ELECTRONIC SUPPLEMENTARY INFORMATION

Metal-metal bond distances and bond orders in dimanganese complexes with bidentate ligands: scope for some very short Mn-Mn bonds

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New J. Chem.

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1. Electron Counting (EC) Diagrams for $(Mn_2)^{+n}$ Core of Dimanganese Complexes

Black arrows indicate electrons originating from the metal centers (ME)

Red arrows indicate electrons originating from the ligands (LE)

The symbol ‖ denotes a metal-metal bond

The box │↑↓│ denotes a dative ligand-metal L→M bond

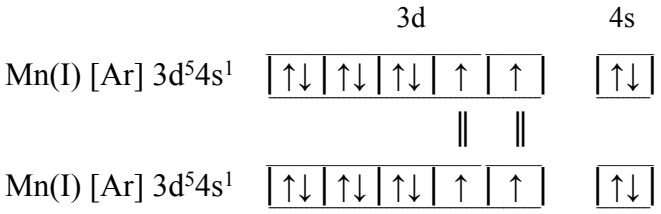
The box │↑↓│ denotes a lone pair

The numbers in parentheses denote the electron populations of the 3d subshells in the core, which ideally is (10,10) but may take on other values in some cases. If the population is (10,10), it is not mentioned explicitly, but the other cases are mentioned.

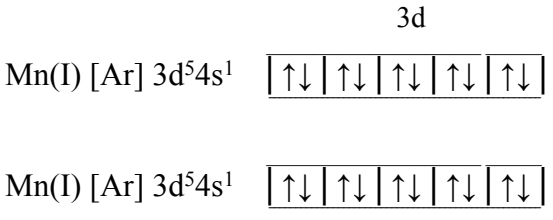
Ligand electrons per metal center number 4, 6 and 8 for *bis*, *tris* and *tetrakis* respectively, with 2 more added per metal center for the water ligated cases (*dihydrates*). 6

(A) Models for Experimentally Known Complexes

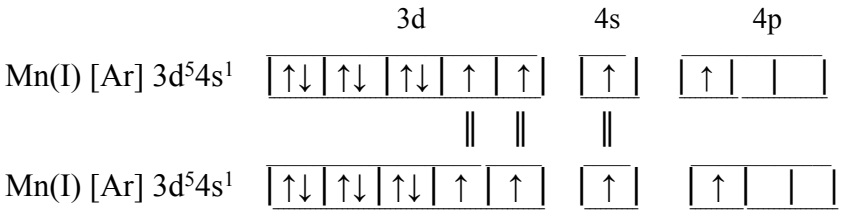
EC M1Aa-1 Dimanganese bis(diimidosilane) dianion A *singlet*: fBO = 2



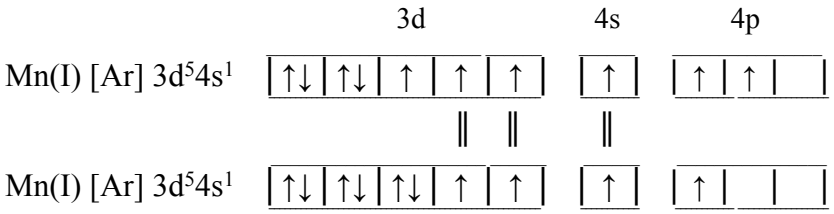
EC M1Aa-2 Dimanganese bis(diimidosilane) dianion A *singlet*: fBO = 0



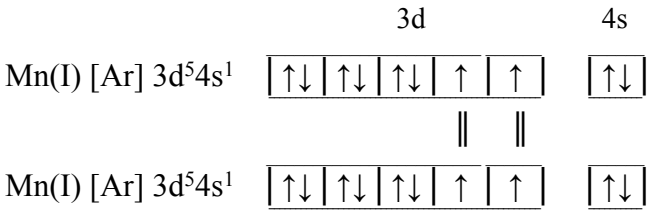
EC M1Ab Dimanganese bis(diimidosilane) dianion A *triplet*: fBO = 3



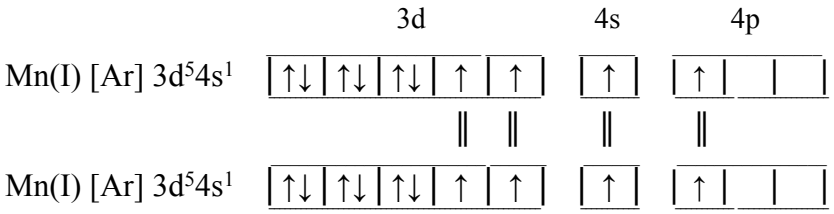
M1Ac Dimanganese bis(diimidosilane) dianion A *quintet*: fBO = 3



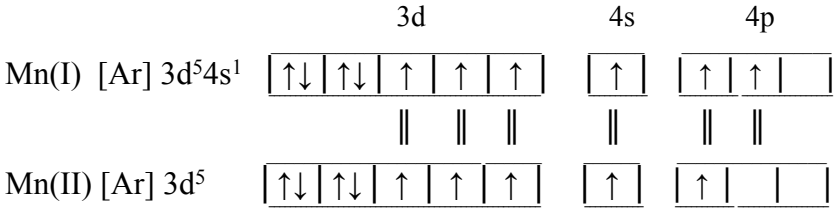
M1Ba-1 Dimanganese bis(diimidosilane) dianion B *singlet*: fBO = 2



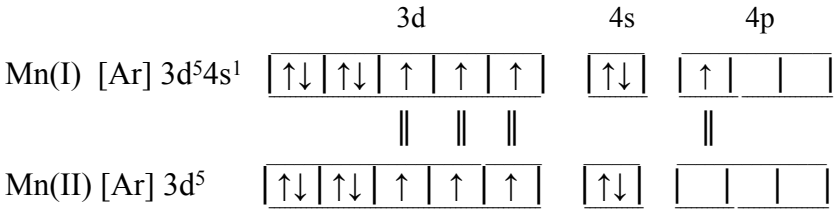
M1Ba-2 Dimanganese bis(diimidosilane) dianion B *singlet*: fBO = 4



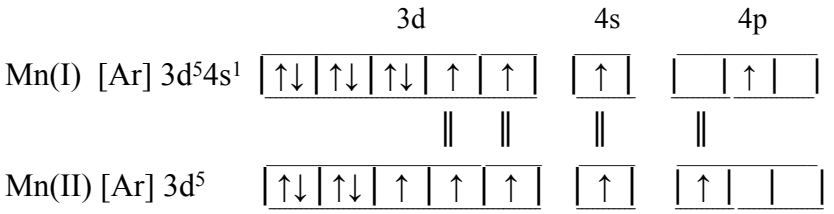
M2Aa-1 Dimanganese bis(diimidosilane) monanion A *doublet*: fBO = 5.5



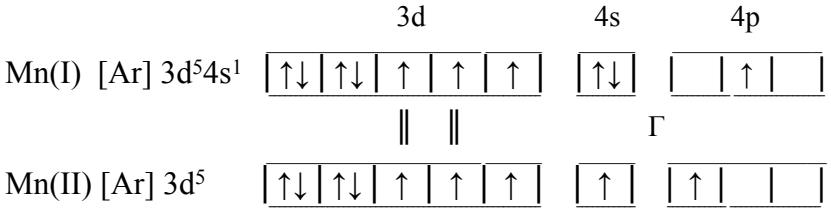
M2Aa-2 Dimanganese bis(diimidosilane) monanion A *doublet*: fBO = 3.5



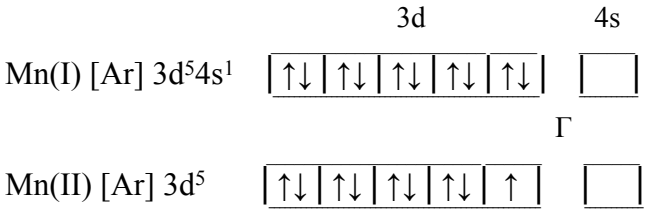
M2Ab Dimanganese bis(diimidosilane) monanion A *quartet*: fBO = 3.5



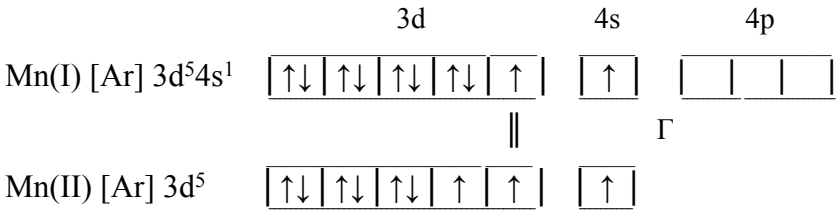
M2Ac Dimanganese bis(diimidosilane) monanion A *sextet*: fBO = 2.5; (9,9)



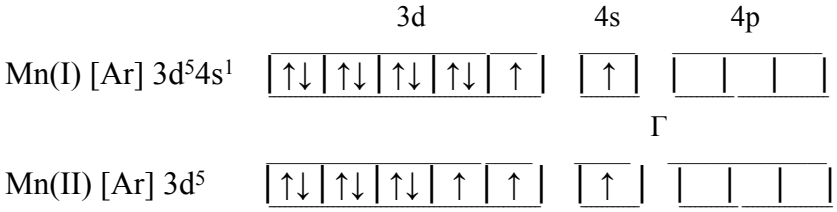
M2Ba Dimanganese bis(diimidosilane) monanion B *doublet*: fBO = 0.5; (10,9)



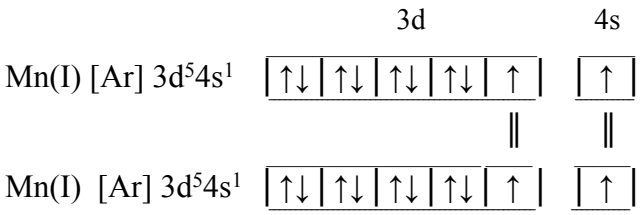
M2Bb Dimanganese bis(diimidosilane) monanion B *quartet*: fBO = 1.5; (10,9)



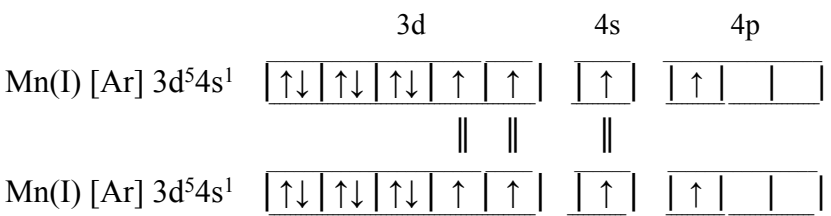
M2Bc Dimanganese bis(diimidosilane) monanion B *sextet*: fBO = 0.5; (9,8)



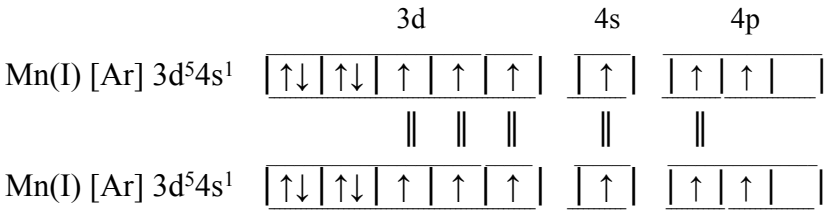
M3Aa Dimanganese bis(β-ketiminate) A *singlet*: fBO = 2



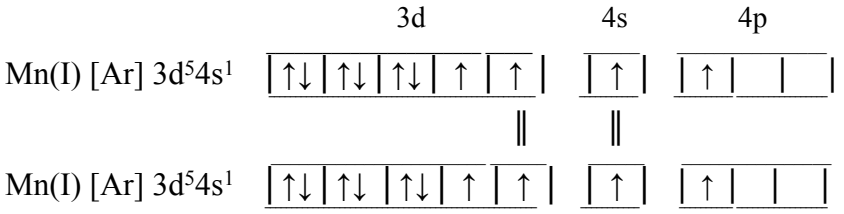
M3Ab-1 Dimanganese bis(β-ketiminate) A *triplet*: fBO = 3



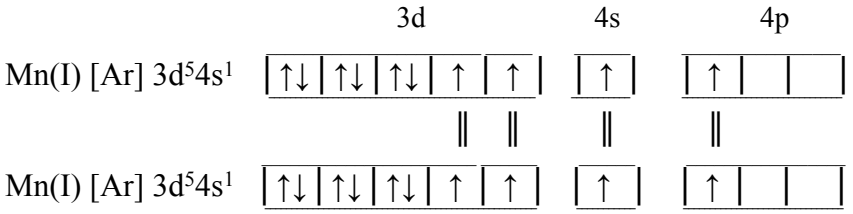
M3Ab-2 Dimanganese bis(β-ketiminate) A *triplet*: fBO = 5



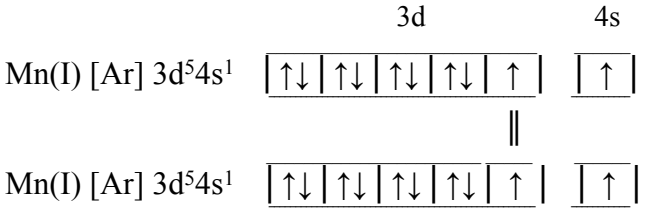
M3Ac Dimanganese bis(β-ketiminate) A *quintet*: fBO = 2; (9,9)



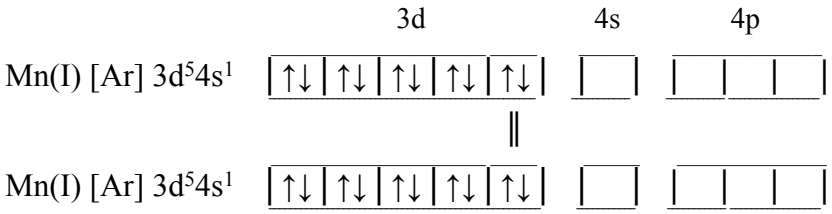
M3Ba Dimanganese bis(β-ketiminate) B *singlet*: fBO = 4



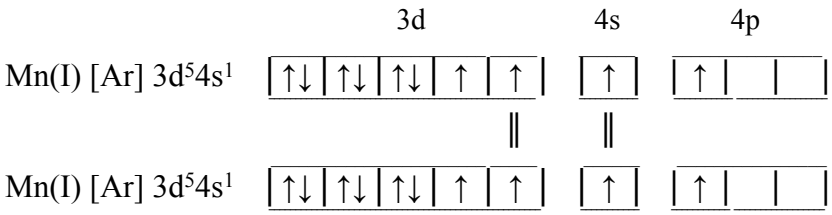
M3Bb Dimanganese bis(β-ketiminate) B *triplet*: fBO = 1



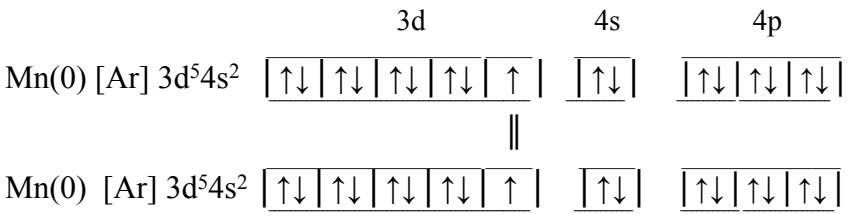
M3Bc-1 Dimanganese bis(β-ketiminate) B *quintet*: fBO = 0



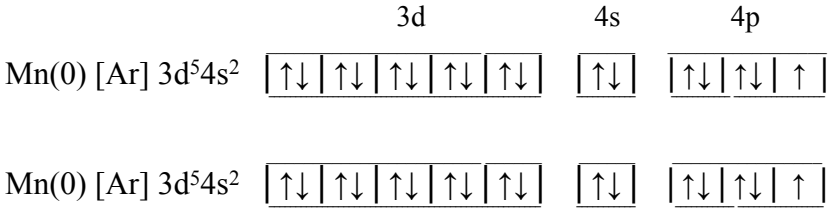
M3Bc-2 Dimanganese bis(β-ketiminate) B *quintet*: fBO = 2



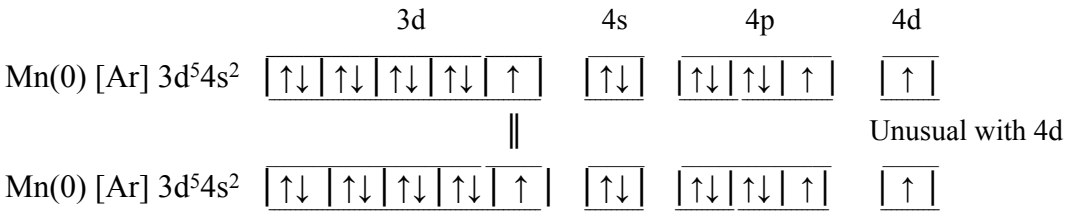
M4a Dimanganese decacarbonyl (LE = 10) *singlet*: fBO = 1



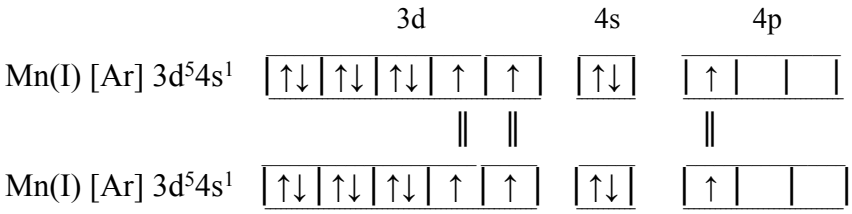
M4b Dimanganese decacarbonyl (LE = 10) *triplet*: fBO = 0



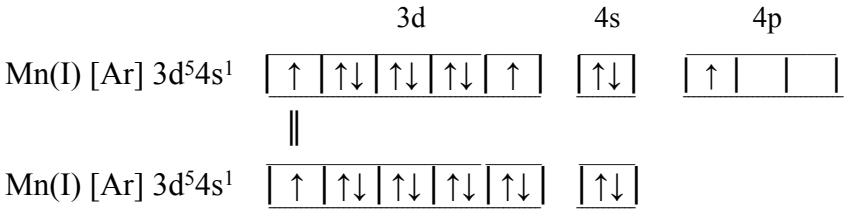
M4c Dimanganese decacarbonyl (LE = 10) *quintet*: fBO = 1



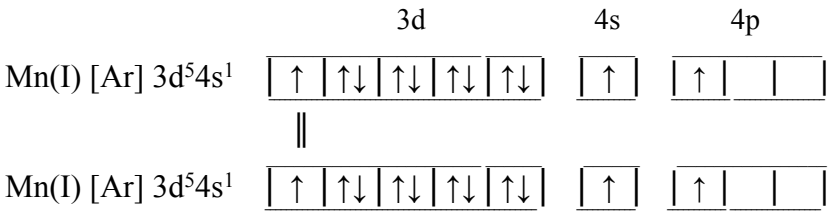
M5a Dimanganese bis(cyclopentadienyl) tricarbonyl (LE = 5) *singlet*: fBO = 3



M5b Dimanganese bis(cyclopentadienyl) tricarbonyl (LE = 5) *triplet*: fBO = 1; (9,9)



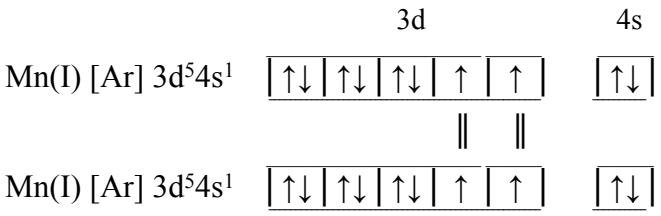
M5c Dimanganese bis(cyclopentadienyl) tricarbonyl (LE = 5) *quintet*: fBO = 1



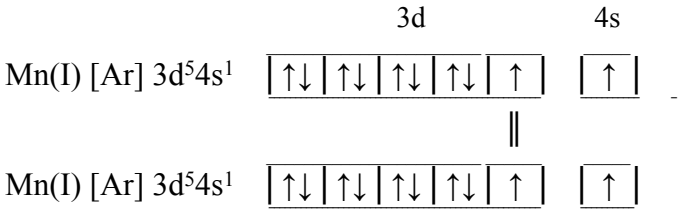
(B) Model Formamidinate Series

Digonal formamidinates: ME = 6 per metal center; LE = 4 to each metal center
LE = 6 to each center for water ligated cases

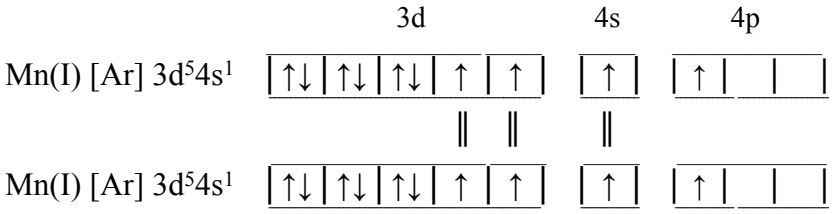
1Aa Dimanganese bis(formamidinate) *singlet*: fBO = 2



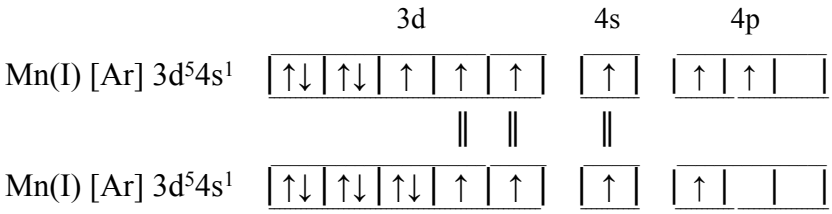
1Ab-1 Dimanganese bis(formamidinate) *triplet*: fBO = 1



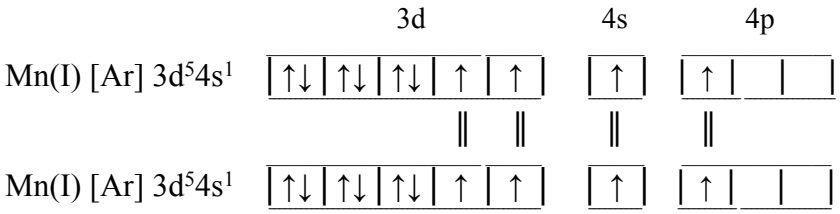
1Ab-2 Dimanganese bis(formamidinate) *triplet*: fBO = 3



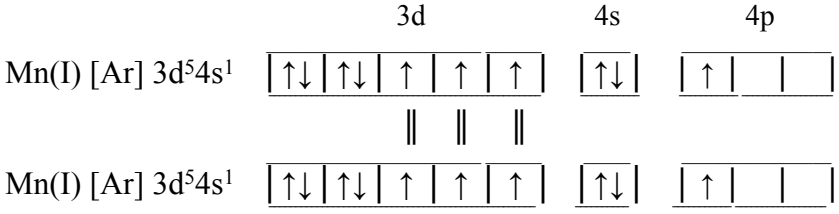
1Ac Dimanganese bis(formamidinate) *quintet*: fBO = 3; (9,10)



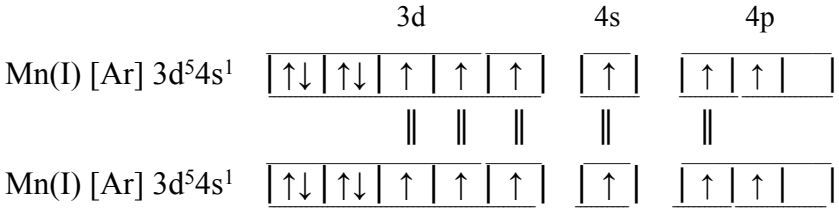
1Ba Dimanganese bis(formamidinate) *singlet*: fBO = 4



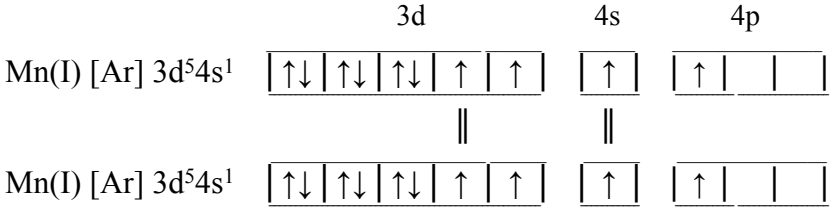
1Bb-1 Dimanganese bis(formamidinate) *triplet*: fBO = 3



