	a_g	81(0)	79(0)
a'	86(0)	87(1)	b_u	86(0)	83(0)
a"	92(1)	90(1)	a_u	92(1)	91(1)
a'	107(0)	105(0)	b_u	107(0)	106(0)
a'	122(0)	119(0)	a_g	122(0)	121(0)
a"	125(0)	124(0)	b_g	125(0)	122(0)
a'	204(0)	218(1)	a_g	204(0)	208(0)
a'	345(22)	379(14)	b_u	344(21)	337(11)
a"	354(0)	356(0)	b_g	352(0)	359(0)
a"	419(0)	424(1)	a_u	419(0)	428(0)
a"	432(0)	427(0)	a_u	432(0)	431(1)
a'	437(19)	457(9)	b_u	437(19)	457(12)
a"	443(0)	455(0)	b_g	443(0)	454(0)
a'	443(0)	459(2)	a_g	443(0)	457(0)
a'	451(0)	475(1)	a_g	451(0)	474(0)
a"	475(62)	495(21)	a_u	475(62)	500(32)
a'	494(30)	510(6)a"	b_u	494(30)	531(4)
a"	503(0)	531(3)a'	b_g	503(0)	509(0)
a'	518(0)	535(5)a'	a_g	518(0)	540(0)
a'	582(21)	576(0)a"	b_u	582(21)	569(10)
a"	607(28)	582(21)a'	a_u	607(28)	607(26)
a'	620(0)	626(39)a"	a_g	620(0)	601(0)
a"	621(0)	627(28)a'	b_g	621(0)	631(0)
a"	634(0)	634(2)a"	b_g	632(0)	633(0)
a'	641(121)	647(15)a"	b_u	641(118	637(39)

a'	674(0)	679(1)	a_g	674(0)	681(0)
a'	713(54)	695(80)	b_u	711(57)	685(113)
a"	1387(0)	1255(0)	b_g	1385(0)	1329(0)
a'	1432(555)	1296(66)	b_u	1431(553)	1375(82)
a"	1445(1)	1475(1)	a_u	1445(1)	1459(4)
a'	1480(0)	1501(1)	a_g	1477(0)	1477(0)
a'	2037(0)	1936(256)	a_g	2037(0)	1950(0)
a'	2043(1704)	1960(1007)	b_u	2044(1707)	1957(1428)
a"	2055(0)	1961(433)	b_g	2055(0)	1964(0)
a"	2059(1950)	1971(1213)	a_u	2059(1950)	1967(1635)
a'	2094(1811)	2004(1782)	b_u	2094(1809)	2004(1792)
a'	2131(0)	2040(6)	a_g	2131(0)	2039(0)

Table S11. Harmonic vibrational frequencies(in cm^{-1}) and Infrared Intensities (in Parentheses in km/mol) for **26-3** and **26-4 .**

_	**26-3**			**26-4**	
_	B3LYP	BP86	_	B3LYP	BP86
a_2	22(0)	20(0)	a	32(0)	29(0)
b_1	49(0)	45(0)	a	35(0)	35(0)
a_1	61(0)	61(0)	a	51(0)	48(0)
b_2	71(0)	56(1)	a	69(0)	67(0)
a_2	79(0)	79(0)	a	76(0)	74(0)
a_1	81(0)	80(0)	a	86(0)	88(0)
b_2	91(0)	85(1)	a	92(0)	90(0)
b_1	93(1)	92(1)	a	94(0)	96(0)
a_1	100(0)	102(0)	a	103(0)	104(0)
b_2	110(0)	110(0)	a	127(0)	135(0)
a_2	120(0)	116(0)	a	134(0)	146(0)
a_1	204(0)	204(0)	a	221(3)	230(1)
b_1	346(1)	355(1)	a	327(1)	314(6)
a_1	372(9)	367(8)	a	357(1)	360(3)
a_2	403(0)	413(0)	a	398(12)	418(0)
b_2	414(6)	416(7)	a	413(0)	420(2)
b_1	430(0)	431(1)	a	435(7)	434(5)
a_2	446(0)	455(0)	a	438(3)	446(2)
b_2	447(10)	478(1)	a	452(34)	462(36)
a_1	455(7)	478(7)	a	462(8)	477(3)
b_1	475(55)	491(19)	a	471(19)	490(0)
a_1	492(30)	528(12)	a	474(23)	499(13)
b_2	495(0)	528(0)	a	504(16)	522(14)
a_2	506(0)	519(0)	a	507(23	527(12)
b_1	552(22)	561(29)	a	591(53)	570(33)
a_1	564(9)	540(0)	a	602(69)	575(38)

b_2	606(46)	606(11)	a	604(52)	600(55)
a_2	620(0)	627(0)	a	628(9)	630(28)
b_1	621(14)	617(11)	a	634(9)	639(10)
a_1	655(2)	657(5)	a	681(36)	662(15)
b_2	669(88)	677(82)	a	709(18)	685(20)
a_1	702(38)	700(34)	a	760(29)	706(29)
a_2	1367(0)	1334(0)	a	1203(2)	1096(15)
b_1	1380(1)	1392(3)	a	1252(364)	1150(76)
b_2	1401(677)	1371(112)	a	1497(9)	1497(3)
a_1	1430(4)	1492(1)	a	1609(51)	1690(30)
b_2	2037(165)	1948(138)	a	2035(92)	1941(395)
a_2	2049(0)	1958(0)	a	2047(755)	1958(573)
b_1	2053(1977)	1961(1646)	a	2048(1743)	1960(1197)
a_1	2058(1415)	1967(1139)	a	2067(1583)	1975(1172)
b_2	2093(1739)	2001(1844)	a	2101(1046)	2012(1158)
a_1	2131(48)	2039(59)	a	2141(74)	2047(47)