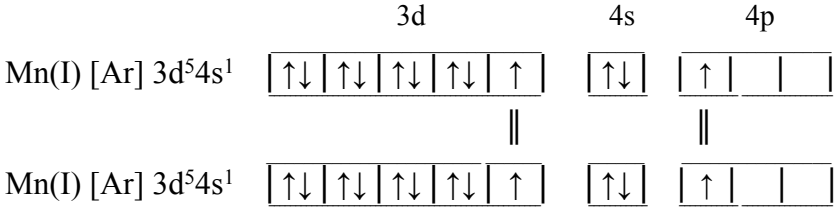
1Bb-2 Dimanganese bis(formamidinate) *triplet*: fBO = 5



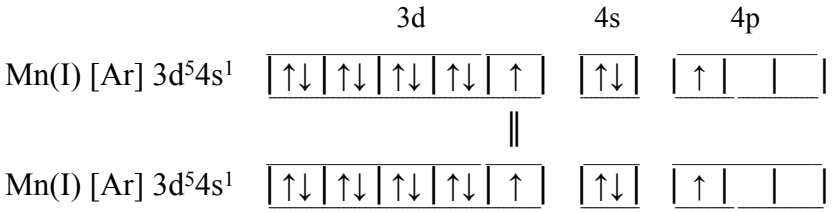
1Bc Dimanganese bis(formamidinate) *quintet*: fBO = 2; (9,9)



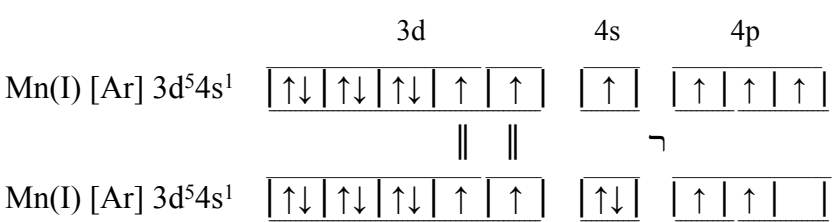
2a Dimanganese bis(formamidinate) dihydrate *singlet*: fBO = 2



2b Dimanganese bis(formamidinate) dihydrate *triplet*: fBO = 1

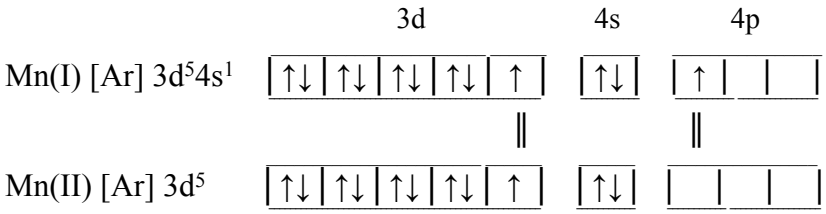


2c Dimanganese bis(formamidinate) dihydrate *quintet*: fBO = 3

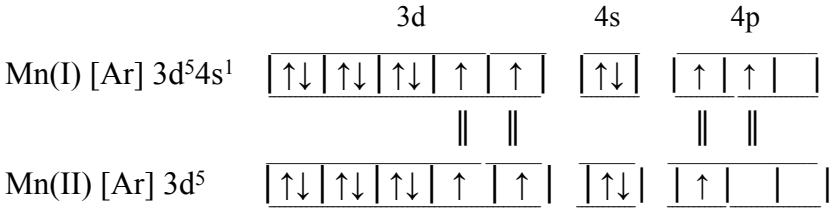


Trigonal formamidinates: ME = 6 for Mn(I), 5 for Mn(II); LE = 6 to each Mn center
LE = 8 to each center for water ligated cases

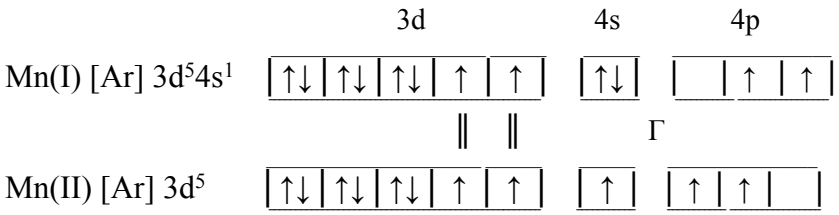
3a-1 Dimanganese tris(formamidinate) *doublet*: fBO = 1.5



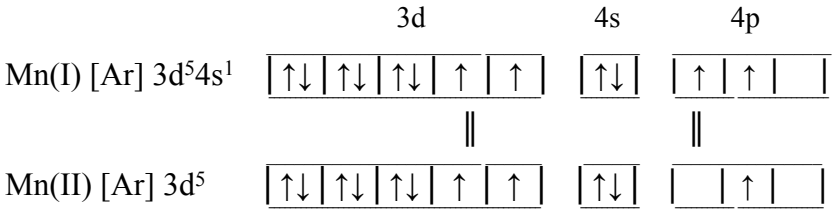
3a-2 Dimanganese tris(formamidinate) *doublet*: fBO = 3.5



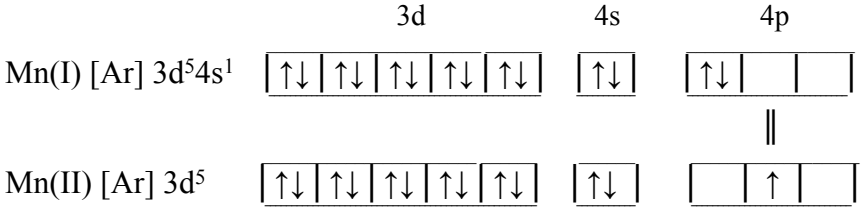
3b Dimanganese tris(formamidinate) *quartet*: fBO = 2.5



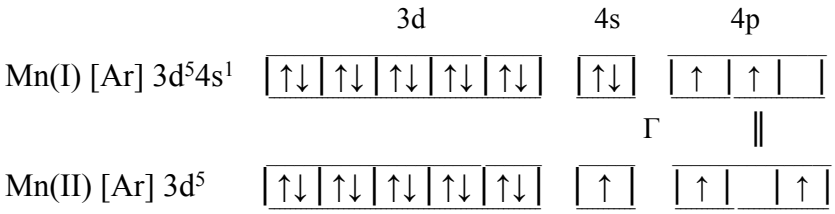
3c Dimanganese tris(formamidinate) *sextet*: fBO = 1.5; (9,9)



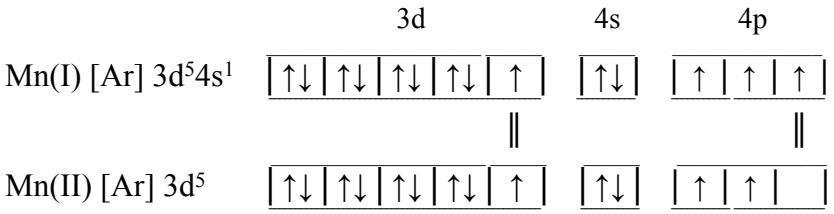
4a Dimanganese tris(formamidinate) dihydrate *doublet*: fBO = 0.5; non-Hund



4b Dimanganese tris(formamidinate) dihydrate *quartet*: fBO = 1.5

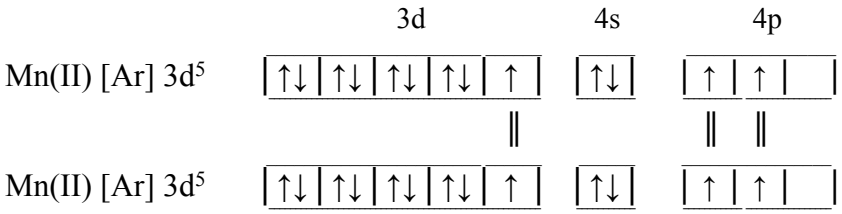


4c Dimanganese tris(formamidinate) dihydrate *sextet*: fBO = 1.5

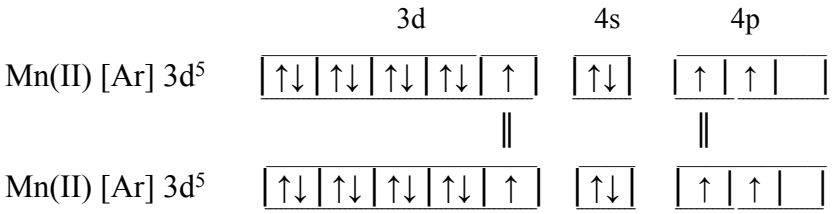


Tetragonal formamidinates: ME = 5 for each Mn center; LE = 8 to each Mn center
LE = 10 to each center for water ligated cases

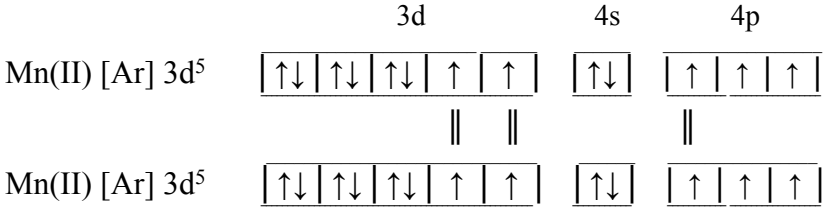
5a Dimanganese tetrakis(formamidinate) *singlet*: fBO = 3



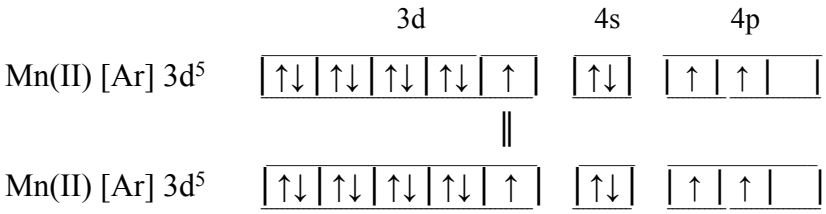
5b Dimanganese tetrakis(formamidinate) *triplet*: fBO = 2



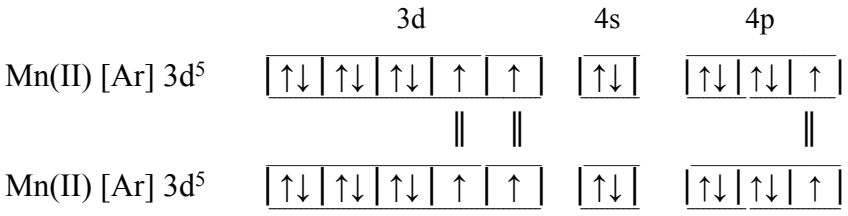
5c-1 Dimanganese tetrakis(formamidinate) *quintet*: fBO = 3



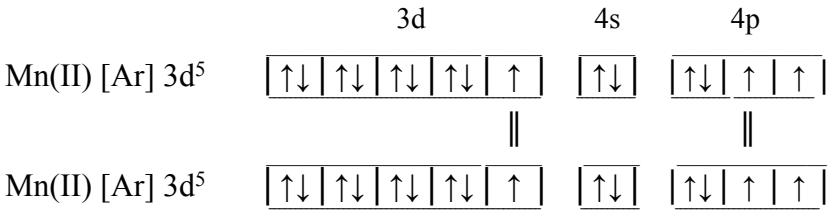
5c-2 Dimanganese tetrakis(formamidinate) *quintet*: fBO = 1



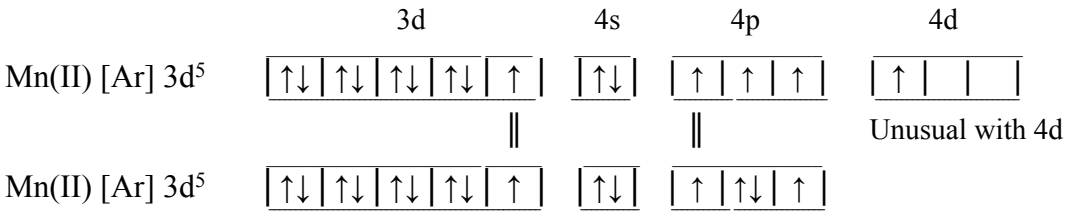
6a Dimanganese tetrakis(formamidinate) dihydrate *singlet*: LE = 10; fBO = 3



6b Dimanganese tetrakis(formamidinate) dihydrate *triplet*: LE = 10; fBO = 2



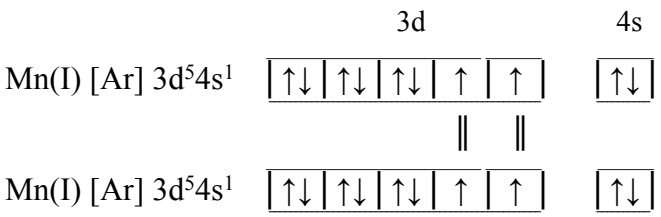
6c Dimanganese tetrakis(formamidinate) dihydrate *quintet*: LE = 10; fBO = 2



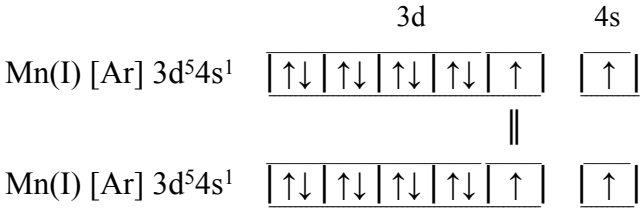
(C) Guanidinate Series

Digonal guanidinates: ME = 6 per metal center; LE = 4 to each metal center
LE = 6 to each center for water ligated cases

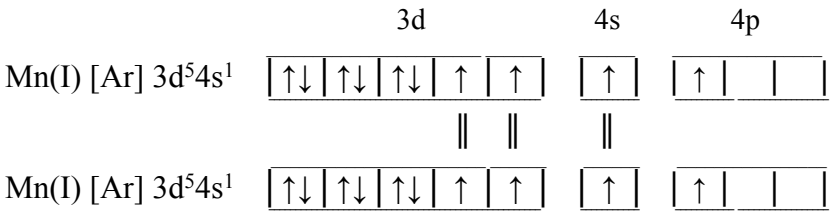
7Aa Dimanganese bis(guanidinate) *singlet*: fBO = 2



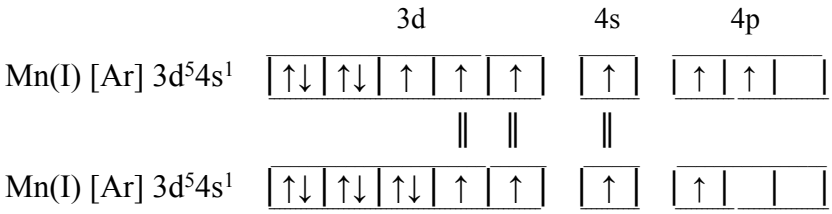
7Ab-1 Dimanganese bis(guanidinate) *triplet*: fBO = 1



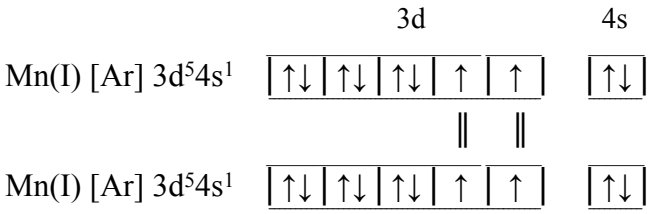
7Ab-2 Dimanganese bis(guanidinate) *triplet*: fBO = 3



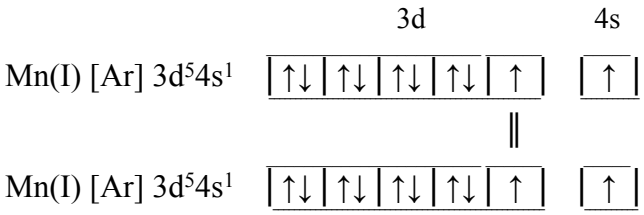
7Ac Dimanganese bis(guanidinate) *quintet*: fBO = 3; (9,10)



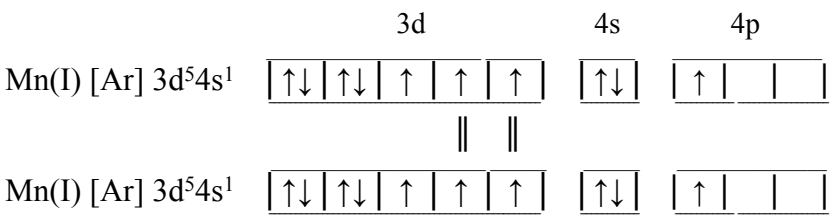
7Ba Dimanganese bis(guanidinate) *singlet*: fBO = 2



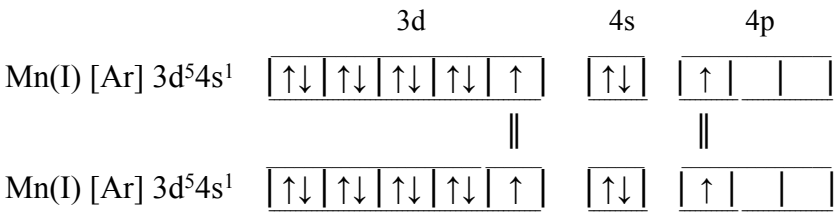
7Bb Dimanganese bis(guanidinate) *triplet*: fBO = 1



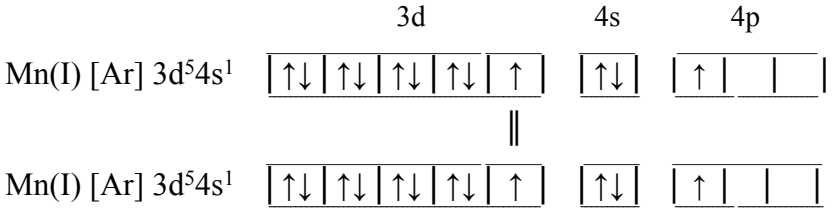
7Bc Dimanganese bis(guanidinate) *quintet*: fBO = 2; (9,9)



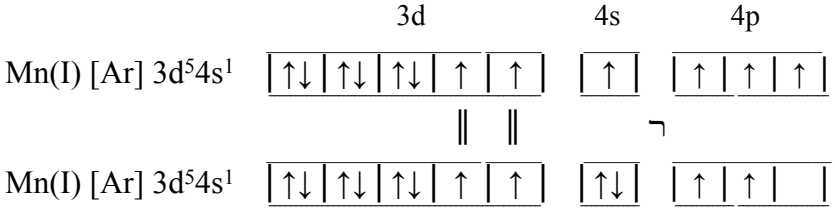
8a Dimanganese bis(guanidinate) dihydrate *singlet*: LE = 6; fBO = 2



8b Dimanganese bis(guanidinate) dihydrate *triplet*: LE = 6; fBO = 1

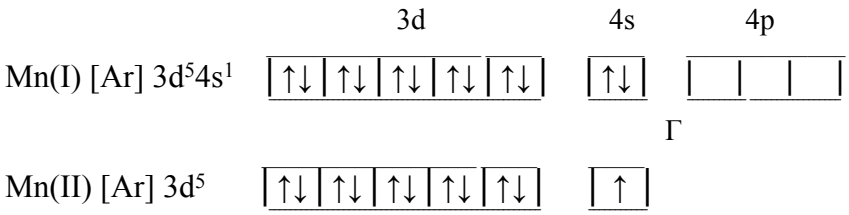


8c Dimanganese bis(guanidinate) dihydrate *quintet*: LE = 6; fBO = 3

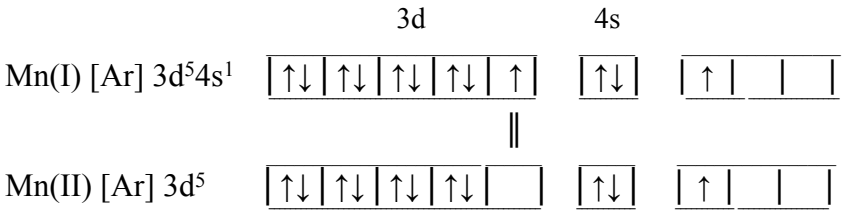


Trigonal guanidinates: ME = 6 for Mn(I), 5 for Mn(II); LE = 6 to each metal center
LE = 8 to each center for water ligated cases

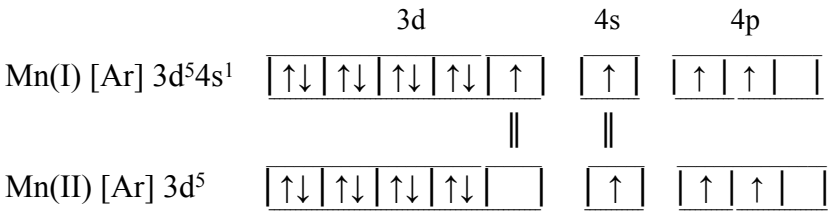
9a Dimanganese tris(guanidinate) *doublet*: fBO = 0.5



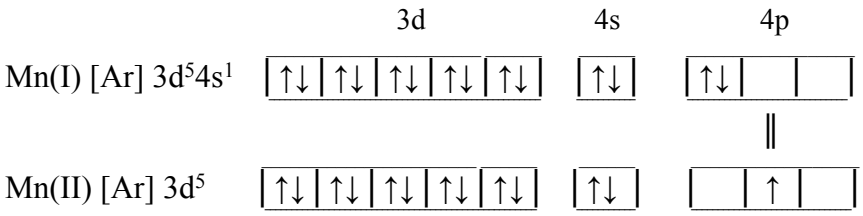
9b Dimanganese tris(guanidinate) *quartet*: fBO = 0.5; (9,9)



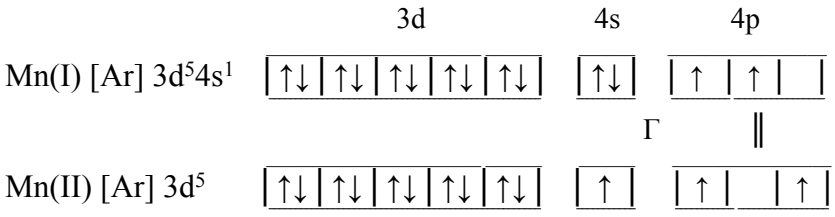
9c Dimanganese tris(guanidinate) *sextet*: fBO = 1.5



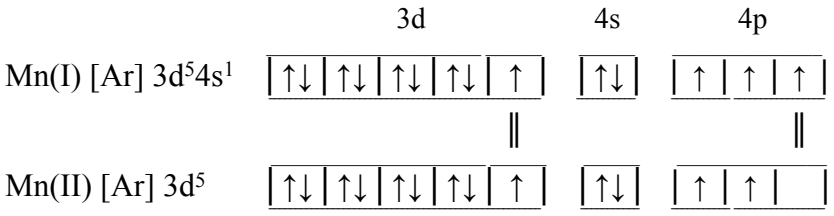
10a Dimanganese tris(guanidinate) dihydrate *doublet*: fBO = 0.5; non-Hund



10b Dimanganese tris(guanidinate) dihydrate *quartet*: fBO = 1.5

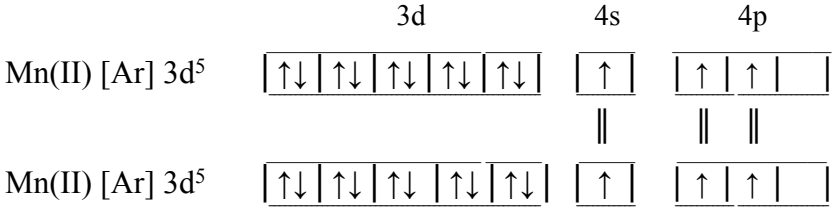


10c Dimanganese tris(guanidinate) dihydrate *sextet*: fBO = 1.5

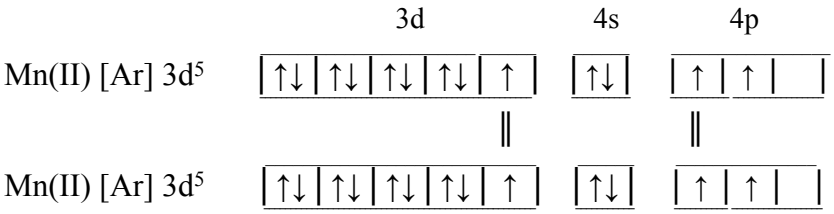


Tetragonal guanidinates: ME = 5 for each Mn(II) center; LE = 8 to each metal center
LE = 10 to each center for water ligated cases

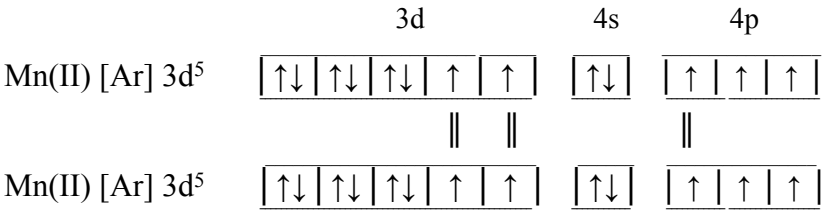
11a Dimanganese tetrakis(guanidinate) *singlet*: fBO = 3



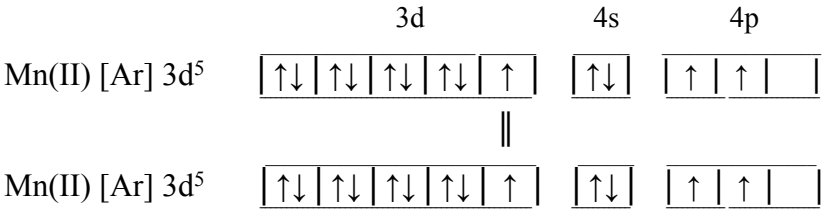
11b Dimanganese tetrakis(guanidinate) *triplet*: fBO = 2



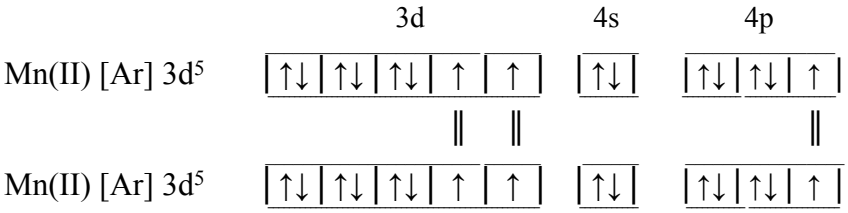
11c-1 Dimanganese tetrakis(guanidinate) *quintet*: fBO = 3



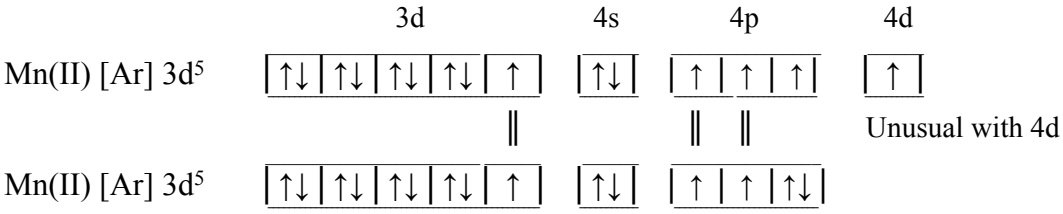
11c-2 Dimanganese tetrakis(guanidinate) *quintet*: fBO = 1



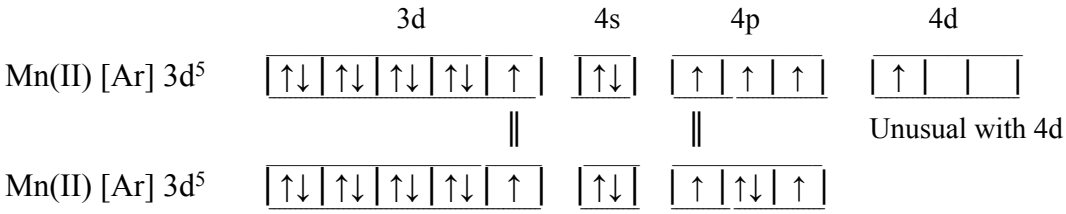
12a Dimanganese tetrakis(guanidinate) dihydrate *singlet*: LE = 10; fBO = 3



12b Dimanganese tetrakis(guanidinate) dihydrate *triplet*: LE = 10; fBO = 3



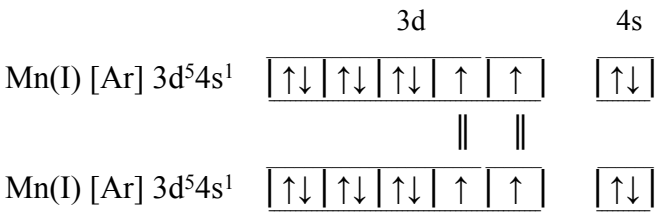
12c Dimanganese tetrakis(guanidinate) dihydrate *quintet*: LE = 10; fBO = 2



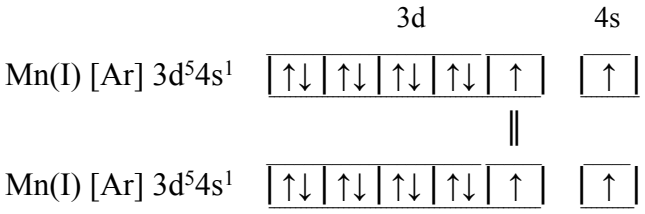
(C) Formate Series

Digonal formates: ME = 6 per metal center; LE = 4 to each metal center
LE = 6 to each center for water ligated cases

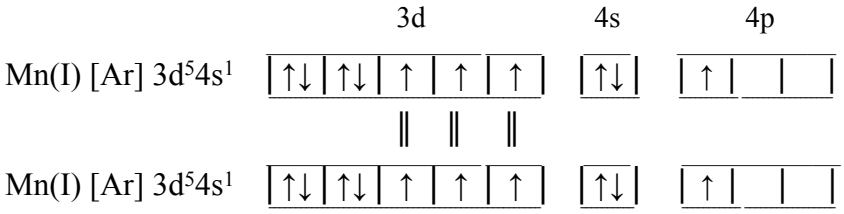
13Aa Dimanganese bridged diformate *singlet*: fBO = 2



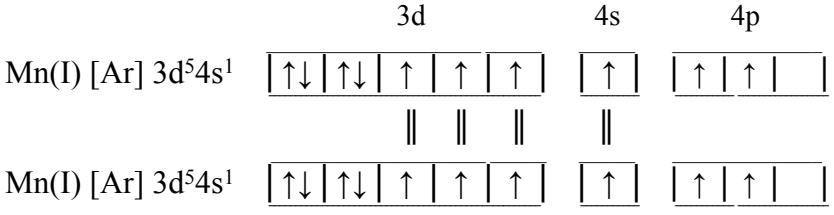
13Ab-1 Dimanganese diformate bridged *triplet*: fBO = 1



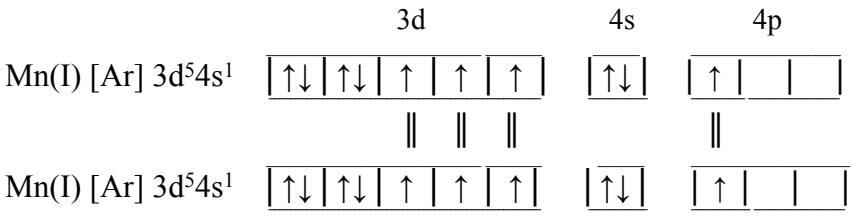
13Ab-2 Dimanganese diformate bridged *triplet*: fBO = 3



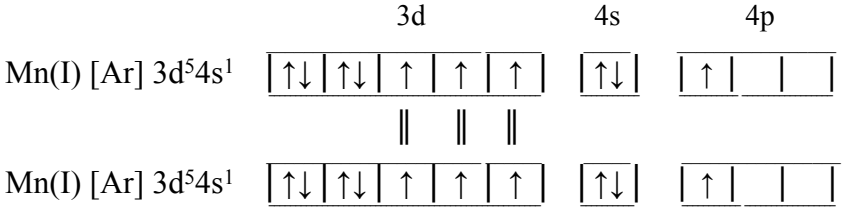
13Ac Dimanganese diformate bridged *quintet*: fBO = 4



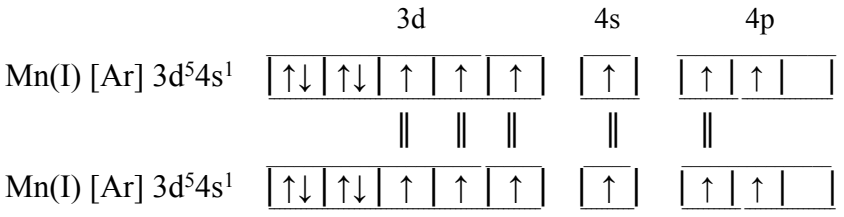
13Ba Dimanganese diformate ipso *singlet*: fBO = 4



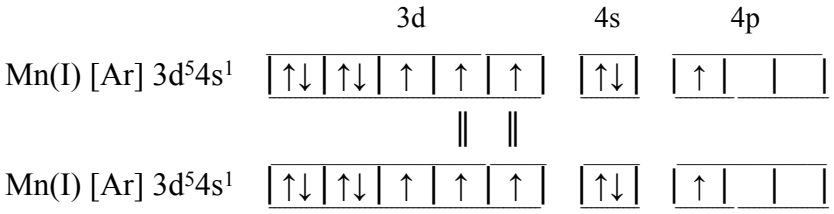
13Bb-1 Dimanganese diformate ipso *triplet*: fBO = 3



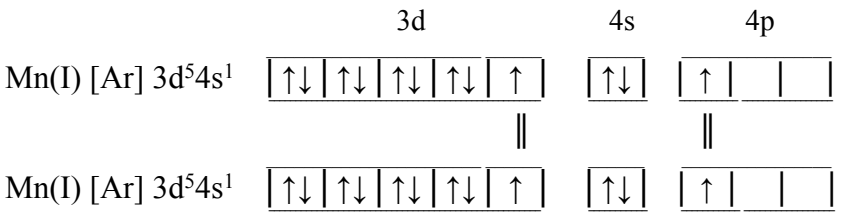
13Bb-2 Dimanganese diformate ipso *triplet*: fBO = 5



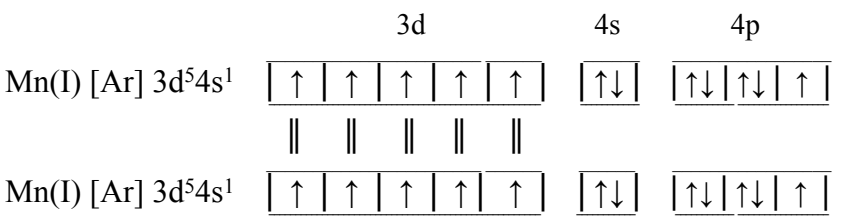
13Bc Dimanganese diformate ipso *quintet*: fBO = 2; (9,9)



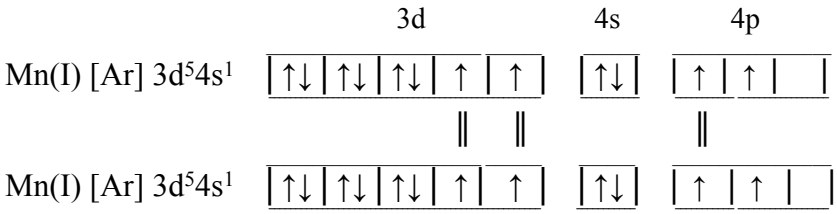
14a Dimanganese diformate dihydrate *singlet*: LE = 6; fBO = 2



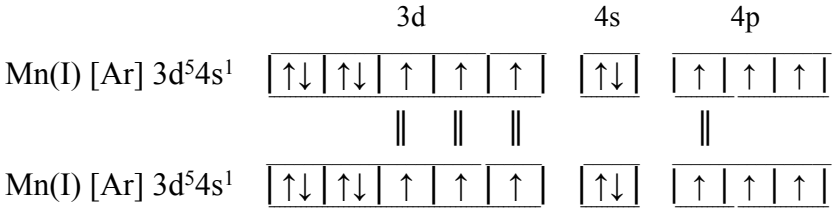
14b-1 Dimanganese diformate dihydrate *triplet*: LE = 6; fBO = 5



14b-2 Dimanganese diformate dihydrate *triplet*: LE = 6; fBO = 3

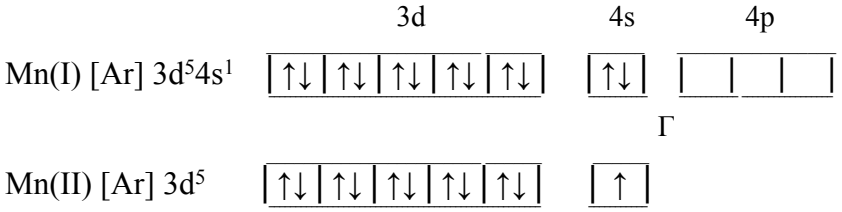


14c Dimanganese diformate dihydrate *quintet*: LE = 6; fBO = 4

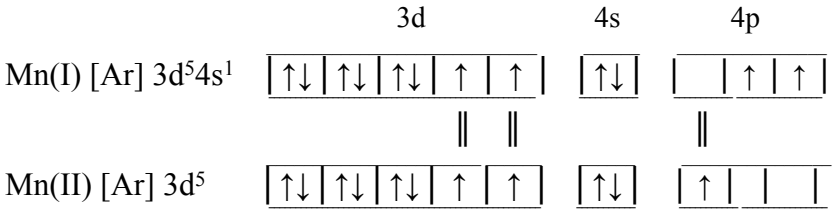


Trigonal formates: ME = 6 for Mn(I), 5 for Mn(II); LE = 6 to each metal center
LE = 8 to each center for water ligated cases

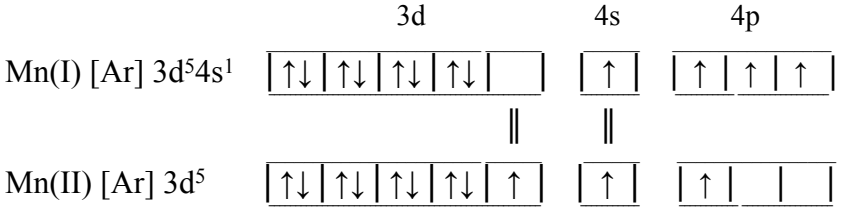
15a Dimanganese triformate *doublet*: fBO = 0.5



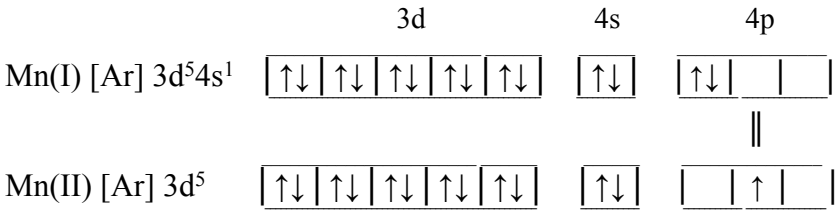
15b Dimanganese triformate *quartet*: fBO = 2.5



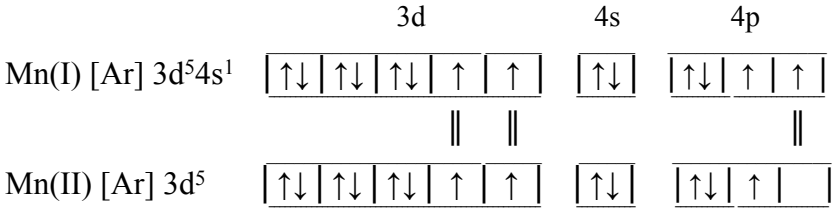
15c Dimanganese triformate *sextet*: fBO = 1.5; (9,9)



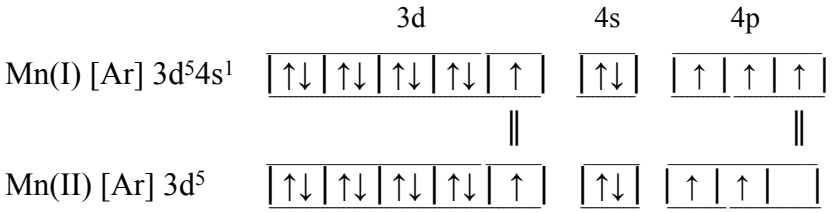
16a Dimanganese triformate dihydrate *doublet*: LE = 8; fBO = 0.5; non-Hund



16b Dimanganese triformate dihydrate *quartet*: LE = 8; fBO = 2.5

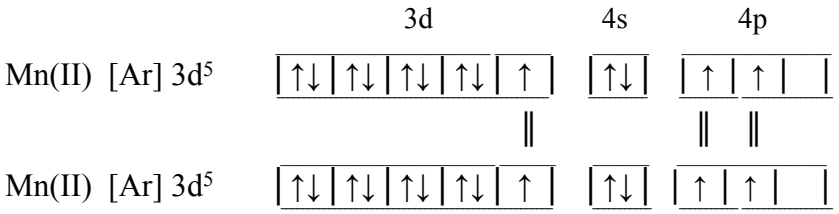


16c Dimanganese tris(formate) dihydrate *sextet*: LE = 8; fBO = 1.5

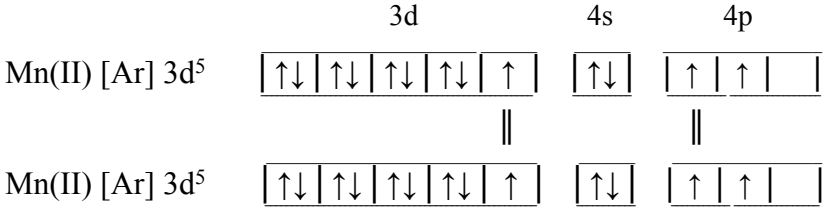


Tetragonal formates: ME = 5 for each Mn(II) center; LE = 8 to each metal center
LE = 10 to each center for water ligated cases

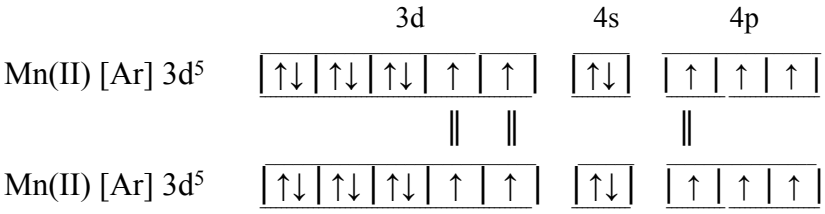
17a Dimanganese tetraformate *singlet*: fBO = 3



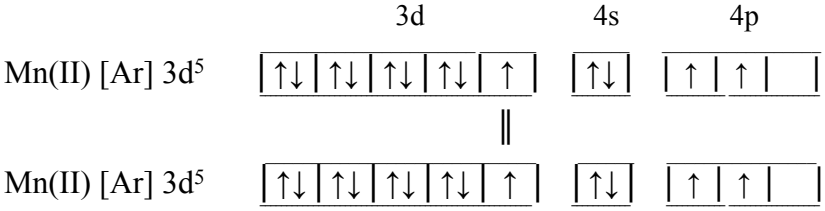
17b Dimanganese tetraformate *triplet*: fBO = 2



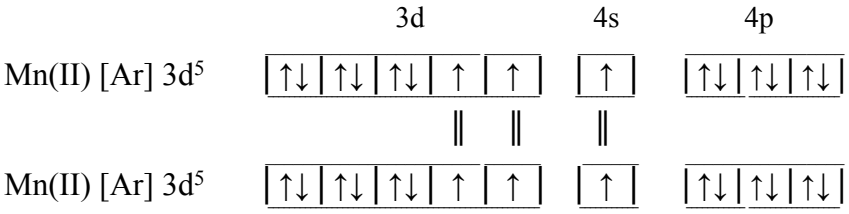
17c-1 Dimanganese tetraformate *quintet*: fBO = 3



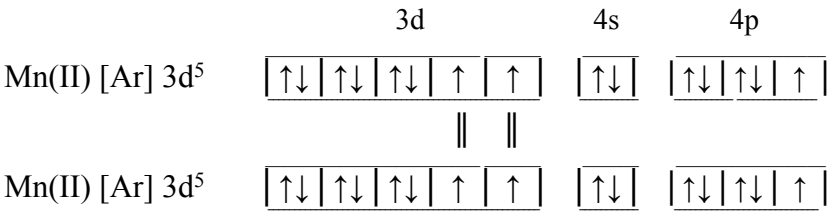
17c-2 Dimanganese tetraformate *quintet*: fBO = 1



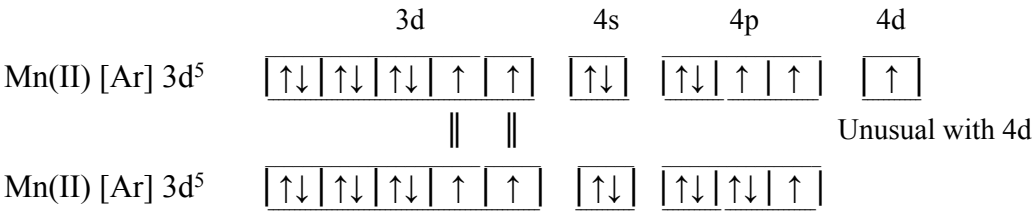
18a Dimanganese tetraformate dihydrate *singlet*: LE = 10; fBO = 3



18b Dimanganese tetraformate dihydrate *triplet*: LE = 10; fBO = 2

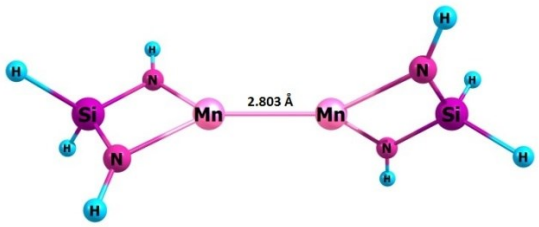


18c Dimanganese tetraformate dihydrate *quintet*: LE = 10; fBO = 2



2. Optimized M06-L Structures for all complexes

Note: M*s* = (2S+1) as spin multiplicity



(a) M1A ($M_S = 1$)

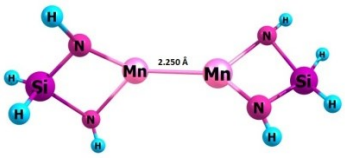
(b) M1A ($M_S = 3$)

(c) M1A ($M_S = 5$)

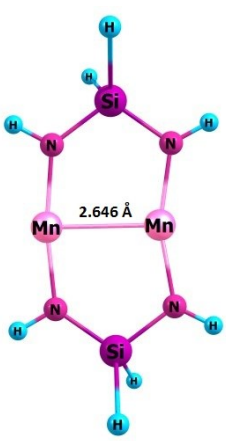
(d) M1B ($M_S = 1$)

(e) M2A ($M_S = 2$)

(f) M2A ($M_S = 2$)

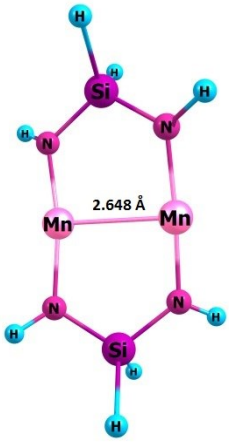


(g) M2A ($M_S = 2$)



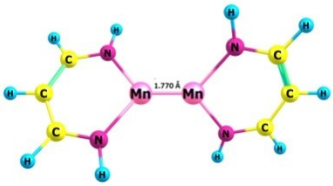
(h) M2B ($M_S = 2$)

(i) M2B ($M_S = 4$)



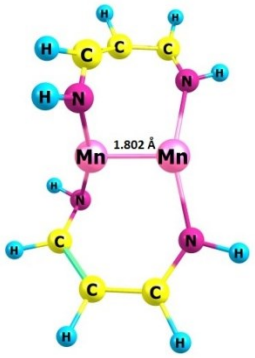
(j) M2B ($M_S = 6$)

(k) M3A ($M_S = 1$)

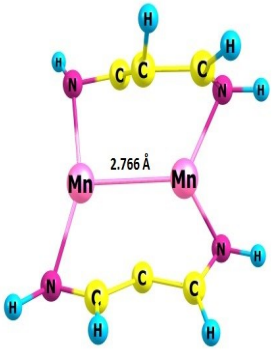


(l) M3A ($M_S = 1$)

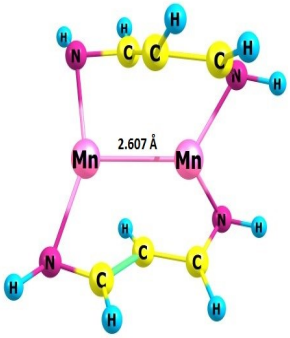
(m) M3A ($M_S = 1$)