Table S12. Harmonic vibrational frequencies(in cm^{-1}) and Infrared Intensities (in Parentheses in km/mol) for **26-5T, 26-6T** and **26-7T .**

26-5T			**26-6T**			**26-7T**	
B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a'	15(0)	45(0)	a"	26(0)	20i(0)	a_2	10i(0)	2(0)
a"	22(0)	25(0)	a'	31(0)	9(1)	b_1	49(0)	45(0)
a"	43(0)	38(0)	a"	32(0)	27(0)	a_1	70(0)	67(0)
a"	71(1)	64(0)	a"	67(0)	61(0)	b_2	71(2)	47(4)
a'	71(0)	71(0)	a'	71(1)	71(0)	a_1	74(0)	74(0)
a'	76(0)	76(0)	a'	79(0)	78(0)	a_2	77(0)	78(0)
a"	86(0)	85(0)	a'	86(0)	91(1)	b_1	85(1)	86(1)
a'	91(2)	95(0)	a"	92(0)	89(0)	b_2	92(1)	90(1)
a'	99(0)	105(0)	a'	102(0)	104(0)	a_1	109(0)	104(0)
a'	103(0)	135(1)	a'	113(0)	152(2)	b_2	114(1)	98(1)
a"	121(2)	119(1)	a"	120(1)	124(1)	a_2	121(0)	116(0)
a'	205(1)	225(0)	a'	186(0)	202(9)	a_1	238(0)	234(0)
a'	327(1)	367(6)	a"	327(1)	318(0)	b_1	290(1)	337(0)
a"	330(215)	342(0)	a"	341(0)	339(0)	a_2	360(0)	367(0)
a"	340(0)	364(1)	a'	341(11)	316(3)	a_1	366(0)	375(0)
a"	367(0)	392(14)	a'	385(21)	402(2)	b_1	370(1)	388(0)
a'	410(3)	424(9)	a'	399(9)	413(5)	b_2	403(6)	381(19)
a'	412(2)	427(1)	a"	410(0)	415(0)	b_1	410(20)	430(5)
a'	425(1)	440(4)	a'	431(15)	444(29)	a_2	410(0)	427(0)
a"	431(33)	433(26)	a"	444(1)	437(4)	b_2	429(88)	420(1)

a'	454(3)	472(18)	a'	447(26)	448(0)	a_1	443(6)	465(4)
a"	459(47)	484(71)	a'	463(9)	482(2)	b_1	465(61)	484(0)
a'	464(34)	477(7)	a"	491(41)	503(20)	a_1	470(12)	487(0)
a"	484(3)	487(3)	a'	505(16)	523(10)	a_2	493(0)	489(0)
a'	554(1)	517(13)	a'	538(43)	551(36)	a_1	507(4)	493(8)
a"	564(0)	552(0)	a"	574(15)	543(3)	b_2	515(0)	457(18)
a'	590(94)	597(72)	a'	607(72)	568(72)	b_2	549(0)	561(18)
a'	625(34)	625(46)	a"	610(9)	580(1)	a_2	556(0)	580(0)
a"	641(59)	586(0)	a'	613(28)	618(23)	b_1	566(36)	574(40)
a"	654(0)	647(53)	a'	671(76)	673(47)	a_1	601(1)	616(0)
a'	676(164)	666(128)	a"	671(12)	642(29)	b_2	607(160)	608(81)
a'	714(109)	739(59)	a'	720(28)	682(37)	a_1	629(65)	627(47)
a"	1314(1)	1157(2)	a"	1187(0)	1098(1)	a_2	1348(0)	1292(0)
a'	1358(473)	1174(21)	a'	1231(605)	1128(264)	b_2	1388(8)	1337(1)
a"	1429(2)	1460(0)	a"	1438(4)	1477(0)	b_1	1510(2)	1481(0)
a'	1453(48)	1490(0)	a'	1461(261)	1487(31)	a_1	1536(0)	1511(0)
a"	1958(2406)	1910(1446)	a'	2027(95)	1935(539)	b_2	2051(2)	1940(152)
a"	2066(1008)	1983(900)	a'	2045(2068)	1960(960)	a_2	2057(0)	1959(0)
a'	2070(1538)	1944(701)	a"	2045(1010)	1964(832)	b_1	2059(2316)	1961(1961)
a'	2078(720)	1995(1426)	a'	2088(836)	1988(801)	a_1	2064(1271)	1973(1037)
a'	2096(736)	2001(561)	a'	2097(1456)	2009(1671)	b_2	2087(3138)	1985(2129)
a'	2149(103)	2058(255)	a'	2145(152)	2048(52)	a_1	2134(34)	2036(50)