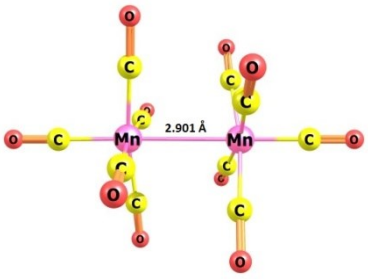
(n) M3B ($M_S = 1$)



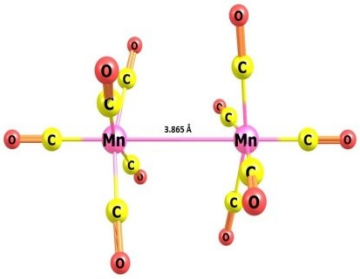
(o) M3B ($M_S = 3$)



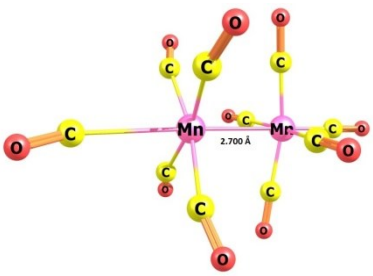
(p) M3B ($M_S = 5$)



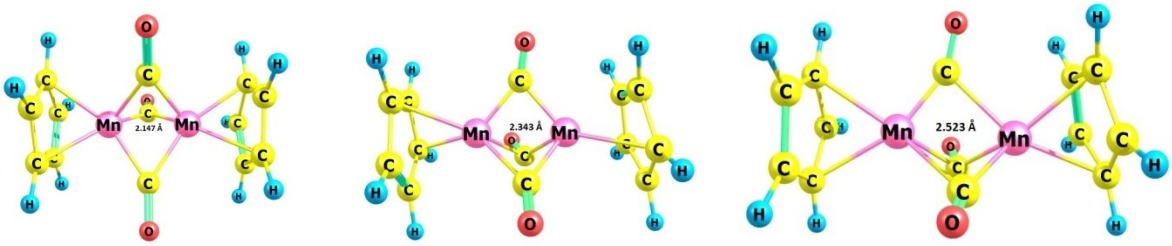
(q) M4 ($M_S = 1$)



(r) M4 ($M_S = 1$)

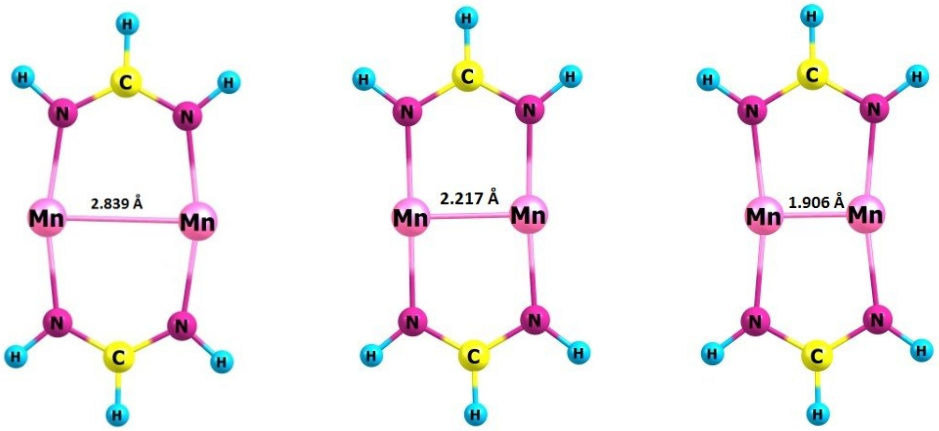


(s) M4 ($M_S = 1$)



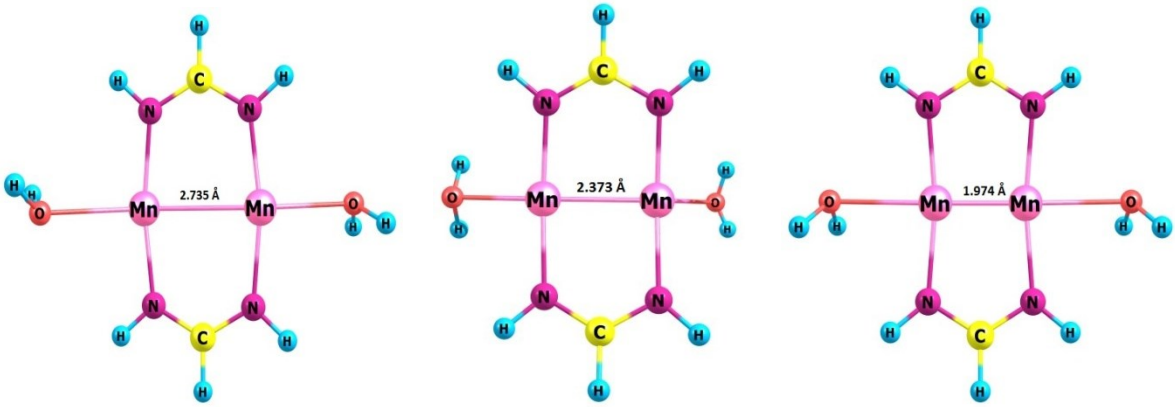
(t) M5 (M_S = 1) **(u) M5** (M_S = 1) **(v) M5** (M_S = 1)

Figure S1 Optimized structures of experimentally known dimanganese complexes [**E1-E5**]

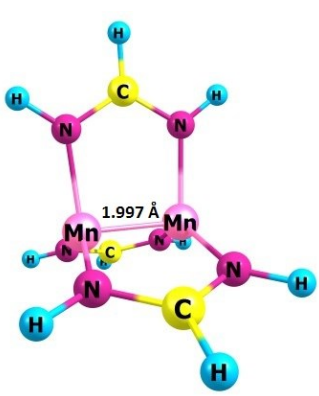


(a) 1A (M_S = 1) **(b) 1A** (M_S = 3) **(c) 1A** (M_S = 5)

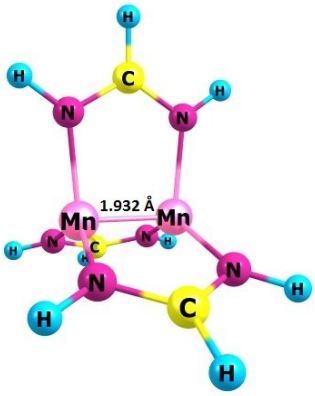
(d) 1B (M_S = 1) **(e) 1B** (M_S = 3) **(f) 1B** (M_S = 5)



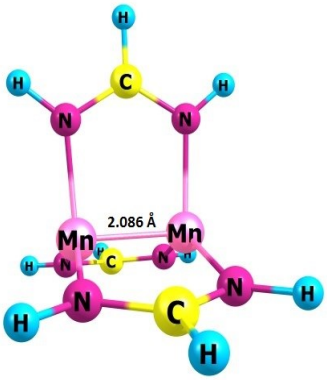
(g) 2 (M_S = 1) **(h) 2** (M_S = 3) **(i) 2** (M_S = 5)



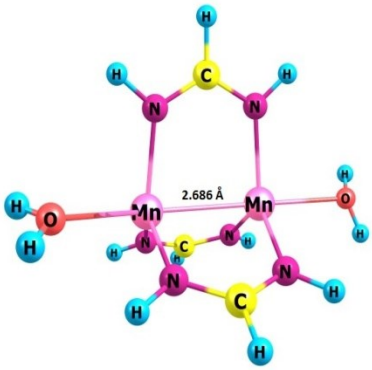
(j) 3 ($M_S = 2$)



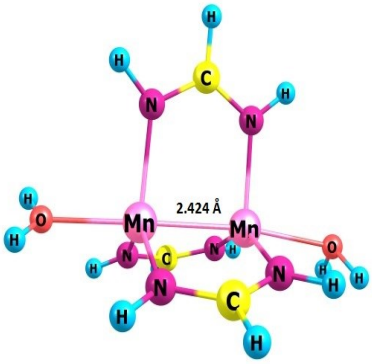
(k) 3 ($M_S = 4$)



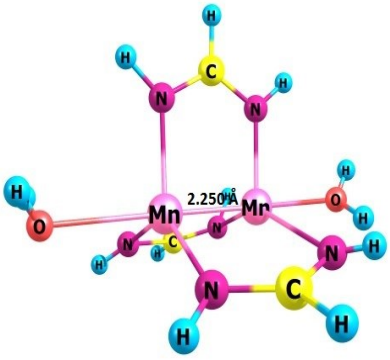
(l) 3 ($M_S = 6$)



(m) 4 ($M_S = 2$)



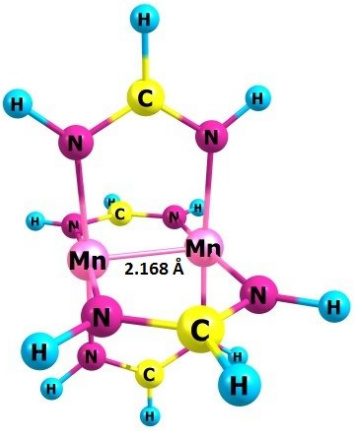
(n) 4 ($M_S = 4$)



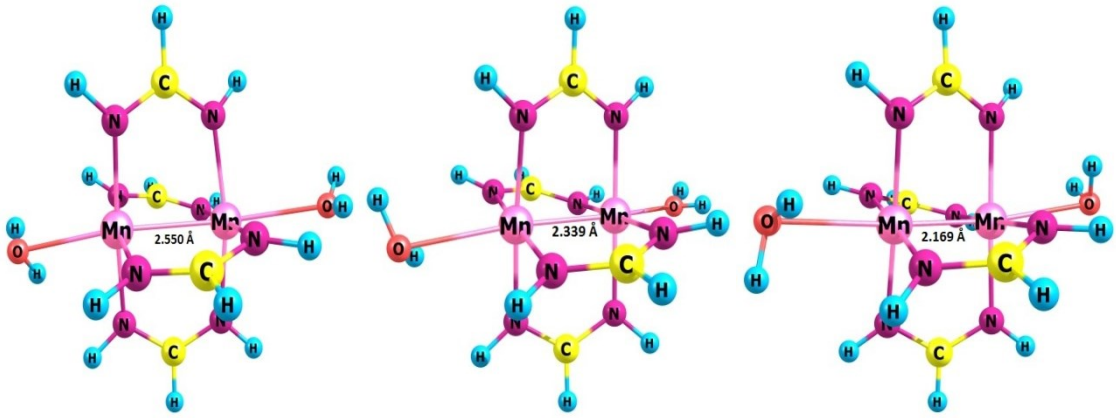
(o) 4 ($M_S = 6$)

(p) 5 ($M_S = 1$)

(q) 5 ($M_S = 3$)

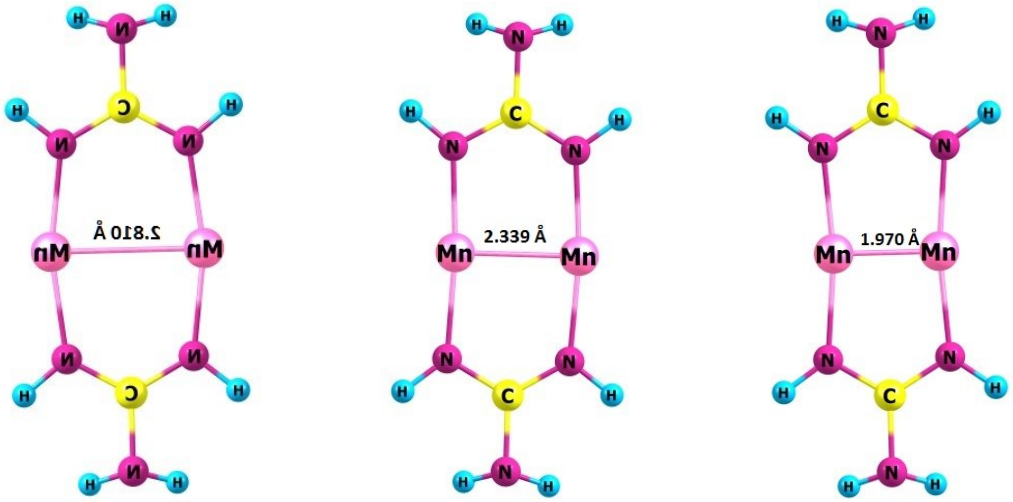


(r) 5 ($M_S = 5$)

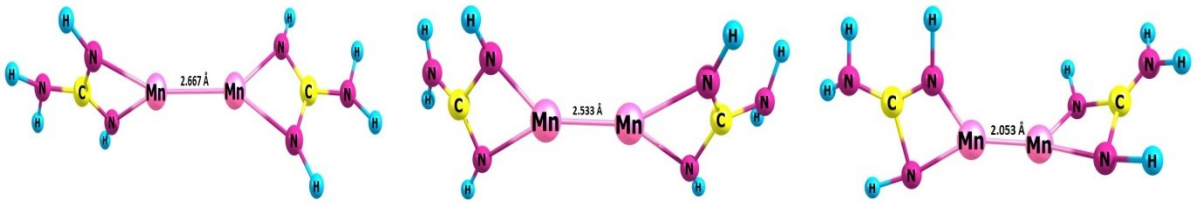


(s) 6 (M_S = 1) **(t) 6** (M_S = 3) **(u) 6** (M_S = 5)

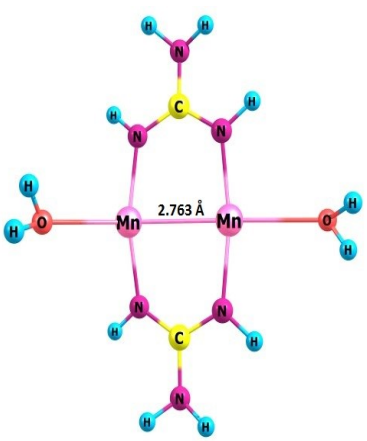
Figure S2 Optimized structures of dimanganese formamidinate complexes



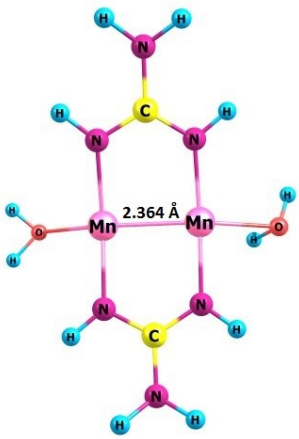
(a) 7A (M_S = 1) **(b) 7A** (M_S = 3) **(c) 7A** (M_S = 5)



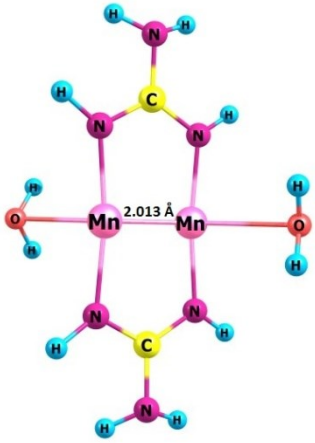
(a) 7B (M_S = 1) **(b) 7B** (M_S = 3) **(c) 7B** (M_S = 5)



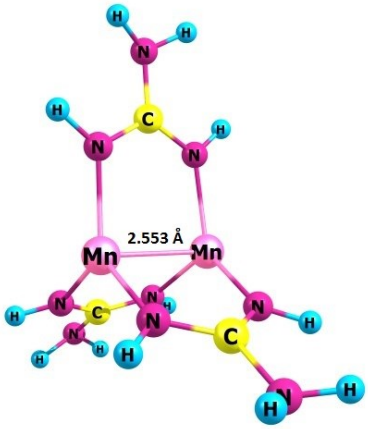
(d) 8 ($M_S = 1$)



(e) 8 ($M_S = 3$)

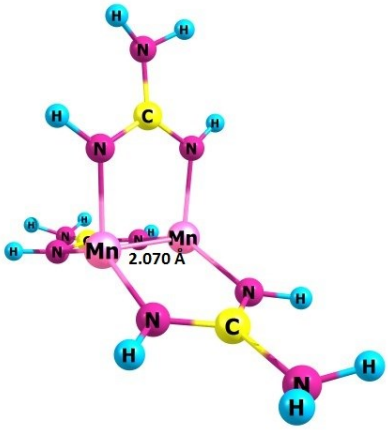


(f) 8 ($M_S = 5$)

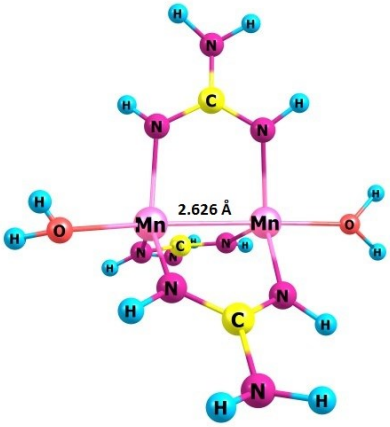


(g) 9 ($M_S = 2$)

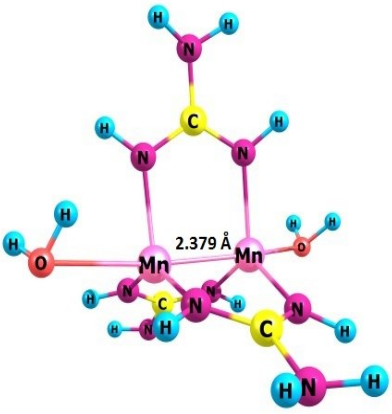
(h) 9 ($M_S = 4$)



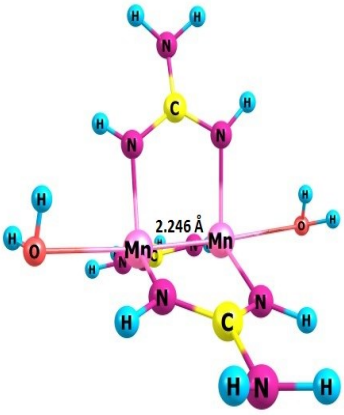
(i) 9 ($M_S = 6$)



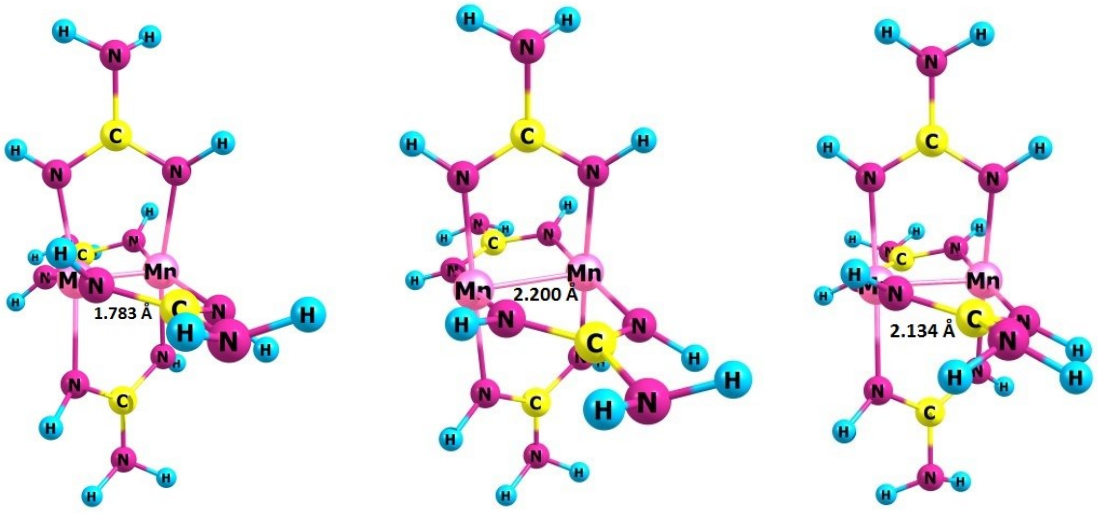
(j) 10 ($M_S = 2$)



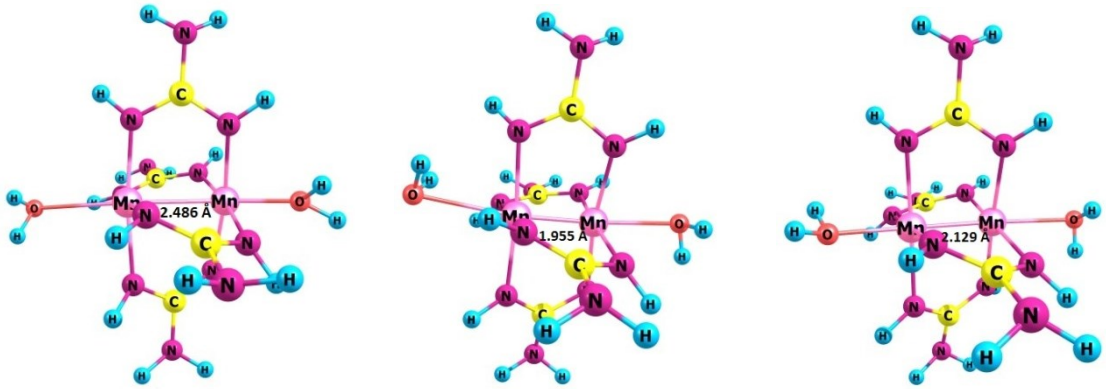
(k) 10 ($M_S = 4$)



(l) 10 ($M_S = 6$)

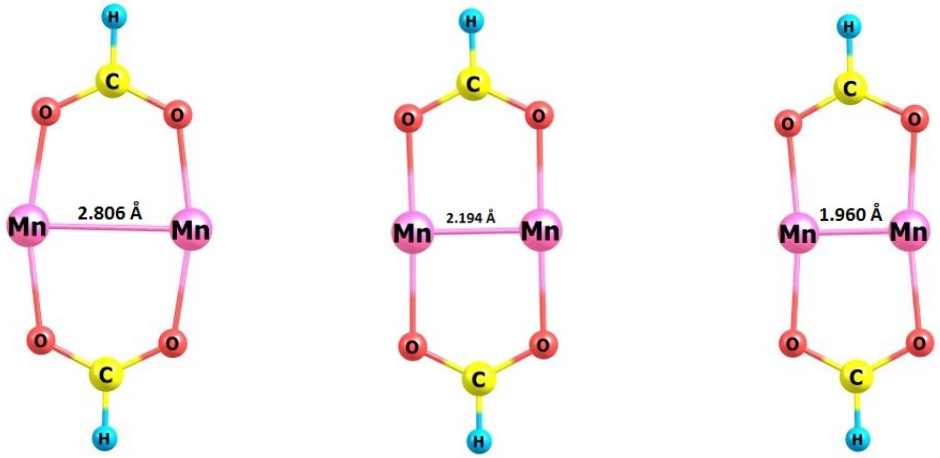


(m) 11 (M_S = 1) **(n) 11** (M_S = 3) **(o) 11** (M_S = 5)

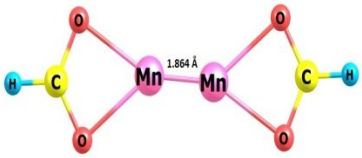


(p) 12 (M_S = 1) **(q) 12** (M_S = 3) **(r) 12**(M_S = 5)

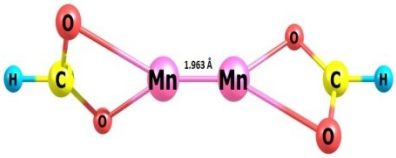
Figure S3 Optimized structures of dimanganese guanidinate complexes



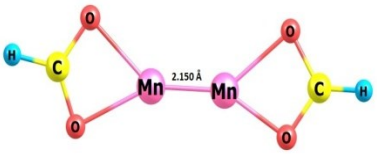
(a) 13A (M_S = 1) **(b) 13A** (M_S = 3) **(c) 13A** (M_S = 5)



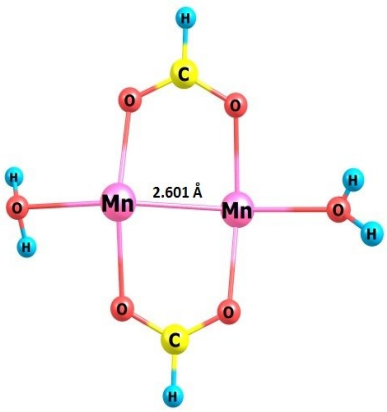
(d) 13B ($M_S = 1$)



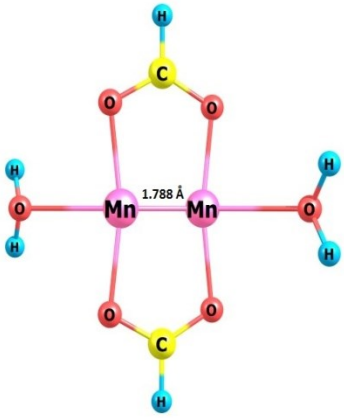
(e) 13B ($M_S = 3$)



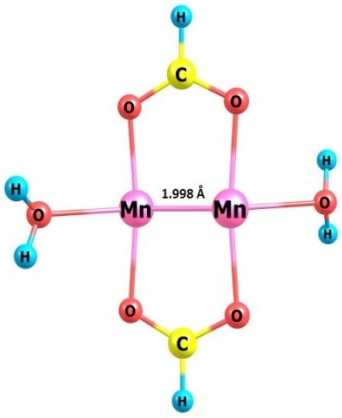
(f) 13B ($M_S = 5$)



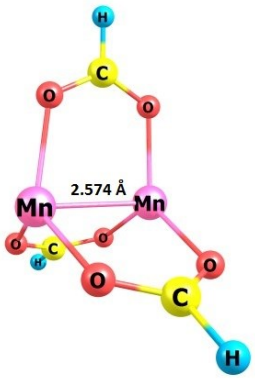
(g) 14 ($M_S = 1$)



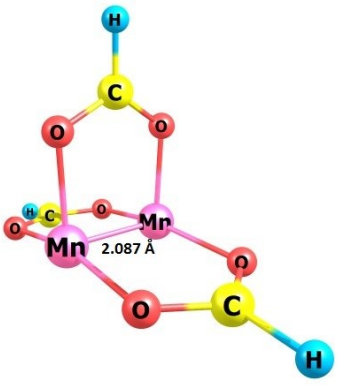
(h) 14 ($M_S = 3$)



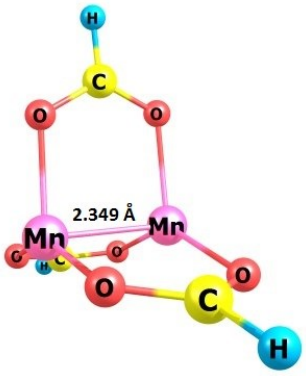
(i) 14 ($M_S = 5$)



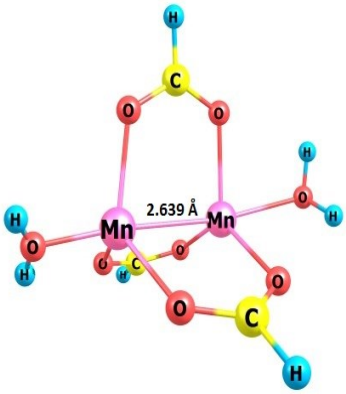
(j) 15 ($M_S = 2$)



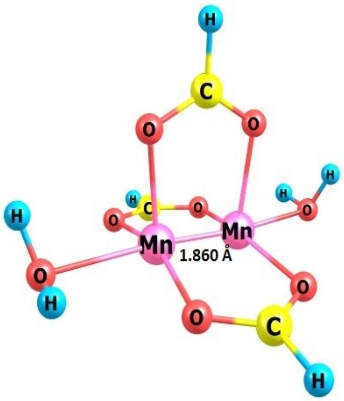
(k) 15 ($M_S = 4$)



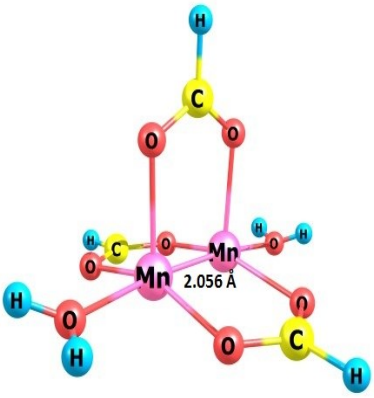
(l) 15 ($M_S = 6$)



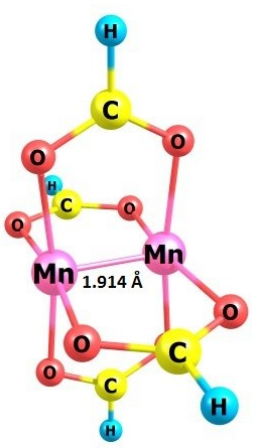
(m) 16 ($M_S = 2$)



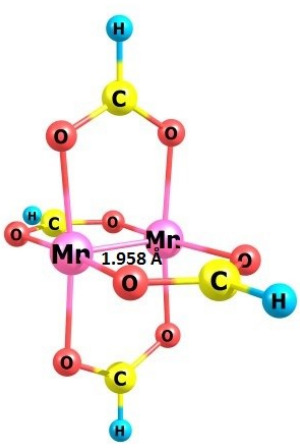
(n) 16 ($M_S = 4$)



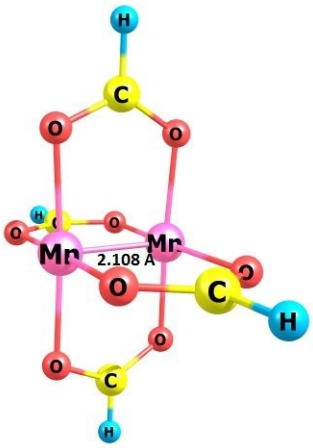
(o) 16 ($M_S = 6$)



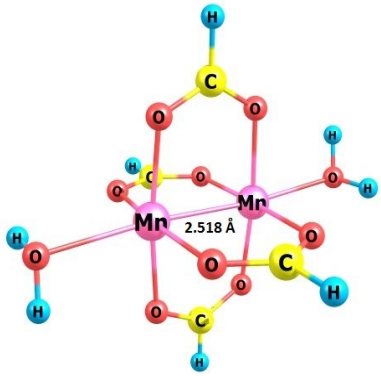
(p) 17 (M_S = 1)



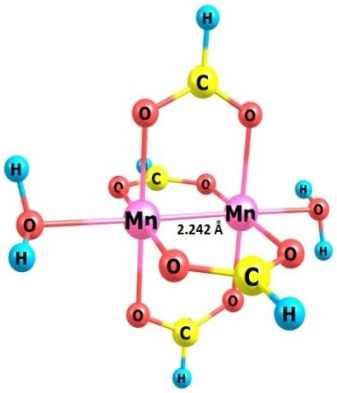
(q) 17 (M_S = 3)



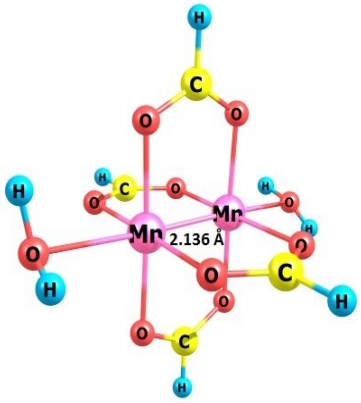
(r) 17 (M_S = 5)



(s) 18 (M_S = 1)



(t) 18 (M_S = 3)



(u) 18 (M_S = 5)

Figure S4 Optimized structures of dimanganese formate complexes

3. Metal-Metal Molecular Orbital Diagrams

These molecular orbital diagrams represent the occupied Metal-Metal (MM) Molecular Orbitals (MOs) which specifically involve the orbitals of one metal (manganese) center with those of another metal (manganese) center in the bimetallic core. Given are the energy levels of the MOs (in eV) along with their occupancies. Singlet species are dealt with by employing a restricted approach with MOs capable of being filled by up to two electrons each. Species with unpaired electrons are treated by unrestricted theory and yield alpha and beta molecular orbitals which are singly occupied. The Mn-Mn Bond Order (BO) derives from the electron occupancies of the bonding and antibonding MOs. The Mn-Mn MOs are shown pictorially alongside the energy level (with occupancy), and may be identified by their serial number in the full list of MOs, or else as per the symmetry (**σ**, **π**, or **δ**). These MM MO diagrams are drawn for all ground state complexes, and also for complexes with bond order values of 4.