Table S13. Atomic coordinates of the optimized structure **15-1.**

_15-1	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	0.000000	0.000000	0.154019	0.000000	0.000000	0.155700
H	0.000000	0.000000	1.728898	0.000000	0.000000	1.732063
C	0.000000	1.844576	0.376009	0.000000	1.828967	0.376175
C	-1.844576	0.000000	0.376009	-1.828967	0.000000	0.376175
C	1.844576	0.000000	0.376009	1.828967	0.000000	0.376175
C	0.000000	-1.844576	0.376009	0.000000	-1.828967	0.376175
O	2.979638	0.000000	0.577351	2.979279	0.000000	0.573302
O	0.000000	-2.979638	0.577351	0.000000	-2.979279	0.573302
O	-2.979638	0.000000	0.577351	-2.979279	0.000000	0.573302
O	0.000000	2.979638	0.577351	0.000000	2.979279	0.573302
C	0.000000	0.000000	-1.702478	0.000000	0.000000	-1.688525
O	0.000000	0.000000	-2.857995	0.000000	0.000000	-2.858409

Table S14. Atomic coordinates of the optimized structure **14-1.**

_14-1	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	0.377917	-0.237922	0.000000	0.423412	-0.181494	0.000000
C	0.413828	-0.566942	1.826636	0.469463	-0.534209	1.803161
C	0.413828	-0.566942	-1.826636	0.469463	-0.534209	-1.803161
C	0.510399	1.619850	0.000000	0.312067	1.661272	0.000000
O	0.413828	-0.859963	-2.943003	0.469463	-0.851501	-2.928748
O	0.577083	2.774506	0.000000	0.213720	2.829016	0.000000
O	0.413828	-0.859963	2.943003	0.469463	-0.851501	2.928748
C	-1.419260	-0.235197	0.000000	-1.331267	-0.367663	0.000000
O	-2.576923	-0.271923	0.000000	-2.497631	-0.509590	0.000000
H	0.416787	-1.817812	0.000000	0.656232	-1.745188	0.000000

Table S15. Atomic coordinates of the optimized structure **14-2.**

14-2	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	0.000000	0.000000	0.228194	0.000000	0.000000	0.234176
H	0.000000	0.000000	-1.296991	0.000000	0.000000	-1.281241
C	0.000000	1.846331	0.044041	0.000000	1.828077	0.045551
C	1.846331	0.000000	0.044041	1.828077	0.000000	0.045551
C	-1.846331	0.000000	0.044041	-1.828077	0.000000	0.045551
C	0.000000	-1.846331	0.044041	0.000000	-1.828077	0.045551
O	-2.981798	0.000000	-0.170776	-2.977704	0.000000	-0.177075
O	0.000000	-2.981798	-0.170776	0.000000	-2.977704	-0.177075
O	2.981798	0.000000	-0.170776	2.977704	0.000000	-0.177075
O	0.000000	2.981798	-0.170776	0.000000	2.977704	-0.177075

Table S16. Atomic coordinates of the optimized structure **14-3T.**

14-3T	B3LYP			BP86		
	X	Y	Z	X	Y	Z
Mn	0.000000	0.000000	0.280227	0.000000	0.000000	0.255214
C	0.000000	1.809437	0.675035	0.000000	1.790075	0.656292
C	0.000000	-1.809437	0.675035	0.000000	-1.790075	0.656292
C	1.604839	0.000000	-0.814669	1.578473	0.000000	-0.773422
O	0.000000	-2.916718	1.008635	0.000000	-2.909969	0.998864
O	2.559798	0.000000	-1.457987	2.549275	0.000000	-1.423740
O	0.000000	2.916718	1.008635	0.000000	2.909969	0.998864
C	-1.604839	0.000000	-0.814669	-1.578473	0.000000	-0.773422
O	-2.559798	0.000000	-1.457987	-2.549275	0.000000	-1.423740
H	0.000000	0.000000	1.859552	0.000000	0.000000	1.823233

Table S17. Atomic coordinates of the optimized structure **13-1.**

13-1	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	-0.525244	-0.596119	0.000000	-0.512757	-0.632131	0.000000
C	1.293164	-1.020420	0.000000	1.305314	-0.965501	0.000000
C	-0.428093	0.650873	1.279558	-0.454304	0.615077	1.230432
C	-0.428093	0.650873	-1.279558	-0.454304	0.615077	-1.230432
O	-0.428093	1.467004	2.103500	-0.454304	1.459046	2.051687
O	-0.428093	1.467004	-2.103500	-0.454304	1.459046	-2.051687
O	2.431465	-1.234082	0.000000	2.473424	-1.088754	0.000000
H	-2.093004	-0.384405	0.000000	-2.079851	-0.419363	0.000000

Table S18. Atomic coordinates of the optimized structure **13-2.**

13-2	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	-0.480633	-0.269273	0.000000	-0.463999	-0.350060	0.000000
C	-0.523707	0.022526	1.823823	-0.507385	-0.024719	1.797282
C	-0.523707	0.022526	-1.823823	-0.507385	-0.024719	-1.797282
C	-0.523707	0.349060	-2.935058	-0.507385	0.349108	-2.911123
O	-0.523707	0.349060	2.935058	-0.507385	0.349108	2.911123
O	1.295227	-0.108981	0.000000	1.243795	0.019029	0.000000
O	2.449212	0.035773	0.000000	2.396478	0.278519	0.000000
H	-0.685440	1.244251	0.000000	-0.827817	1.120077	0.000000