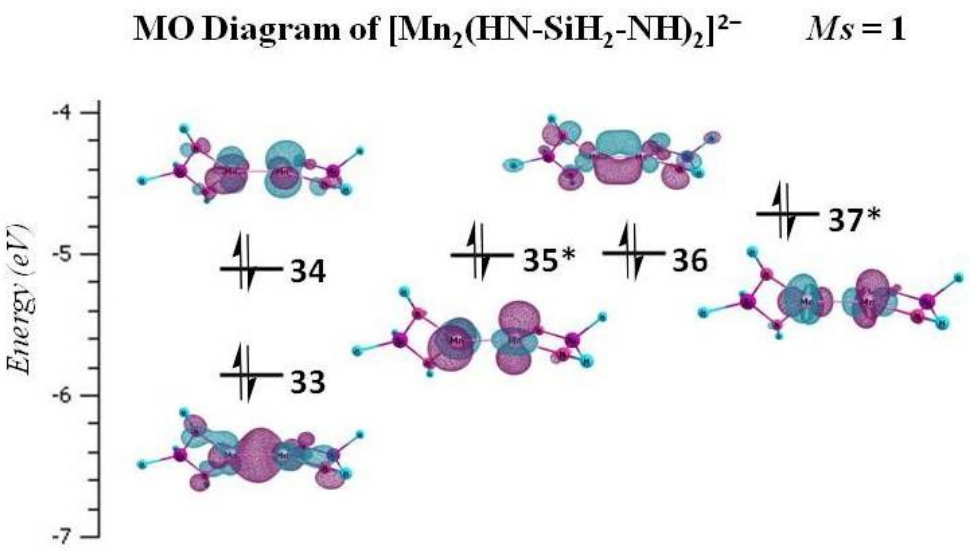


Figure S5: MM MOs of **M1A singlet BO = 1**

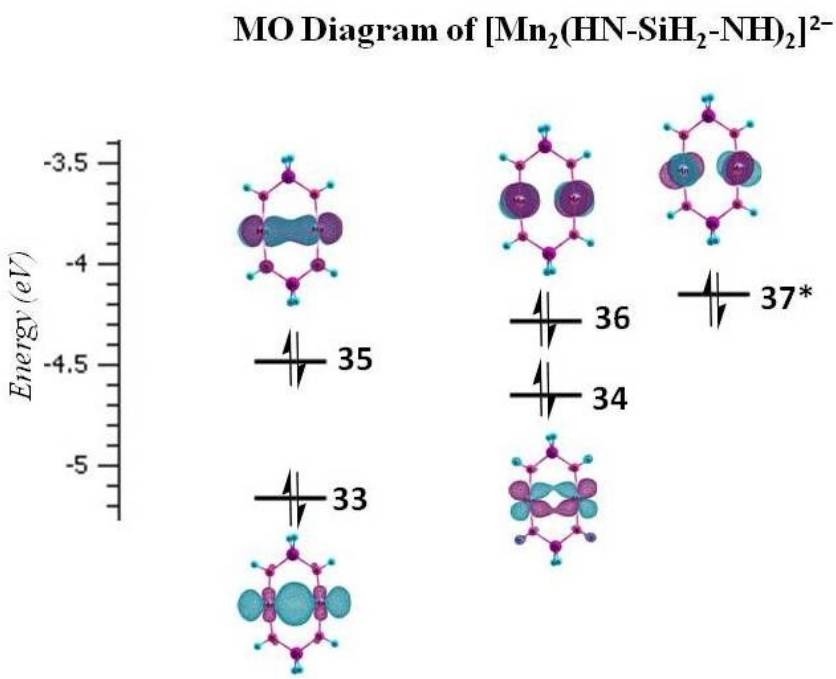


Figure S6: MM MOs of **M1B singlet BO = 3**

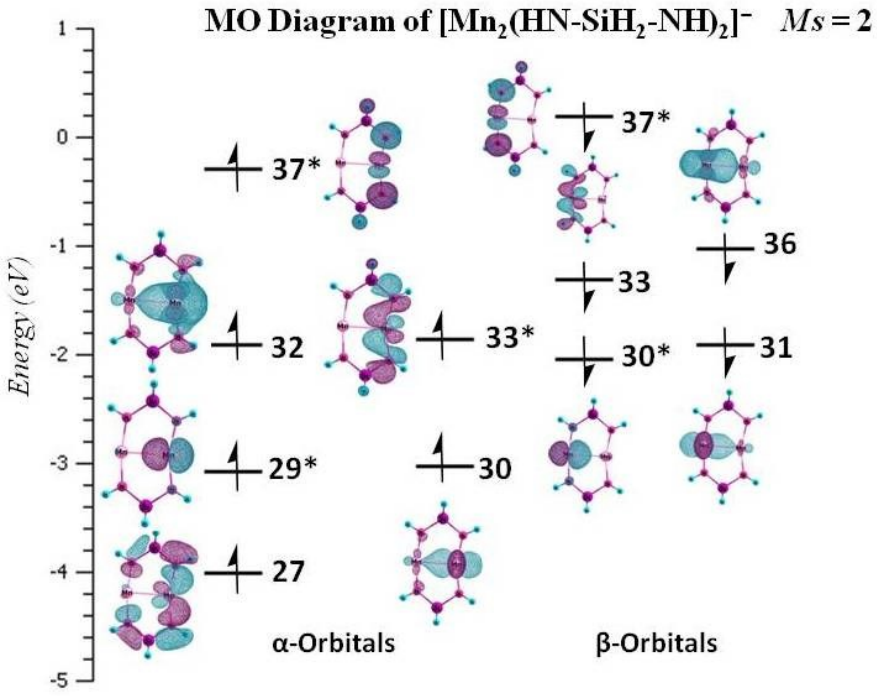


Figure S7: MM MOs of **M2B doublet BO = 0.5**

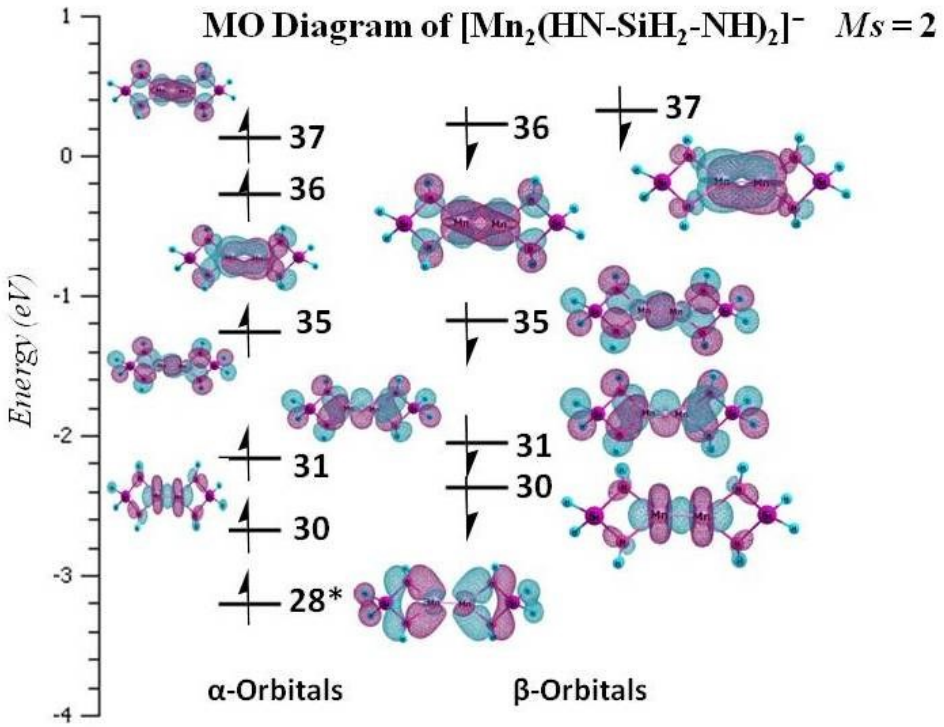


Figure S8: MM MOs of **M2A doublet BO = 4.5**

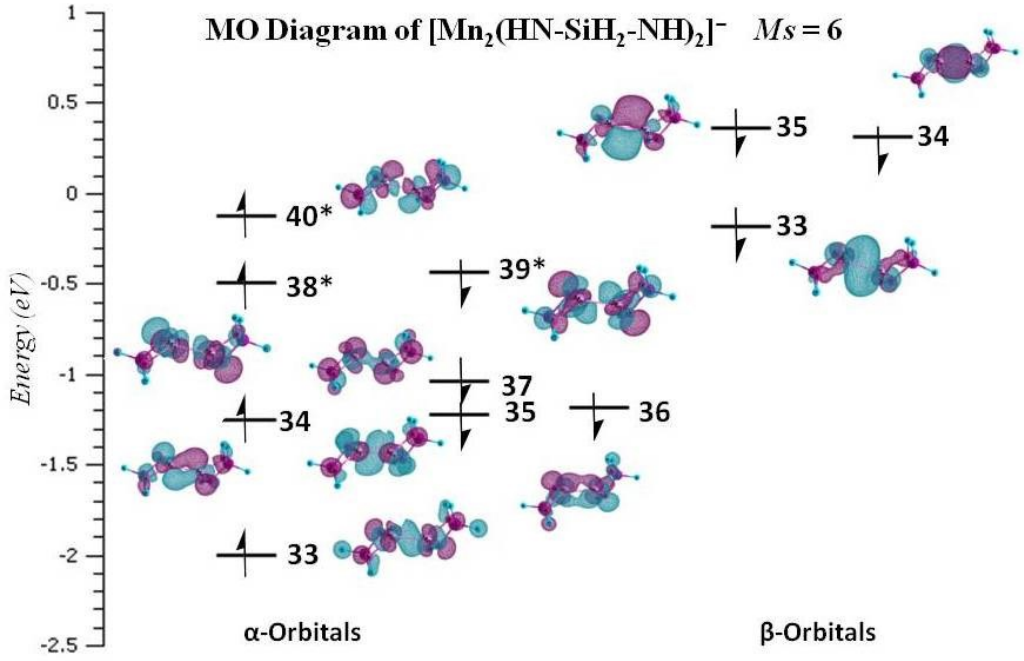


Figure S9: MM MOs of **M2A sextet BO = 2.5**

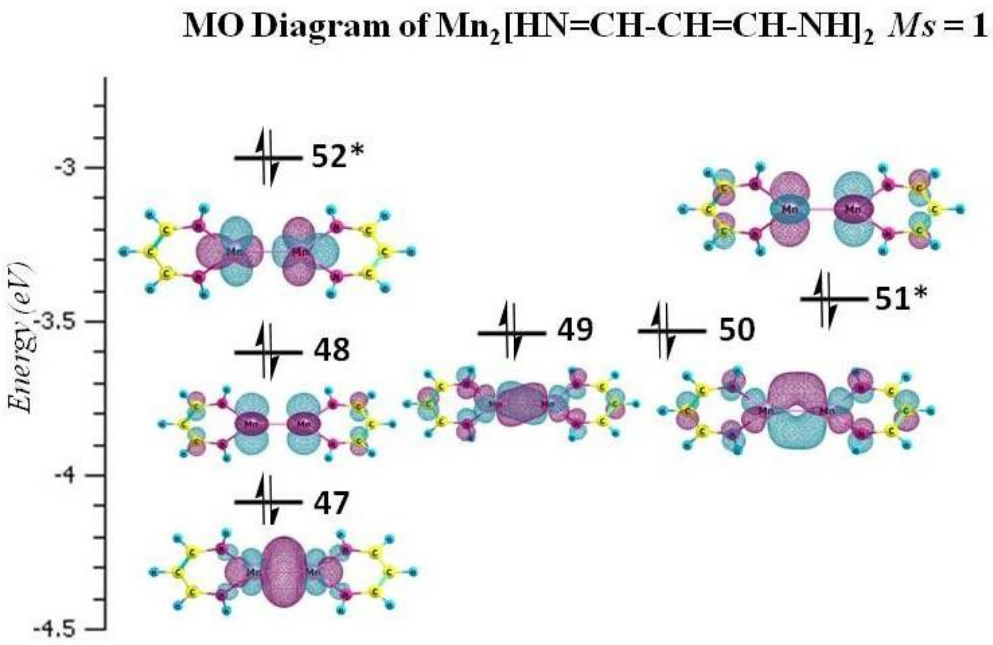


Figure S10: MM MOs of **M3A singlet BO = 2**

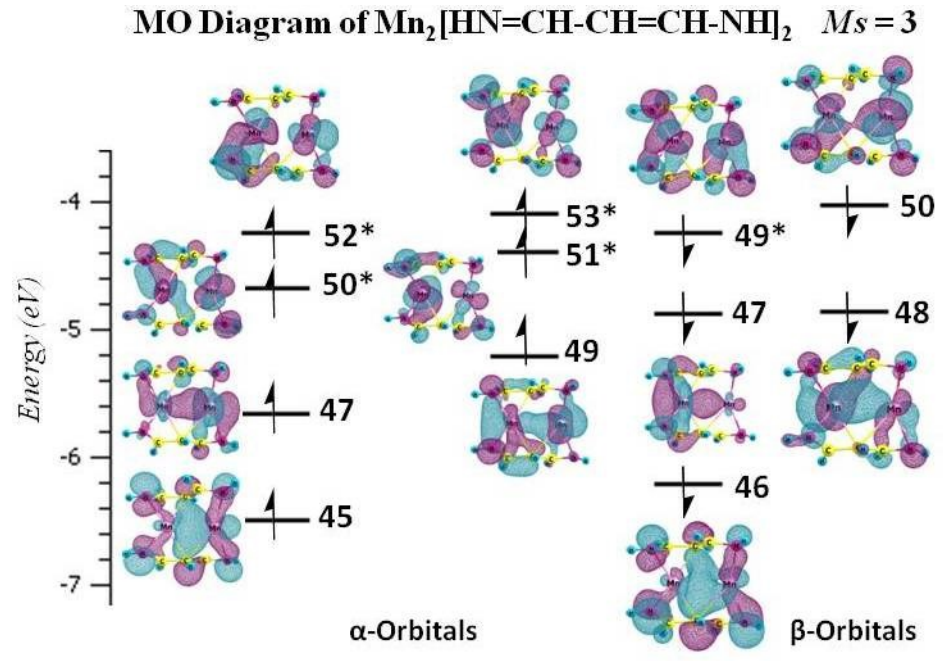


Figure S11: MM MOs of **M3B triplet BO = 1**

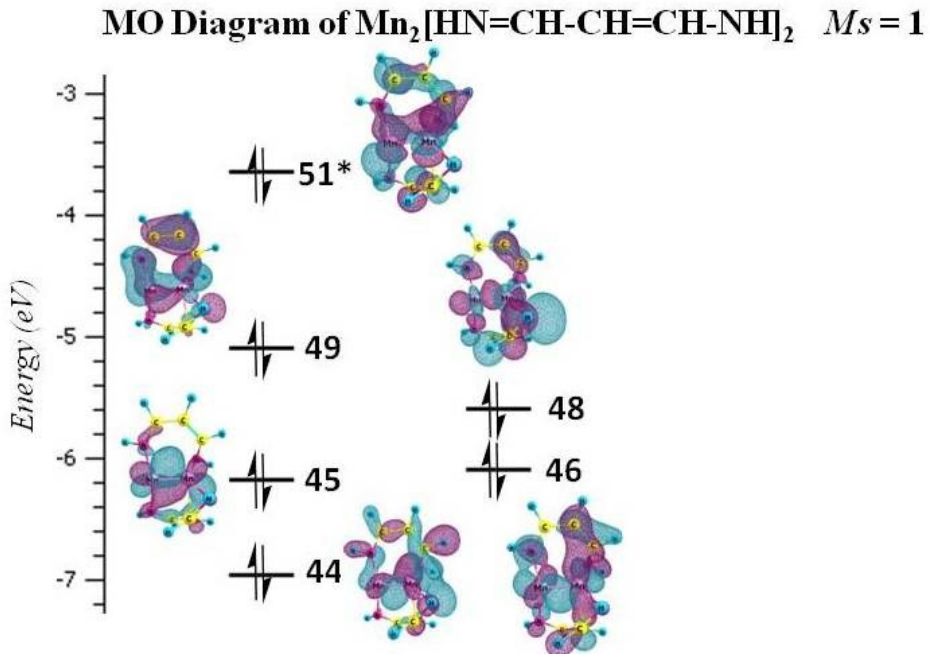


Figure S12: MM MOs of **M3B singlet BO = 4**

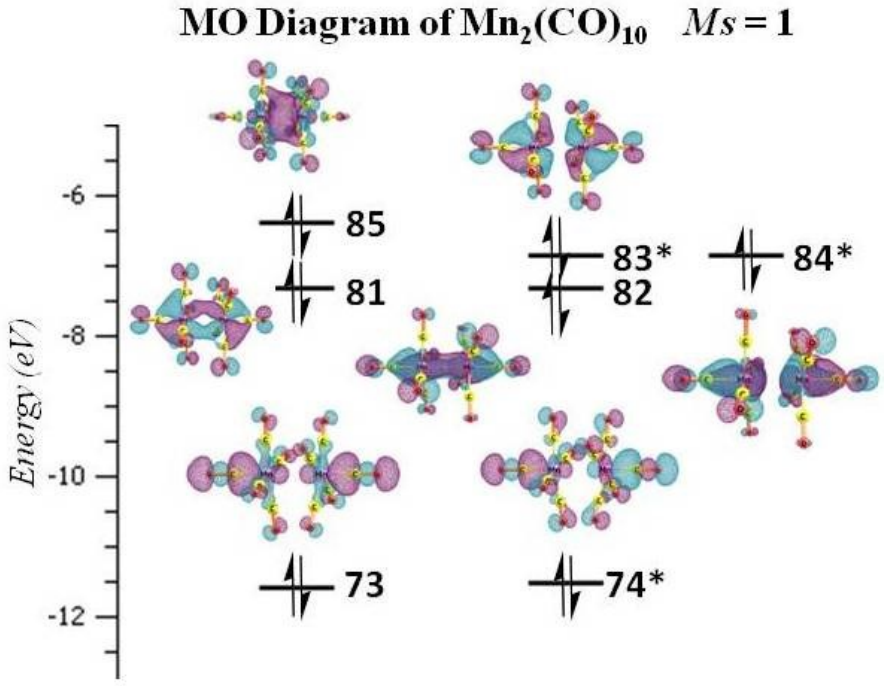


Figure S13: MM MOs of **M4 singlet BO = 1**

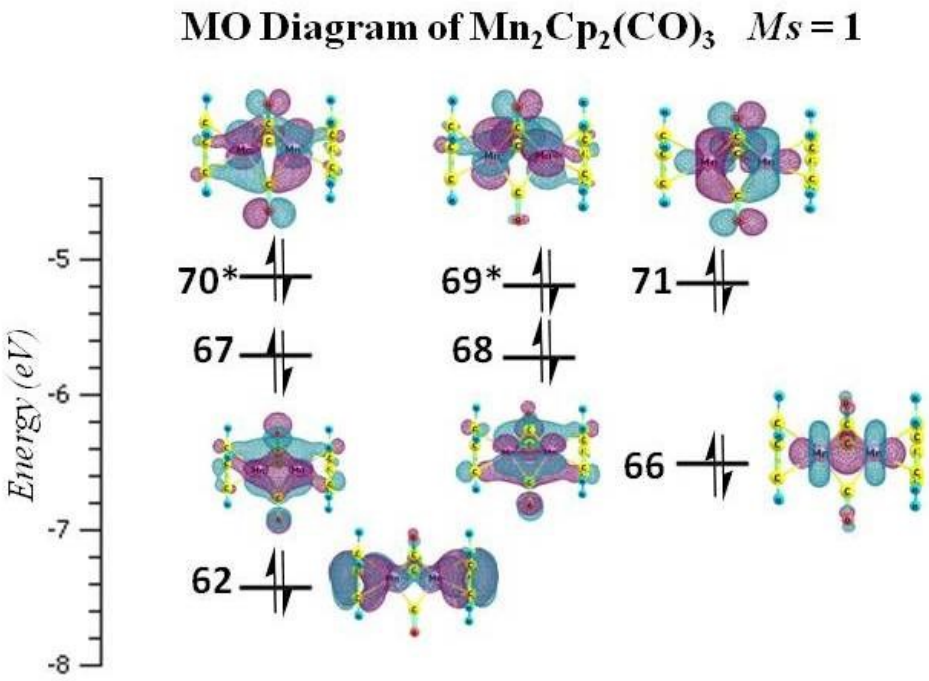


Figure S14: MM MOs of **M5 singlet BO = 3**

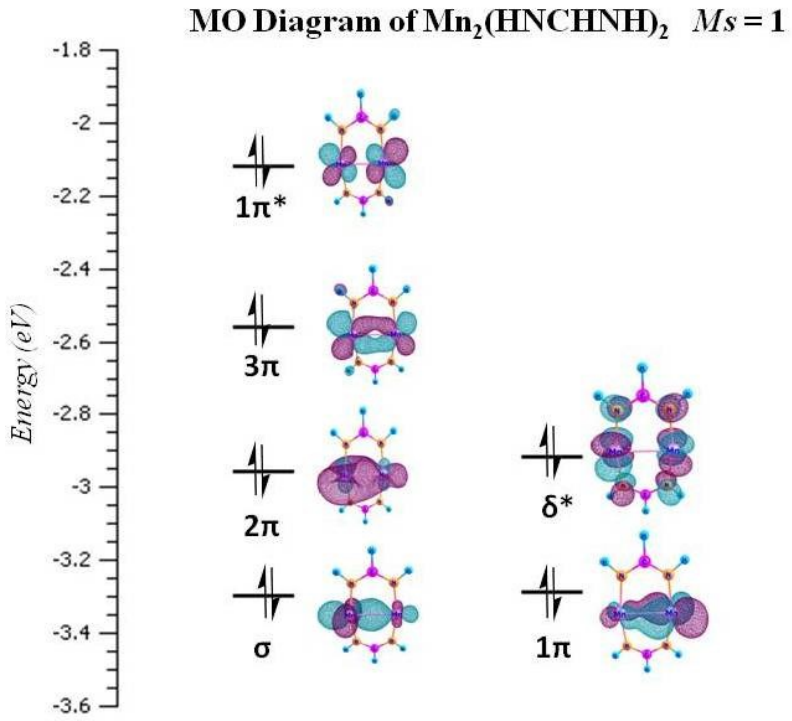


Figure S15: MM MOs of **1A singlet (**configuration $\sigma^2\pi^6\pi^{*2}\delta^{*2}$**) BO = 2**

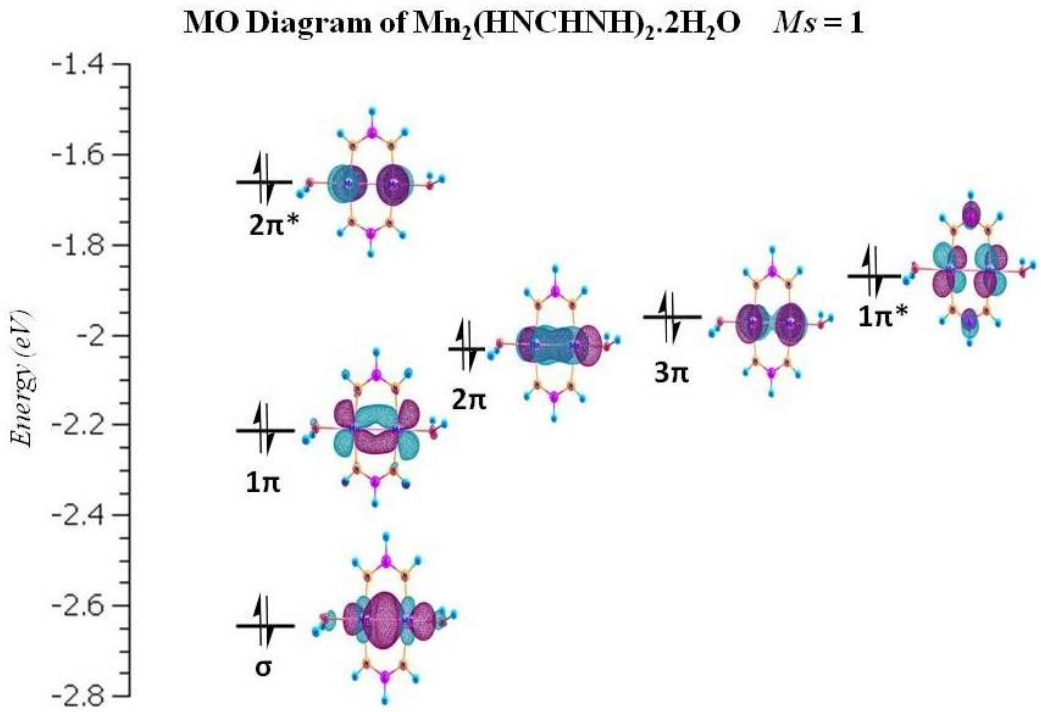


Figure S16: MM MOs of **2 singlet** (configuration $\sigma^2\pi^6\pi^{*4}$) **BO = 2**

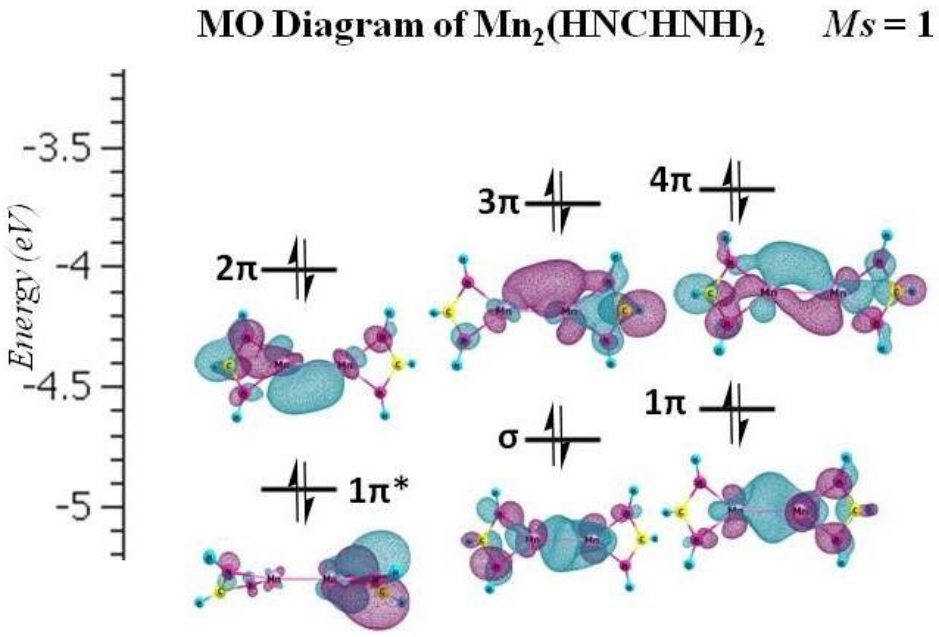


Figure S17: MM MOs of **1B singlet (**configuration $\sigma^2\pi^8\pi^{*2}$) **BO = 4**

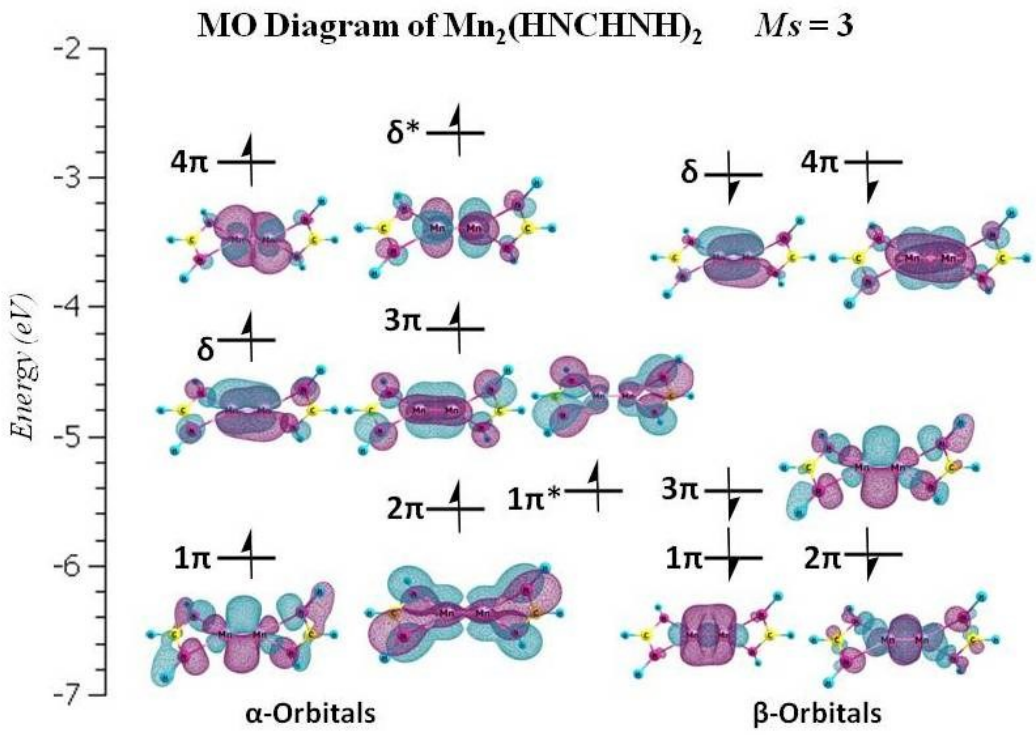


Figure S18: MM MOs of **1B triplet (**configuration $\pi^8\delta^2\pi^{*1}\delta^{*1}$) **BO = 4**

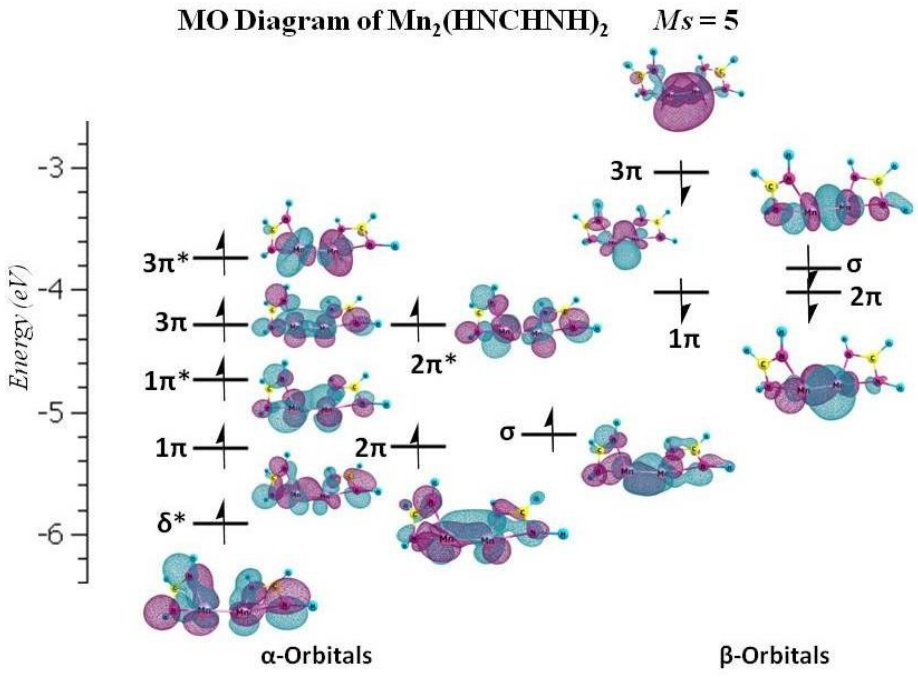


Figure S19: MM MOs of **1B quintet (**configuration $\sigma^2\pi^6\pi^{*3}\delta^{*1}$) **BO = 2**

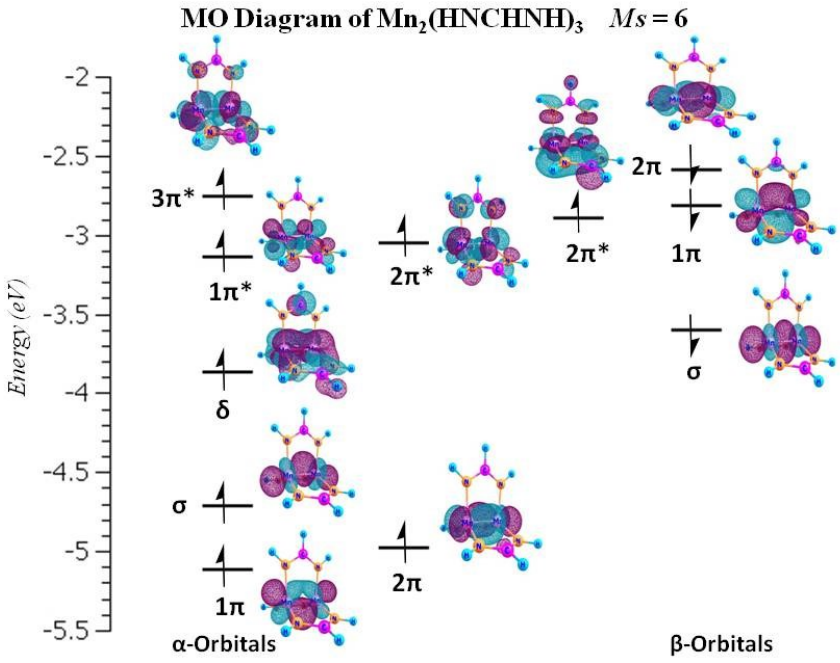


Figure S20: MM MOs of **3 sextet** (configuration $\sigma^2\pi^4\delta^1\pi^{*4}$) **BO = 1.5**

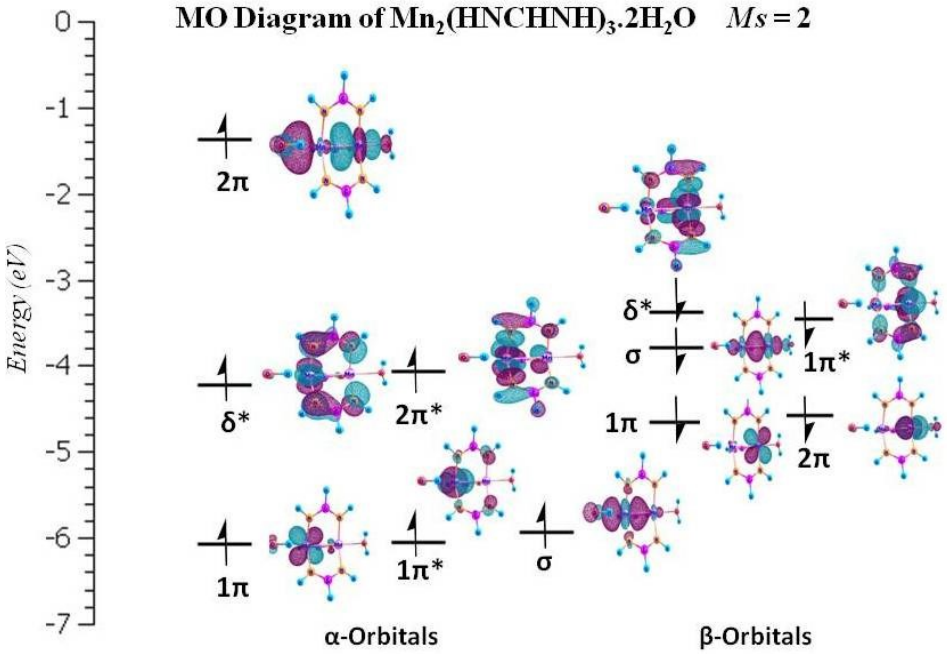


Figure S21: MM MOs of **4 doublet** (configuration $\sigma^2\pi^4\pi^{*3}\delta^{*2}$) **BO = 0.5**

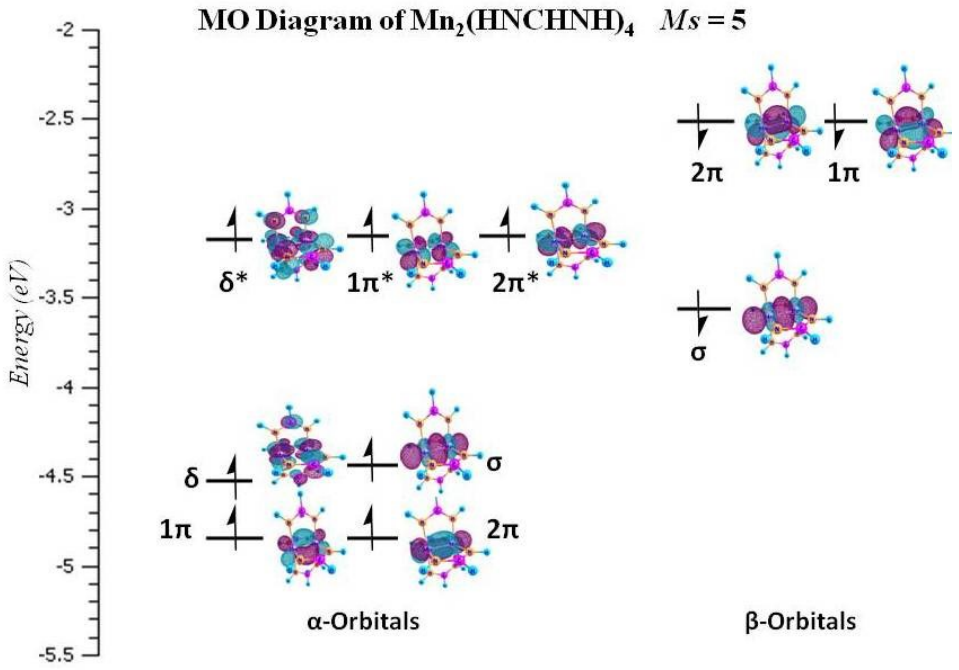


Figure S22: MM MOs of **5 quintet** (configuration $\sigma^2\pi^4\delta^1\pi^{*2}\delta^{*1}$) **BO = 2**

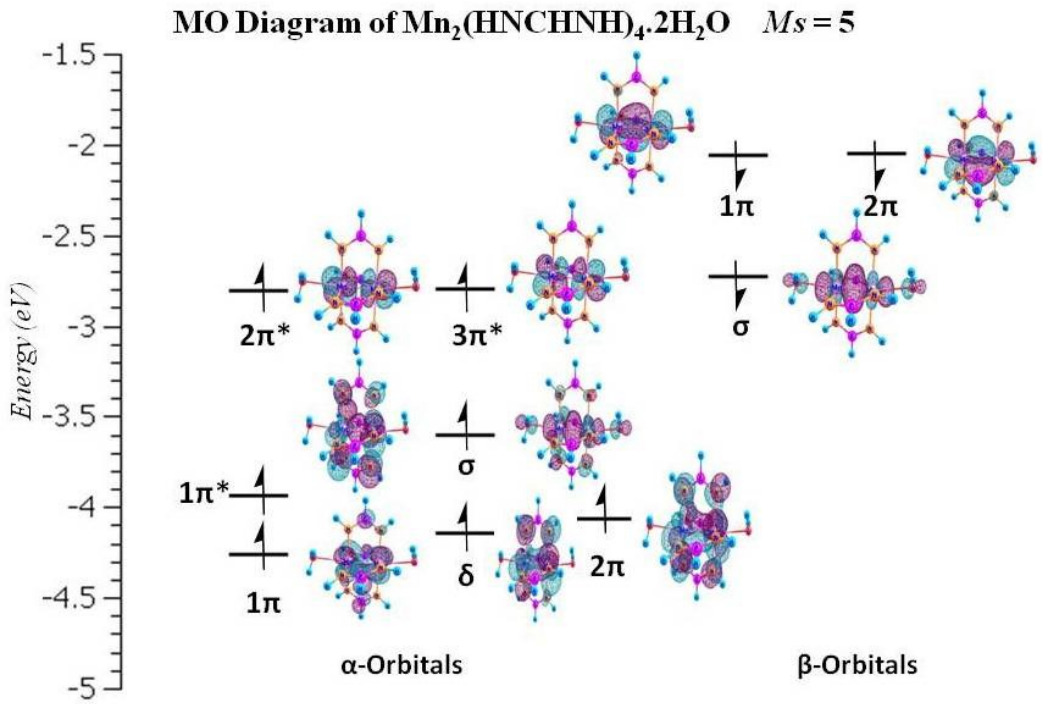


Figure S23: MM MOs of **6 quintet** (configuration $\sigma^2\pi^4\delta^1\pi^{*3}$) **BO = 2**