Table S19. Atomic coordinates of the optimized structure **13-3T.**

13-3T	a	B3LYP			BP86	
	X	Y	Z	X	Y	Z
Mn	0.000000	0.000000	0.331501	0.000000	0.000000	0.319999
H	0.000000	0.000000	1.931592	0.000000	0.000000	1.916957
C	0.000000	1.834482	0.631306	0.000000	1.815669	0.631242
C	0.000000	-1.834482	0.631306	0.000000	-1.815669	0.631242
O	0.000000	-2.963356	0.891044	0.000000	-2.957486	0.900853
O	0.000000	2.963356	0.891044	0.000000	2.957486	0.900853
C	0.000000	0.000000	-1.631699	0.000000	0.000000	-1.612710
O	0.000000	0.000000	-2.782663	0.000000	0.000000	-2.778653

Table S20. Atomic coordinates of the optimized structure **13-4.**

13-4	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	0.000000	0.000000	0.283962	0.000000	0.000000	0.275382
H	0.000000	0.000000	1.878808	0.000000	0.000000	1.865653
C	0.000000	1.826643	0.625348	0.000000	1.805010	0.627250
C	0.000000	-1.826643	0.625348	0.000000	-1.805010	0.627250
O	0.000000	-2.941869	0.930339	0.000000	-2.934187	0.940709
O	0.000000	2.941869	0.930339	0.000000	2.934187	0.940709
C	0.000000	0.000000	-1.578167	0.000000	0.000000	-1.566027
O	0.000000	0.000000	-2.737306	0.000000	0.000000	-2.741550

Table S21. Atomic coordinates of the optimized structure **29-1.**

29-1	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	0.023730	-1.429978	0.000000	0.046045	-1.409311	0.000000
Mn	0.328897	1.540246	0.000000	0.305031	1.512303	0.000000
C	-1.268101	-1.133916	1.310818	-1.241140	-1.127960	1.300221
C	0.331870	1.425738	1.863437	0.298195	1.438778	1.848884
C	0.331870	1.425738	-1.863437	0.298195	1.438778	-1.848884
C	1.343163	-1.449533	-1.311048	1.352121	-1.453718	-1.306517
C	1.343163	-1.449533	1.311048	1.352121	-1.453718	1.306517
C	-0.194483	-3.231082	0.000000	-0.177590	-3.199092	0.000000
C	-1.497355	1.698589	0.000000	-1.500714	1.699696	0.000000
O	-2.075509	-0.989205	2.123773	-2.064227	-1.009741	2.121230
O	0.324393	1.396280	3.017832	0.280487	1.453502	3.017885
O	2.164526	-1.488766	2.123720	2.176934	-1.523073	2.133214
O	2.164526	-1.488766	-2.123720	2.176934	-1.523073	-2.133214
O	0.324393	1.396280	-3.017832	0.280487	1.453502	-3.017885
O	-0.334360	-4.379778	0.000000	-0.324382	-4.361645	0.000000
O	-2.646976	1.826390	0.000000	-2.660272	1.866009	0.000000
H	1.830675	0.737938	0.000000	1.757348	0.659564	0.000000
C	0.608325	3.330037	0.000000	0.618837	3.283637	0.000000
O	0.770547	4.476614	0.000000	0.813108	4.440381	0.000000
H	2.043296	1.533877	0.000000	1.993719	1.486010	0.000000
C	-1.268101	-1.133916	-1.310818	-1.241140	-1.127960	-1.300221
O	-2.075509	-0.989205	-2.123773	-2.064227	-1.009741	-2.121230

Table S22. Atomic coordinates of the optimized structure **29-2.**

29-2	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
C	1.524006	1.557122	-1.078314	1.434360	1.609377	-0.938581
O	1.470432	2.501729	-1.728244	1.435795	2.606222	-1.538640
C	1.252682	-1.009879	-1.566158	1.057580	-0.861502	-1.590692
O	1.095364	-1.628805	-2.519702	0.927767	-1.413019	-2.608202
Mn	1.591659	0.008793	-0.016652	1.494130	0.008663	0.002240
Mn	-1.719280	0.028152	-0.113637	-1.599471	0.036462	-0.101429
C	3.422844	-0.177709	-0.178844	3.279006	-0.203962	-0.295520
C	-3.493155	-0.012001	-0.464252	-3.363445	0.041591	-0.431434
C	-1.713461	1.851323	-0.394238	-1.617816	1.852584	-0.337416
C	-1.617210	-1.784873	-0.430708	-1.569113	-1.757404	-0.485947
C	1.715007	1.067990	1.523755	1.774553	0.939205	1.578177
C	1.400134	-1.524993	1.048743	1.370855	-1.588808	0.940989
O	-1.568789	-2.907209	-0.712178	-1.610993	-2.883393	-0.807307
O	-1.709490	2.979430	-0.652069	-1.675039	2.999839	-0.565108
O	1.753467	1.723614	2.466232	1.941509	1.532873	2.565918
O	1.262123	-2.456588	1.705803	1.298464	-2.586189	1.535658

O	-4.624658	-0.032027	-0.715220	-4.516336	0.054315	-0.647060
O	4.567262	-0.289404	-0.267711	4.426535	-0.341069	-0.470011
H	-1.452295	0.061335	-1.671704	-1.362671	0.128768	-1.662648
H	-0.004097	0.258777	0.278154	-0.058725	0.272589	0.651145
C	-1.937417	-0.002043	1.719192	-1.882928	-0.068404	1.706810
O	-2.079915	-0.019910	2.870054	-2.083125	-0.132772	2.861365

Table S23. Atomic coordinates of the optimized structure **28-1.**

28-1	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	-1.361141	0.000000	0.000000	-1.351601	0.000000	0.000000
Mn	1.361141	0.000000	0.000000	1.351601	0.000000	0.000000
C	-1.433033	1.867563	0.000000	-1.435772	1.848268	0.000000
C	1.433033	1.867563	0.000000	1.435772	1.848268	0.000000
C	2.584814	0.000000	1.360925	2.576310	0.000000	1.329438
C	1.433033	-1.867563	0.000000	1.435772	-1.848268	0.000000
C	-1.433033	-1.867563	0.000000	-1.435772	-1.848268	0.000000
C	-2.584814	0.000000	1.360925	-2.576310	0.000000	1.329438
C	-2.584814	0.000000	-1.360925	-2.576310	0.000000	-1.329438
C	2.584814	0.000000	-1.360925	2.576310	0.000000	-1.329438
O	-1.581141	3.010382	0.000000	-1.607823	3.002820	0.000000
O	1.581141	3.010382	0.000000	1.607823	3.002820	0.000000
O	3.326646	0.000000	2.247732	3.347412	0.000000	2.211444
O	-3.326646	0.000000	2.247732	-3.347412	0.000000	2.211444
O	-1.581141	-3.010382	0.000000	-1.607823	-3.002820	0.000000
O	1.581141	-3.010382	0.000000	1.607823	-3.002820	0.000000
O	-3.326646	0.000000	-2.247732	-3.347412	0.000000	-2.211444
O	3.326646	0.000000	-2.247732	3.347412	0.000000	-2.211444
H	0.000000	0.000000	-1.084224	0.000000	0.000000	-1.089518
H	0.000000	0.000000	1.084224	0.000000	0.000000	1.089518

Table S24. Atomic coordinates of the optimized structure **27-1.**

27-1	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	0.026916	1.182331	0.000000	-0.034703	1.159143	0.000000
Mn	0.055781	-1.228810	0.000000	0.254252	-1.163740	0.000000
C	1.829677	1.675100	0.000000	1.547908	2.106547	0.000000
C	1.649347	-2.060242	0.000000	1.847772	-1.946119	0.000000
C	-0.568641	-2.313956	1.329334	-0.297316	-2.284036	1.294142
C	-1.751879	0.608742	0.000000	-1.671824	0.240800	0.000000
C	-0.346488	2.346325	1.380744	-0.657903	2.188482	1.372159
C	-0.346488	2.346325	-1.380744	-0.657903	2.188482	-1.372159
C	-0.568641	-2.313956	-1.329334	-0.297316	-2.284036	-1.294142
O	2.948092	1.943000	0.000000	2.555410	2.690844	0.000000

O	2.700221	-2.548189	0.000000	2.920676	-2.424673	0.000000
O	-0.965383	-2.971624	2.195295	-0.657903	-2.992176	2.158318
O	-0.568641	3.040083	2.276336	-1.042558	2.814742	2.281430
O	-2.886822	0.390074	0.000000	-2.797057	-0.085259	0.000000
O	-0.568641	3.040083	-2.276336	-1.042558	2.814742	-2.281430
O	-0.965383	-2.971624	-2.195295	-0.657903	-2.992176	-2.158318
H	0.501853	0.028758	-1.128275	0.702949	0.122928	-1.101085
H	0.501853	0.028758	1.128275	0.702949	0.122928	1.101085

Table S25. Atomic coordinates of the optimized structure **27-2.**

27-2	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	-0.036832	1.271670	0.000000	-0.892188	0.856442	0.000000
Mn	-0.071387	-1.216169	0.000000	0.802885	-0.892998	0.000000
C	1.288000	-2.461217	0.000000	2.627335	-0.831398	0.000000
C	-0.073203	-1.117319	1.859848	0.728168	-0.826131	1.846473
C	-1.438376	-2.449436	0.000000	0.716766	-2.713915	0.000000
C	-1.405172	2.489010	0.000000	-2.691003	0.747236	0.000000
C	-0.073203	-1.117319	-1.859848	0.728168	-0.826131	-1.846473
O	2.164007	-3.213671	0.000000	3.794598	-0.759686	0.000000
O	-0.073203	-1.067676	3.012037	0.700530	-0.804600	3.013281
O	-2.284579	3.239755	0.000000	-3.860677	0.657201	0.000000
O	-2.323421	-3.191696	0.000000	0.626967	-3.880330	0.000000
O	-0.073203	-1.067676	-3.012037	0.700530	-0.804600	-3.013281
H	-1.241363	-0.016117	0.000000	-0.872830	-0.893153	0.000000
H	1.114491	-0.010431	0.000000	0.835108	0.793229	0.000000
C	0.872401	2.165687	1.278676	-0.931496	2.125184	1.242182
C	0.872401	2.165687	-1.278676	-0.931496	2.125184	-1.242182
O	1.456153	2.687261	2.132163	-0.931496	2.934360	2.094494
O	1.456153	2.687261	-2.132163	-0.931496	2.934360	-2.094494