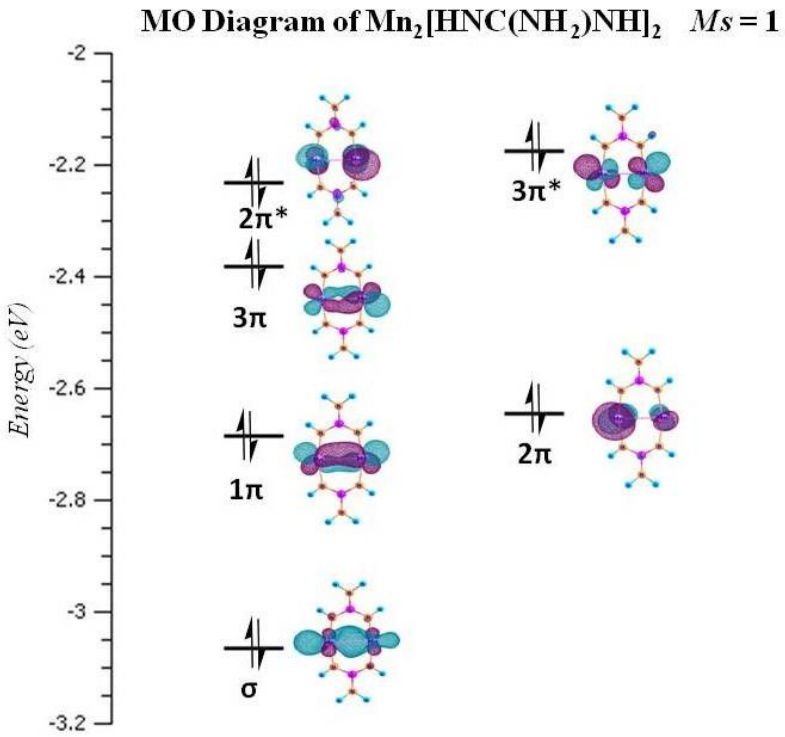


Figure S24: MM MOs of **7A singlet** (configuration $\sigma^2\pi^6\pi^{*4}$) **BO = 2**

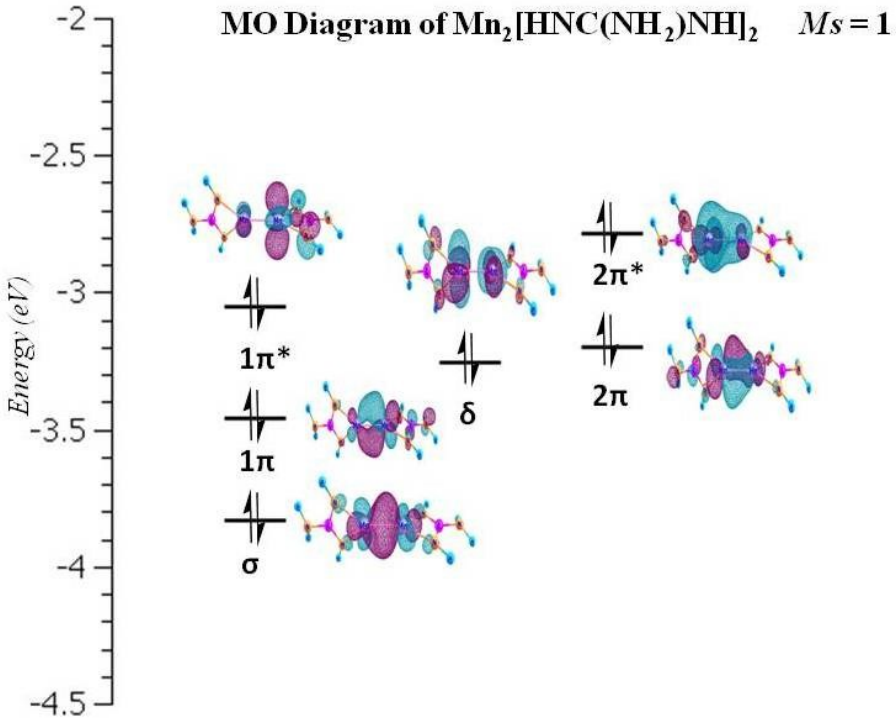


Figure S25: MM MOs of **7B singlet** (configuration $\sigma^2\pi^6\delta^2\pi^{*4}$) **BO = 2**

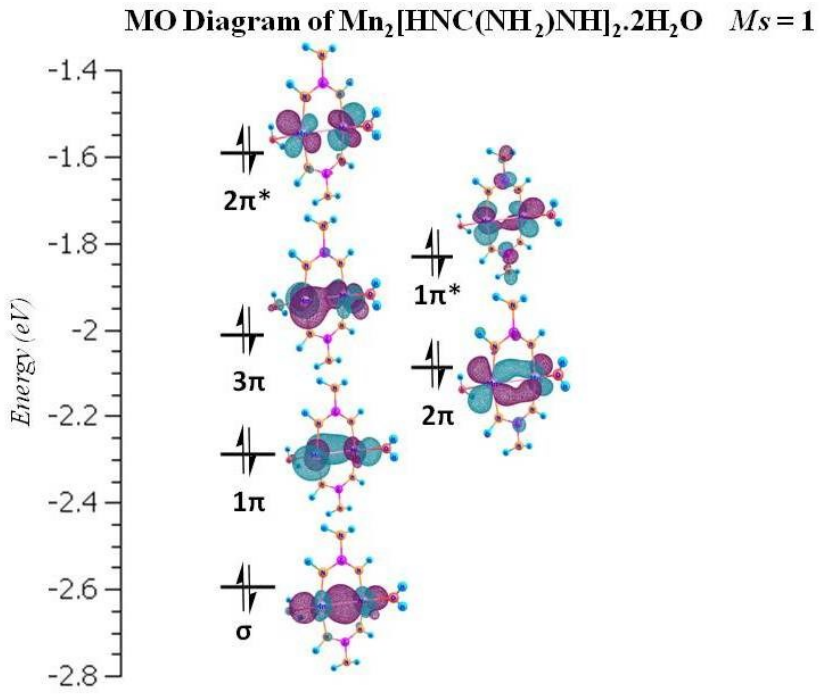


Figure S26: MM MOs of **8 singlet** (configuration $\sigma^2\pi^6\pi^{*4}$) **BO = 2**

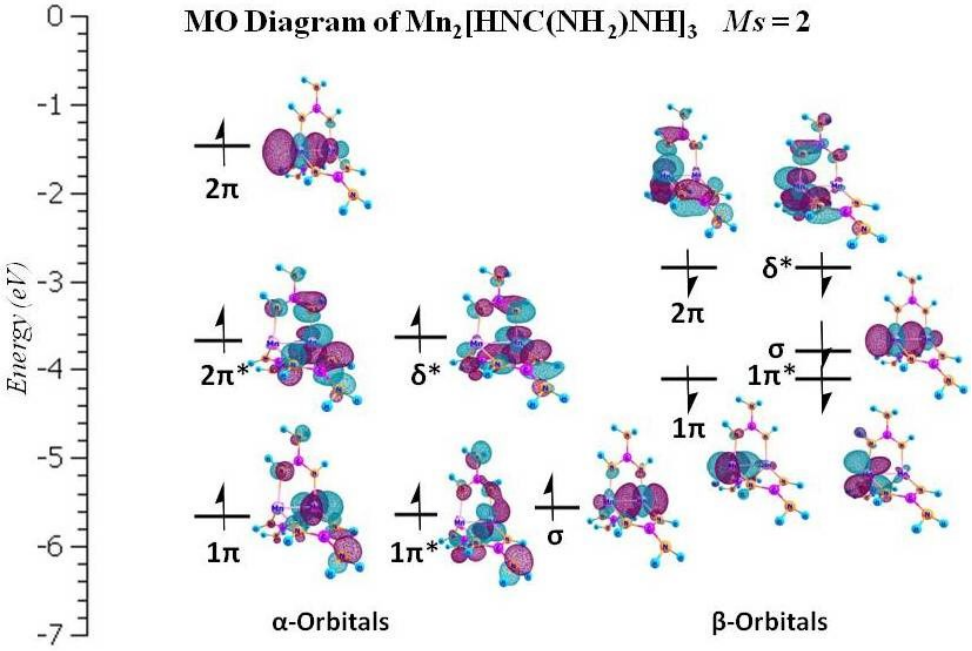


Figure S27: MM MOs of **9 doublet** (configuration $\sigma^2\pi^3\pi^{*4}\delta^{*2}$) **BO = 0.5**

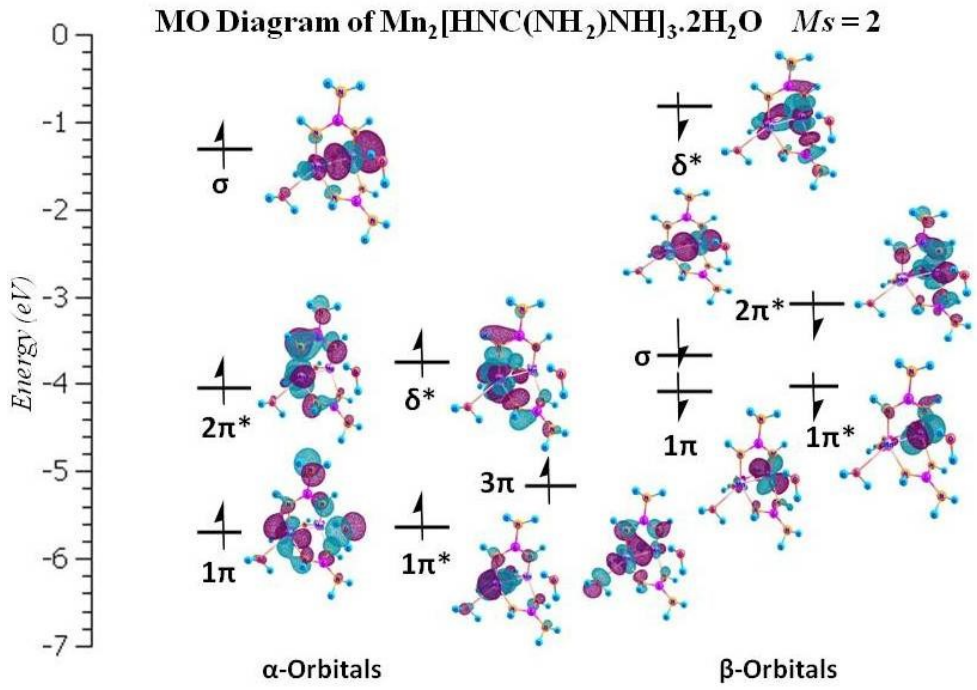


Figure S28: MM MOs of **10 doublet** (configuration $\sigma^2\pi^3\pi^{*4}\delta^{*2}$) **BO = 0.5**

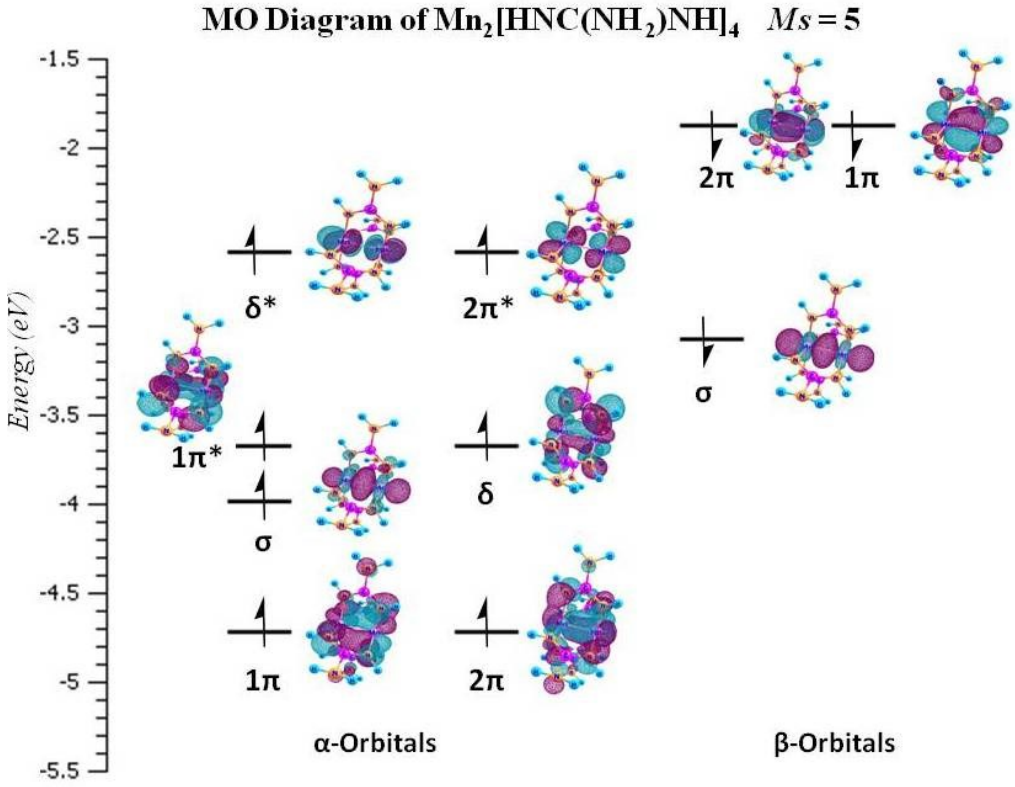


Figure S29: MM MOs of **11 quintet** (configuration $\sigma^2\pi^4\delta^1\pi^{*2}\delta^{*1}$) **BO = 2**

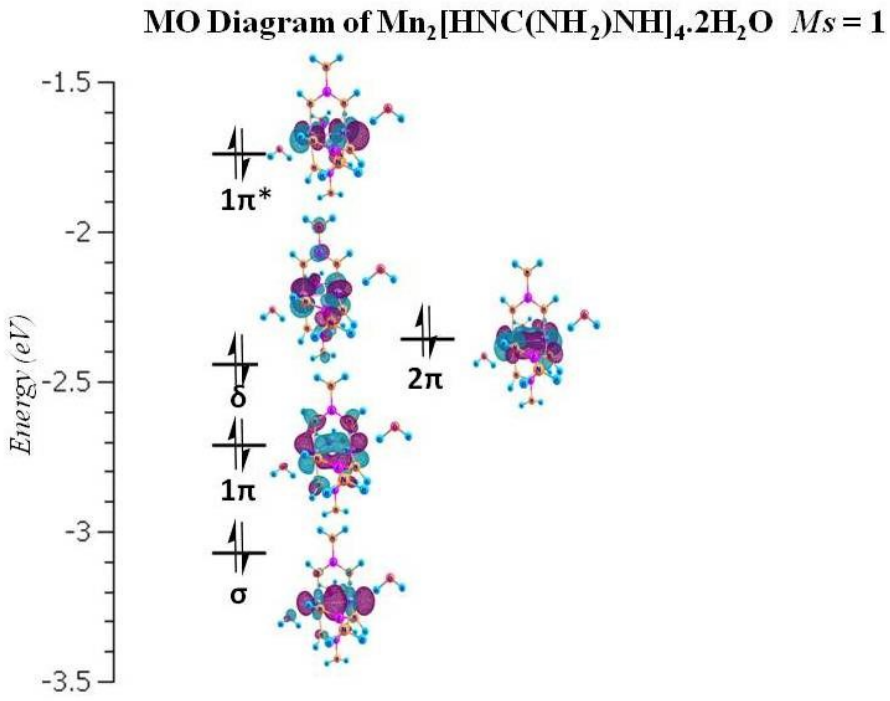


Figure S30: MM MOs of **12 singlet** (configuration $\sigma^2\pi^4\delta^2\pi^{*2}$) **BO = 3**

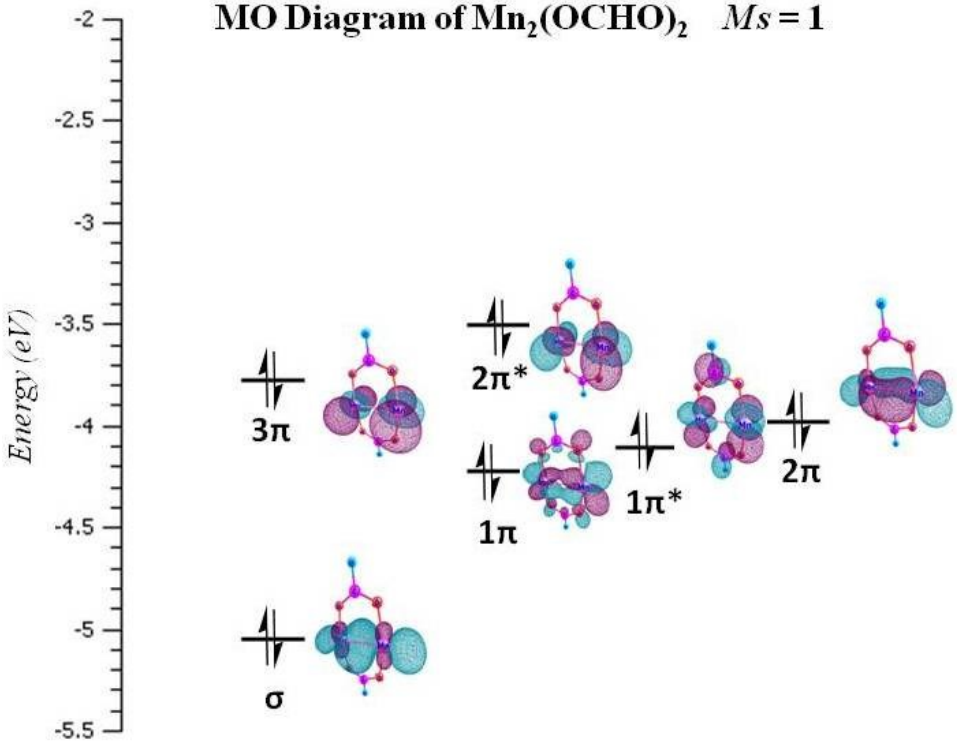


Figure S31: MM MOs of **13A singlet** (configuration $\sigma^2\pi^4\pi^{*4}$) **BO = 2**

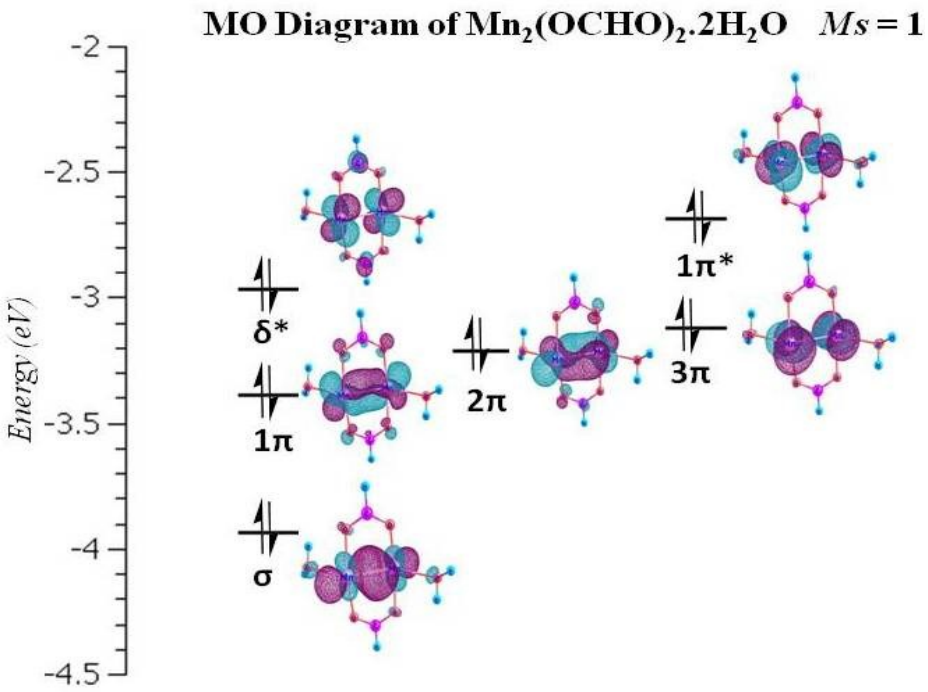


Figure S32: MM MOs of **14 singlet** (configuration $\sigma^2\pi^6\pi^{*2}\delta^{*2}$) **BO = 2**

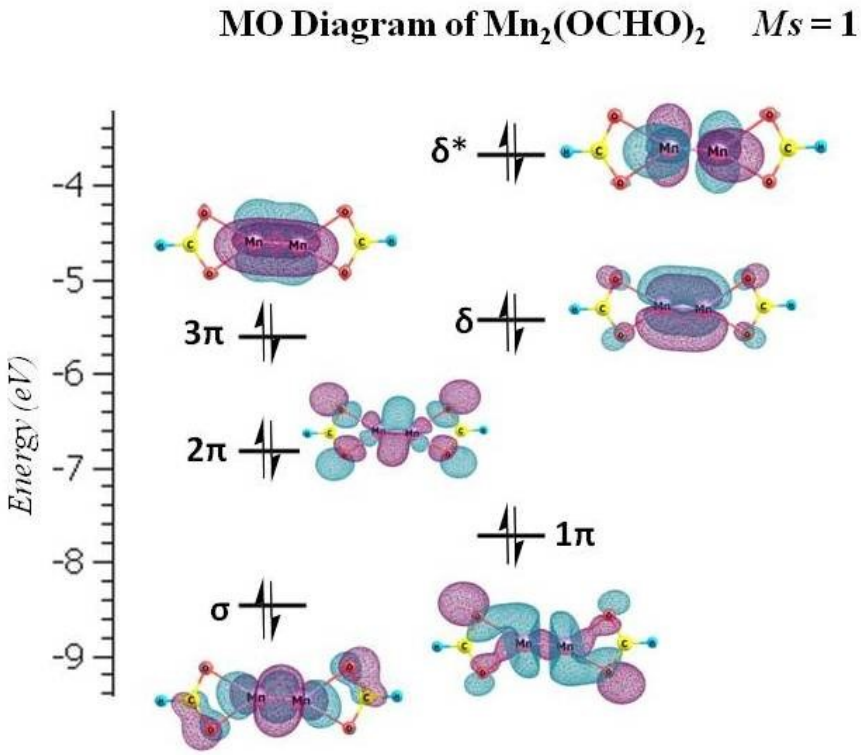


Figure S33: MM MOs of **13B singlet** (configuration $\sigma^2\pi^6\delta^2\delta^{*2}$) **BO = 4**

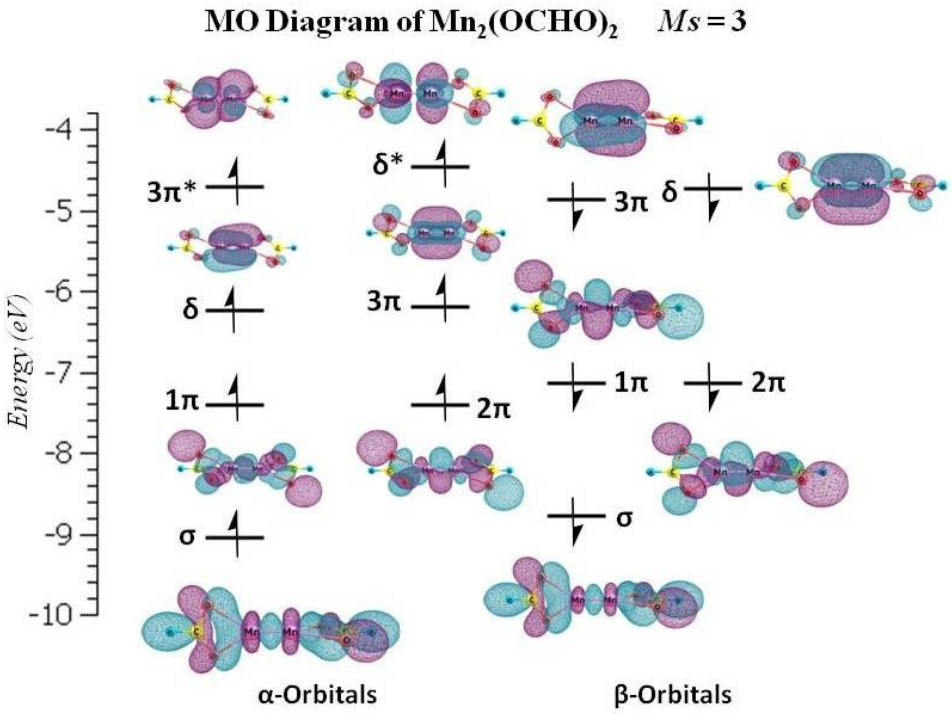


Figure S34: MM MOs of **13B triplet** (configuration $\sigma^2\pi^6\delta^2\pi^{*1}\delta^{*1}$) **BO = 4**