Table S26. Atomic coordinates of the optimized structure **27-5.**

27-5	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	0.030342	-1.098738	0.000000	0.013399	-1.081603	0.000000
Mn	-0.452821	1.538535	0.000000	-0.481270	1.527449	0.000000
C	0.034032	-1.147608	1.867421	0.002844	-1.147821	1.849639
C	-0.536992	1.677075	1.866830	-0.521510	1.689298	1.839968
C	-0.536992	1.677075	-1.866830	-0.521510	1.689298	-1.839968
C	0.034032	-1.147608	-1.867421	0.002844	-1.147821	-1.849639
C	1.612372	-2.020716	0.000000	1.593661	-1.966654	0.000000
C	-1.050554	-2.572414	0.000000	-0.981522	-2.583393	0.000000
C	0.678512	2.959870	0.000000	0.661930	2.899467	0.000000
O	0.050550	-1.264439	3.014031	0.006911	-1.295859	3.007396

O	-0.611700	1.883466	3.000068	-0.553940	1.934413	2.984765
O	2.629580	-2.570987	0.000000	2.627751	-2.517520	0.000000
O	0.050550	-1.264439	-3.014031	0.006911	-1.295859	-3.007396
O	-0.611700	1.883466	-3.000068	-0.553940	1.934413	-2.984765
O	-1.769629	-3.478549	0.000000	-1.656657	-3.541713	0.000000
O	1.465893	3.811965	0.000000	1.473484	3.752477	0.000000
H	-1.315208	-0.011890	0.000000	-1.341966	-0.028211	0.000000
H	0.842382	0.459056	0.000000	0.814178	0.524984	0.000000

Table S27. Atomic coordinates of the optimized structure **27-3T.**

27-3T	B3LYP			BP86		
	X	Y	Z	X	Y	Z
Mn	0.772576	0.953037	0.000000	0.488887	-1.094298	0.000000
Mn	-0.793630	-1.087376	0.000000	-0.677397	1.147244	0.000000
C	0.706185	0.886520	1.859014	0.464330	-1.023434	1.846688
C	-0.809412	-2.094055	1.656370	-1.463640	1.647629	1.629814
C	-2.628764	-1.129991	0.000000	0.101286	2.772892	0.000000
C	0.706185	0.886520	-1.859014	0.464330	-1.023434	-1.846688
C	0.454053	2.760065	0.000000	2.244311	-1.559466	0.000000
C	2.602987	1.104807	0.000000	-0.109096	-2.809995	0.000000
C	-0.809412	-2.094055	-1.656370	-1.463640	1.647629	-1.629814
O	0.664469	0.849103	3.011340	0.464330	-1.001414	3.014059
O	-0.809412	-2.728280	2.616815	-2.005866	2.013044	2.598967
O	-3.788417	-1.108276	0.000000	0.654722	3.809747	0.000000
O	0.216781	3.891681	0.000000	3.383431	-1.831456	0.000000
O	0.664469	0.849103	-3.011340	0.464330	-1.001414	-3.014059
O	3.757720	1.164379	0.000000	-0.522001	-3.905805	0.000000
O	-0.809412	-2.728280	-2.616815	-2.005866	2.013044	-2.598967
H	0.919874	-0.742534	0.000000	-1.115612	-0.547997	0.000000
H	-0.894038	0.666730	0.000000	0.936418	0.547475	0.000000

Table S28. Atomic coordinates of the optimized structure **27-4T.**

27-4T	B3LYP			BP86		
	X	Y	Z	X	Y	Z
Mn	0.000000	0.000000	-1.178676	0.000000	0.000000	-1.152073
Mn	0.000000	0.000000	1.583440	0.000000	0.000000	1.576244
C	0.000000	1.861423	-1.258157	0.000000	1.844613	-1.256838
C	0.000000	1.877080	1.624549	0.000000	1.852062	1.625628
C	0.000000	-1.877080	1.624549	0.000000	-1.852062	1.625628
C	0.000000	-1.861423	-1.258157	0.000000	-1.844613	-1.256838
C	-1.383679	0.000000	-2.373071	-1.359356	0.000000	-2.346979
C	1.383679	0.000000	-2.373071	1.359356	0.000000	-2.346979
C	0.000000	0.000000	3.506825	0.000000	0.000000	3.456978
O	0.000000	3.005098	-1.414468	0.000000	2.997184	-1.450942
O	0.000000	3.026645	1.728043	0.000000	3.016173	1.743566
O	-2.283836	0.000000	-3.101066	-2.256719	0.000000	-3.101429
O	0.000000	-3.005098	-1.414468	0.000000	-2.997184	-1.450942

O	0.000000	-3.026645	1.728043	0.000000	-3.016173	1.743566
O	2.283836	0.000000	-3.101066	2.256719	0.000000	-3.101429
O	0.000000	0.000000	4.657954	0.000000	0.000000	4.624524
H	1.086802	0.000000	0.128167	1.080365	0.000000	0.168396
H	-1.086802	0.000000	0.128167	-1.080365	0.000000	0.168396

Table S29. Atomic coordinates of the optimized structure **26-1.**

26-1	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	-0.156488	1.232809	0.000000	0.233525	1.055292	0.000000
Mn	0.157571	-1.233212	0.000000	0.190138	-1.319163	0.000000
C	1.580811	1.670134	0.000000	1.883021	1.684983	0.000000
C	0.522792	-2.424768	1.353315	-0.067142	-2.514785	1.350048
C	-1.580323	-1.668153	0.000000	-1.526259	-0.916922	0.000000
C	-0.523412	2.423878	1.353242	-0.250814	2.200327	1.314417
C	-0.523412	2.423878	-1.353242	-0.250814	2.200327	-1.314417
C	0.522792	-2.424768	-1.353315	-0.067142	-2.514785	-1.350048
O	2.713335	1.920852	0.000000	2.992234	2.073999	0.000000
O	0.742693	-3.146634	2.229437	-0.250814	-3.245199	2.247236
O	-0.744384	3.145488	2.229312	-0.548179	2.923322	2.189325
O	-2.713172	-1.917422	0.000000	-2.679566	-0.671491	0.000000
O	-0.744384	3.145488	-2.229312	-0.548179	2.923322	-2.189325
O	0.742693	-3.146634	-2.229437	-0.250814	-3.245199	-2.247236
H	0.001592	-0.000116	-1.166595	0.682938	-0.154068	-1.133745
H	0.001592	-0.000116	1.166595	0.682938	-0.154068	1.133745

Table S30. Atomic coordinates of the optimized structure **26-2.**

26-2	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	0.121982	1.236757	0.000000	0.081716	1.210557	0.000000
Mn	-0.121982	-1.236757	0.000000	-0.081716	-1.210557	0.000000
C	1.913071	1.276074	0.000000	1.842074	1.245746	0.000000
C	-0.028444	-2.479380	1.353447	-0.013519	-2.452631	1.323358
C	-1.913071	-1.276074	0.000000	-1.842074	-1.245746	0.000000
C	0.028444	2.479380	1.353447	0.013519	2.452631	1.323358
C	0.028444	2.479380	-1.353447	0.013519	2.452631	-1.323358
C	-0.028444	-2.479380	-1.353447	-0.013519	-2.452631	-1.323358
O	3.072988	1.268397	0.000000	3.018880	1.254096	0.000000
O	0.028444	-3.231647	2.229740	0.013519	-3.230156	2.200425
O	-0.028444	3.231647	2.229740	-0.013519	3.230156	2.200425
O	-3.072988	-1.268397	0.000000	-3.018880	-1.254096	0.000000
O	-0.028444	3.231647	-2.229740	-0.013519	3.230156	-2.200425
O	0.028444	-3.231647	-2.229740	0.013519	-3.230156	-2.200425
H	0.000000	0.000000	-1.167137	0.000000	0.000000	-1.192664
H	0.000000	0.000000	1.167137	0.000000	0.000000	1.192664

Table S31. Atomic coordinates of the optimized structure **26-3.**

26-3	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	0.000000	1.284513	-0.362464	0.000000	1.261002	-0.389869
Mn	0.000000	-1.284513	-0.362464	0.000000	-1.261002	-0.389869
H	1.142415	0.000000	-0.404780	1.154850	0.000000	-0.501505
H	-1.142415	0.000000	-0.404780	-1.154850	0.000000	-0.501505
C	-1.346729	2.505121	-0.604577	-1.317139	2.486429	-0.574345
C	0.000000	1.571436	1.408723	0.000000	1.524743	1.351542
C	1.346729	2.505121	-0.604577	1.317139	2.486429	-0.574345
C	-1.346729	-2.505121	-0.604577	-1.317139	-2.486429	-0.574345
C	0.000000	-1.571436	1.408723	0.000000	-1.524743	1.351542
C	1.346729	-2.505121	-0.604577	1.317139	-2.486429	-0.574345
O	0.000000	1.745791	2.553664	0.000000	1.721669	2.510163
O	2.218804	3.249540	-0.760021	2.189424	3.262515	-0.690636
O	-2.218804	3.249540	-0.760021	-2.189424	3.262515	-0.690636
O	0.000000	-1.745791	2.553664	0.000000	-1.721669	2.510163
O	-2.218804	-3.249540	-0.760021	-2.189424	-3.262515	-0.690636
O	2.218804	-3.249540	-0.760021	2.189424	-3.262515	-0.690636

Table S32. Atomic coordinates of the optimized structure **26-4.**

26-4	B3LYP			BP86		
_	X	Y	Z	X	Y	Z
Mn	-1.354000	-0.027207	-0.479698	-1.332581	-0.013717	-0.467937
Mn	0.948590	0.082707	0.019967	0.904944	0.157816	0.017739
H	-0.029886	0.641061	-1.317119	-0.079145	0.831099	-1.262089
H	-0.568276	0.292731	0.903957	-0.648238	0.388379	0.910514
C	-2.727520	-0.663535	0.557798	-2.570652	-0.813689	0.577869
C	-2.024354	1.725356	-0.406397	-2.283808	1.572325	-0.416156
C	-0.694306	-1.763436	-0.670674	-0.466155	-1.657815	-0.687065
C	1.731350	-0.693479	1.474606	1.689583	-0.633858	1.431190
C	1.696608	1.675824	0.388777	1.715829	1.694270	0.399459
C	2.320392	-0.359383	-1.094044	2.263685	-0.285609	-1.062352
O	-2.394504	2.812778	-0.332591	-2.863256	2.582903	-0.349943
O	-0.440401	-2.879735	-0.845207	-0.182597	-2.772180	-0.927936
O	-3.539269	-1.053335	1.285164	-3.313682	-1.316476	1.335369
O	2.128078	2.727186	0.617223	2.214913	2.729222	0.646110
O	2.196536	-1.192991	2.410060	2.179994	-1.152836	2.363570
O	3.164607	-0.645074	-1.833894	3.130556	-0.580094	-1.798561

Table S33. Atomic coordinates of the optimized structure **26-5T.**

26-5T	B3LYP			BP86		
	X	Y	Z	X	Y	Z
Mn	0.000012	1.004542	0.000000	0.520611	-0.821667	0.000000
Mn	0.000076	-1.516550	0.000000	-0.426635	1.363952	0.000000
C	1.855027	0.882060	0.000000	-1.341468	-0.773767	0.000000
C	0.000054	-2.674590	1.467396	-0.995360	2.377363	1.426398
C	-1.854976	0.881669	0.000000	2.360440	-0.725916	0.000000
C	-0.000122	2.249176	1.353495	0.535231	-2.041229	1.348808
C	-0.000122	2.249176	-1.353495	0.535231	-2.041229	-1.348808
C	0.000054	-2.674590	-1.467396	-0.995360	2.377363	-1.426398
O	3.005688	0.794843	0.000000	-2.510525	-0.900256	0.000000
O	0.000043	-3.313772	2.432112	-1.302374	2.976887	2.386714
O	-0.000204	3.003984	2.228809	0.535231	-2.797098	2.242826
O	-3.005621	0.794232	0.000000	3.525181	-0.653646	0.000000
O	-0.000204	3.003984	-2.228809	0.535231	-2.797098	-2.242826
O	0.000043	-3.313772	-2.432112	-1.302374	2.976887	-2.386714
H	0.000179	-0.216593	-1.171274	0.607689	0.480980	-1.089859
H	0.000179	-0.216593	1.171274	0.607689	0.480980	1.089859

Table S34. Atomic coordinates of the optimized structure **26-6T.**

26-6T	B3LYP			BP86		
	X	Y	Z	X	Y	Z
Mn	0.672077	1.219344	0.000000	0.673850	1.159899	0.000000
Mn	-0.520798	-0.924743	0.000000	-0.664149	-0.742499	0.000000
H	-0.292238	0.319496	1.146028	-0.493769	0.559966	1.105411
H	-0.292238	0.319496	-1.146028	-0.493769	0.559966	-1.105411
C	2.075733	2.559543	0.000000	2.379301	1.999067	0.000000
C	-0.726507	2.474723	0.000000	-0.242884	2.761533	0.000000
C	1.984650	-0.111852	0.000000	1.645350	-0.463171	0.000000
C	-0.533659	-2.156703	-1.349575	-0.675480	-1.969816	-1.325090
C	-2.309962	-0.813108	0.000000	-2.441808	-0.704657	0.000000
C	-0.533659	-2.156703	1.349575	-0.675480	-1.969816	1.325090
O	-1.616876	3.205594	0.000000	-0.867540	3.748517	0.000000
O	2.859264	-0.871668	0.000000	2.493159	-1.277460	0.000000
O	2.920860	3.339455	0.000000	3.441383	2.480465	0.000000
O	-3.463066	-0.685672	0.000000	-3.614665	-0.630194	0.000000
O	-0.533659	-2.917568	-2.223155	-0.675480	-2.752776	-2.199585
O	-0.533659	-2.917568	2.223155	-0.675480	-2.752776	2.199585

Table S35. Atomic coordinates of the optimized structure **26-7T.**

26-7T	B3LYP			BP86		
	X	Y	Z	X	Y	Z
Mn	0.000000	1.173779	-0.392860	0.000000	1.175486	-0.410387
Mn	0.000000	-1.173779	-0.392860	0.000000	-1.175486	-0.410387
H	1.138627	0.000000	-0.847896	1.132518	0.000000	-0.891749
H	-1.138627	0.000000	-0.847896	-1.132518	0.000000	-0.891749
C	-1.427172	2.351840	-0.583703	-1.397856	2.346831	-0.565217
C	0.000000	1.413183	1.428527	0.000000	1.419465	1.384035
C	1.427172	2.351840	-0.583703	1.397856	2.346831	-0.565217
C	-1.427172	-2.351840	-0.583703	-1.397856	-2.346831	-0.565217
C	0.000000	-1.413183	1.428527	0.000000	-1.419465	1.384035
C	1.427172	-2.351840	-0.583703	1.397856	-2.346831	-0.565217
O	0.000000	1.649828	2.562051	0.000000	1.665347	2.530976
O	2.356872	3.024099	-0.712108	2.332658	3.045479	-0.663624
O	-2.356872	3.024099	-0.712108	-2.332658	3.045479	-0.663624
O	0.000000	-1.649828	2.562051	0.000000	-1.665347	2.530976
O	-2.356872	-3.024099	-0.712108	-2.332658	-3.045479	-0.663624
O	2.356872	-3.024099	-0.712108	2.332658	-3.045479	-0.663624

Complete Gaussian 03 reference (Reference 40)

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