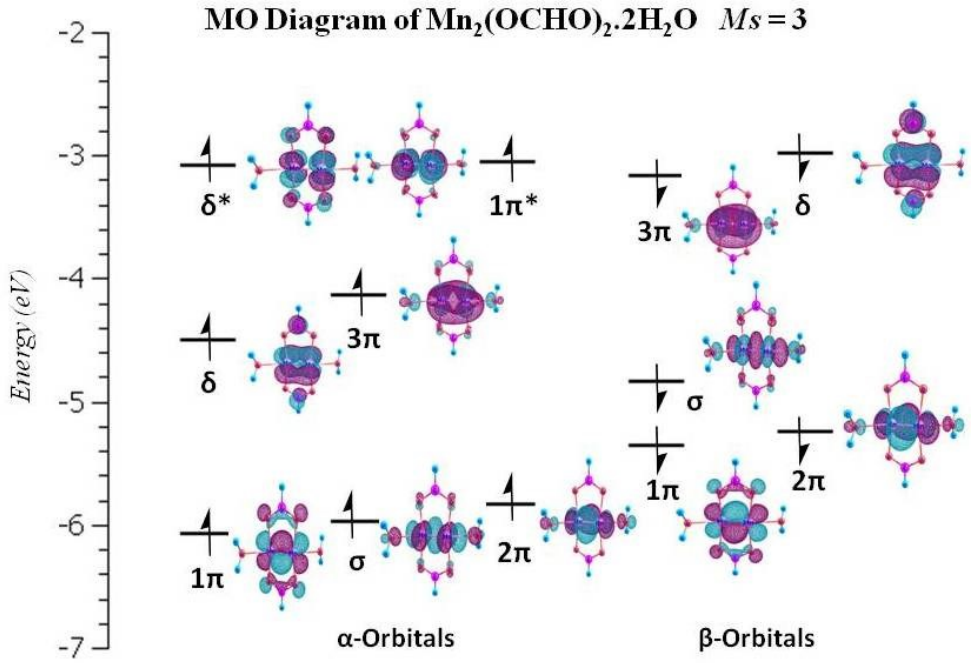


Figure S35: MM MOs of **14 triplet** (configuration $\sigma^2\pi^6\delta^2\pi^{*1}\delta^{*1}$) **BO = 4**

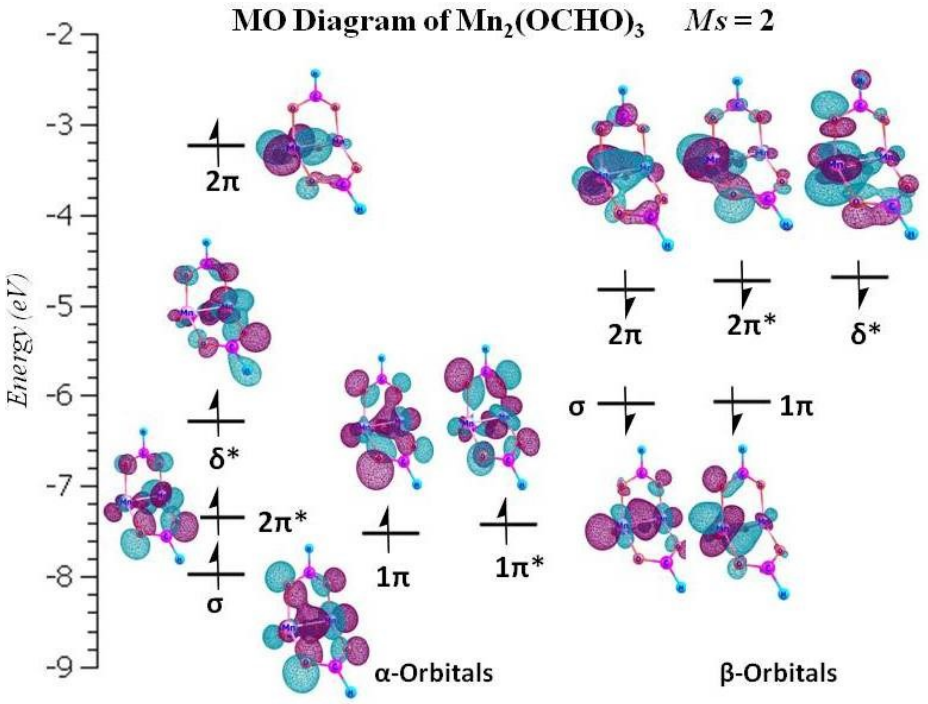


Figure S36: MM MOs of **15 doublet** (configuration $\sigma^2\pi^4\pi^{*3}\delta^{*2}$) **BO = 0.5**

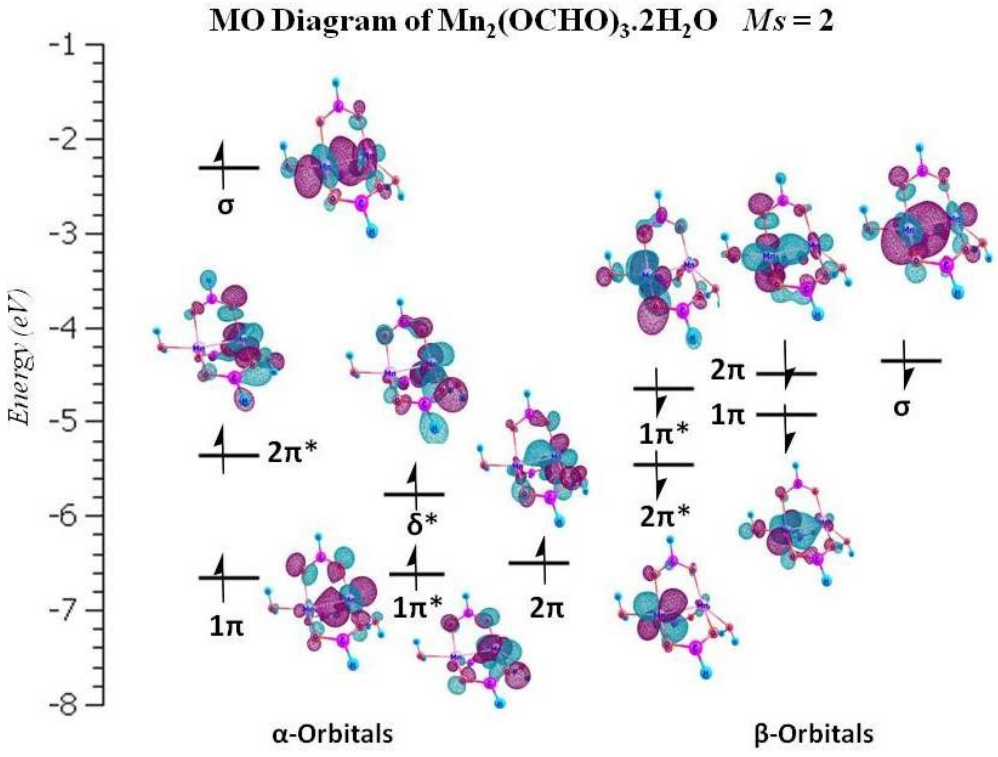


Figure S37: MM MOs of **16 doublet** (configuration $\sigma^2\pi^4\pi^{*4}\delta^{*1}$) **BO = 0.5**

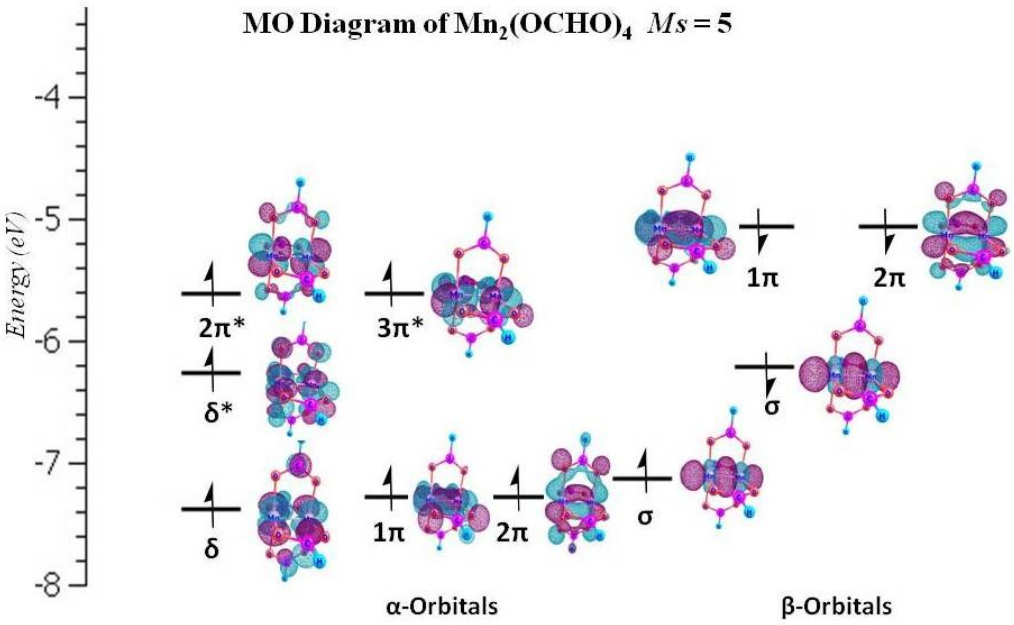


Figure S38: MM MOs of **17 quintet** (configuration $\sigma^2\pi^4\delta^1\pi^{*2}\delta^{*1}$) **BO = 2**

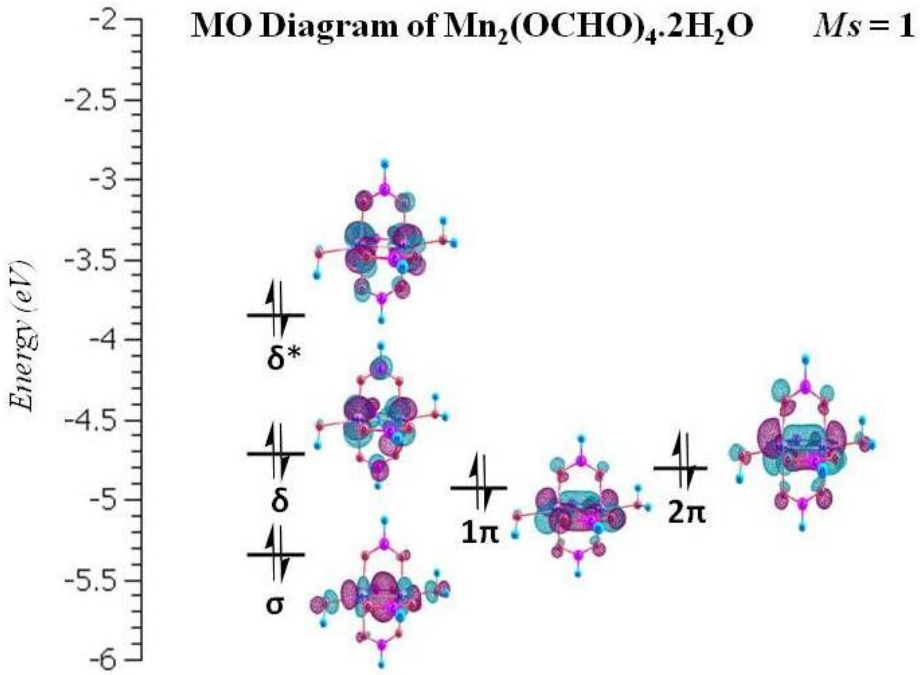


Figure S39: MM MOs of **18 singlet** (configuration $\sigma^2\pi^4\delta^2\delta^{*2}$) **BO = 3**

4. Tables: Total Energies; Results for Metal-Ligand Bonds

Note **Qc** = Charge; **M*s*** = (2S+1) spin multiplicity; $\mathbf{E_{Tot}}$ = total electronic energy; $\mathbf{E_{ZP}}$ = zero point energy; $\mathbf{E_{Tot}(cr)}$ = corrected total energy. The 6-31+G** basis set was used for carbon, oxygen, nitrogen hydrogen and silicon atoms, and the pseudo-potential LANL2DZ basis set for the manganese atoms. Vibrational frequency analysis confirmed the optimized structures as true minima with Nimag = 0 for all cases and generated zero point energy (ZPE) corrections to the total electronic energies, using a scaling factor of 0.978.

Table S1 Energy terms for models for complexes **E1** to **E5** with results related to Mn-Mn bonds present

No Complex	Q_c	M_s	$E_{Tot(uc)}$ (hartree)	$E_{ZP(us)}$ (hartree)	$E_{Tot}(cr)$ (hartree)	$E_{Tot}(cr)$ (kcal/mol)
A M1a	0	1	-1010.752306	0.091104	-1010.663206	-634200.26
		3	-1011.468675	0.093164	-1010.539085	-634122.37
		5	-1011.474938	0.092226	-1010.554708	-634132.17
B M1b	0	1	-1011.613535	0.092462	-1010.690949	-634217.67
C M2a	0	2	-1010.730283	0.094865	-1010.637505	-634184.13
		4	-1010.739790	0.095369	-1010.646519	-634189.78
		6	-1010.755891	0.095392	-1010.662598	-634199.87
D M2b	0	2	-1010.877935	0.093169	-1010.786816	-634277.82
		4	-1010.823272	0.094751	-1010.730606	-634242.55
		6	-1010.822501	0.094986	-1010.729605	-634241.92
E M3a	0	1	-661.594912	0.166769	-661.431812	-415054.41
		3	-661.510610	0.167799	-661.346503	-415000.88
		5	-661.513992	0.163331	-661.354254	-415005.74
F M3b	0	1	-661.476641	0.165993	-661.314299	-414980.67
		3	-661.542036	0.162483	-661.383128	-418023.86
		5	-661.526428	0.165364	-661.364702	-415012.30
G M4	0	1	-1341.387654	0.085409	-1341.302168	-841679.18
		3	-1341.328324	0.085097	-1341.245099	-841643.37
		5	-1341.256355	0.076547	-1341.181492	-841603.45
H M5	0	1	-935.054618	0.196190	-934.862744	-586634.78
		3	-935.026611	0.194444	-934.836444	-586618.28
		5	-935.038410	0.193126	-934.849533	-586626.50

Table S2 Energy terms for dimanganese formamidinates $[Mn_2(HNCHNH)_x]$ (x = 2, 3, 4)

No Complex	Q_C	M_s	$E_{Tot(uc)}$ (hartree)	$E_{ZP(us)}$ (hartree)	$E_{Tot}(cr)$ (hartree)	$E_{Tot}(cr)$ (kcal/mol)
1A $Mn_2(HNCHNH)_2$	0	1	-506.782957	0.098920	-506.686213	-317950.16
(lantern type)		3	-506.751717	0.099614	-506.654294	-317930.13
		5	-506.722983	0.099863	-506.625317	-317911.94
1B $Mn_2(HNCHNH)_2$	0	1	-506.49843	0.096148	-506.500545	-317833.65
(axially dicoordinated)		3	-506.529526	0.096700	-506.531653	-317853.17
		5	-506.538720	0.095726	-506.540826	-317858.92
2 $Mn_2(HNCHNH)_2.2H_2O$	0	1	-659.640181	0.145296	-659.498083	-413840.98
		3	-659.632773	0.147044	-659.488964	-413835.26
		5	-659.58636	0.146454	-659.443128	-413806.50
3 $Mn_2(HNCHNH)_3$	0	2	-656.168576	0.148369	-656.023471	-411660.63
		4	-656.188191	0.147958	-656.043488	-411673.20
		6	-656.21095	0.149046	-656.065183	-411686.80
4 $Mn_2(HNCHNH)_3.2H_2O$	0	2	-809.137366	0.193933	-809.327032	-507859.99
		4	-809.0928	0.196794	-809.285264	-507833.79
		6	-809.100865	0.197754	-809.294268	-507839.44
5 $Mn_2(HNCHNH)_4$	0	1	-805.63414	0.198927	-805.439589	-505420.60
		3	-805.655746	0.198334	-805.461775	-505434.51
		5	-805.679648	0.197346	-805.486643	-505450.12
6 $Mn_2(HNCHNH)_4.2H_2O$	0	1	-958.546946	0.246406	-958.787931	-601648.05
		3	-958.541209	0.245242	-958.781056	-601643.74
		5	-958.547706	0.244758	-958.787079	-601647.52

Table S3 Energy terms for dimanganese guanidinates $[Mn_2(HNC(NH_2)NH)_x]$ (x = 2, 3, 4)

No Complex	Q_C	M_s	$E_{Tot(uc)}$ (hartree)	$E_{ZP(us)}$ (hartree)	E_{Tot}(cr) (hartree)	E_{Tot}(cr) (kcal/mol)
7A $Mn_2[HNC(NH_2)NH]_2$ (lantern type)	0	1	-617.515934	0.132942	-617.379070	-387410.92
		3	-617.497733	0.133056	-617.367604	-387403.73
		5	-617.457707	0.133814	-617.326837	-387378.15
7B $Mn_2[HNC(NH_2)NH]_2$ (axially dicoordinated)	0	1	-617.492475	0.129776	-617.365554	-387402.44
		3	-617.443529	0.130081	-617.316309	-387371.54
		5	-617.375998	0.130765	-617.316309	-387328.74
8 $Mn_2[HNC(NH_2)NH]_2.2H_2O$	0	1	-770.38158	0.181877	-770.559456	-483532.99
		3	-770.364788	0.181300	-770.542099	-483522.10
		5	-770.332309	0.182616	-770.510907	-483502.53
9 $Mn_2[HNC(NH_2)NH]_3$	0	2	-822.364689	0.197461	-822.171572	-515920.06
		4	-822.321651	0.198873	-822.127153	-515892.19
		6	-822.308032	0.199815	-822.112613	-516883.06
10 $Mn_2[HNC(NH_2)NH]_3.2H_2O$	0	2	-975.237028	0.248279	-975.479845	-612122.38
		4	-975.188206	0.247563	-975.430323	-612091.30
		6	-975.184391	0.248282	-975.427210	-612089.35
11 $Mn_2[HNC(NH_2)NH]_4$	0	1	-1027.091554	0.265903	-1026.831501	-644346.01
		3	-1027.132832	0.265379	-1026.873291	-644372.23
		5	-1027.143056	0.265793	-1026.883110	-644378.40
12 $Mn_2[HNC(NH_2)NH]_4.2H_2O$	0	2	-1180.008112	0.315992	-1180.317152	-740659.63
		4	-1180.978361	0.316800	-1180.288191	-740641.46
		6	-1180.011995	0.315416	-1180.320472	-740661.72

Table S4 Energy terms for dimanganese formates $[Mn_2(OCHO)_x]$ (x = 2, 3, 4)

No Complex	Q_C	M_s	$E_{Tot(uc)}$ (hartree)	$E_{ZP(us)}$ (hartree)	$E_{Tot}(cr)$ (hartree)	$E_{Tot}(cr)$ (kcal/mol)
13A $Mn_2(OCHO)_2$	0	1	-586.288356	0.048977	-586.240256	-367871.16
(lantern type)		3	-586.263785	0.049671	-586.215207	-367855.32
		5	-586.236341	0.050433	-586.187017	-367837.63
13B $Mn_2(OCHO)_2$	0	1	-586.064004	0.048056	-586.665061	-367761.10
(axially dicoordinated)		3	-586.099604	0.048900	-586.100679	-367783.45
		5	-586.099687	0.047533	-586.100732	-367783.48
14 $Mn_2(OCHO)_2.2H_2O$	0	1	-739.174991	0.097979	-739.270814	-463899.09
		3	-739.115481	0.100019	-739.213299	-463862.99
		5	-739.124001	0.099258	-739.221075	-463867.88
15 $Mn_2(OCHO)_3$	0	2	-775.545303	0.072489	-775.474410	-486617.17
		4	-775.455501	0.075326	-775.381832	-486559.08
		6	-775.489919	0.072989	-775.418536	-486582.11
16 $Mn_2(OCHO)_3.2H_2O$	0	2	-928.435596	0.121915	-928.554829	-582676.51
		4	-928.343897	0.124195	-928.465359	-582620.37
		6	-928.365723	0.122932	-928.485950	-582633.29
17 $Mn_2(OCHO)_4$	0	1	-964.686088	0.101790	-964.586537	-605286.73
		3	-964.703098	0.101954	-964.603387	-605297.30
		5	-964.725658	0.100944	-964.626935	-605312.08
18 $Mn_2(OCHO)_4.2H_2O$	0	1	-1117.615899	0.150058	-1117.762656	-701406.12
		3	-1117.565797	0.152469	-1117.714912	-701376.16
		5	-1117.613807	0.150023	-1117.760529	-701404.79

5. Cartesian Coordinates for All Optimized Structures

Cartesian Coordinates, Electronic Total Energies and Zero-point Energies for all the complexes in the three lowest-lying spin states

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M1A. $[Mn_2(HN\text{-}SiH_2\text{-}NH)_2]^{2-}$ (Ms=1) (*ipso* coordinated)

Mn	-1.40194600	-0.00040300	-0.00034900
Mn	1.40192900	0.00014300	-0.00019400
N	3.03586300	0.88322900	0.92927000
N	-3.03598200	-0.88303900	0.92940900
N	-3.03618100	0.88287400	-0.92958100
N	3.03624500	-0.88312100	-0.92910300
Si	4.16483100	0.00004400	0.00030200
Si	-4.16479600	0.00031700	0.00040700
H	5.15912100	0.87101300	-0.77891700
H	-5.15956700	-0.87059500	-0.77825500
H	5.15893400	-0.87080000	0.77988500
H	-5.15835700	0.87179100	0.77996600
H	-3.22092100	1.77164800	-1.37295900
H	-3.22110900	-1.77127800	1.37367400
H	3.22133600	-1.77124500	-1.37360300
H	3.22086400	1.77130000	1.37390300

Zero-point correction= 0.091104 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1010.661202

$[Mn_2(HN\text{-}SiH_2\text{-}NH)_2]^{2-}$ (Ms=3)

Mn	0.00010600	0.89336600	0.00012800
Mn	-0.00010600	-0.89336600	0.00012800
N	0.58784200	-2.36642700	1.19434600
N	-0.58784200	2.36642700	1.19434600
N	0.58784200	2.36620500	-1.19432600
N	-0.58784200	-2.36620500	-1.19432600
Si	0.00016800	-3.45830200	-0.00013400
Si	-0.00016800	3.45830200	-0.00013400
H	1.07228200	-4.42843800	-0.49107600
H	-1.07228200	4.42843800	-0.49107600
H	-1.07179400	-4.42853500	0.49083700
H	1.07179400	4.42853500	0.49083700
H	1.51760600	2.45788900	-1.58862500
H	-1.51832400	2.45615700	1.58739700
H	-1.51760600	-2.45788900	-1.58862500
H	1.51832400	-2.45615700	1.58739700

Zero-point correction= 0.093164 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1010.537035

$[Mn_2(HN\text{-}SiH_2\text{-}NH)_2]^{2-}$ (Ms=5)

Mn	-0.24128500	0.93134100	-0.07637100
Mn	0.24128500	-0.93134100	-0.07637100
N	-0.37395500	-2.39937400	-1.28213500
N	0.37395500	2.39937400	-1.28213500
N	0.24128500	2.28433700	1.31637800
N	-0.24128500	-2.28433700	1.31637800
Si	-1.04377000	-3.19098800	0.09231400
Si	1.04377000	3.19098800	0.09231400
H	-2.56770200	-3.24387100	0.17323500
H	2.56770200	3.24387100	0.17323500
H	-0.72384200	-4.68311000	0.13924900

H	0.72384200	4.68311000	0.13924900
H	0.69656300	2.08228500	2.19671300
H	0.90888500	2.28008500	-2.13202800
H	-0.69656300	-2.08228500	2.19671300
H	-0.90888500	-2.28008500	-2.13202800

Zero-point correction= 0.092260 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1010.552678

M1B. $[Mn_2(HN\text{-}SiH_2\text{-}NH)_2]^{2-}$ (Ms=1) (digonal type)

N	1.93101600	1.39672900	0.00202500
N	1.93588900	-1.39557100	0.00081100
H	3.89895000	0.00610800	-1.16901600
H	2.41360500	2.28911200	-0.00417600
H	2.42134500	-2.28632900	0.00252500
N	-1.93105600	-1.39678500	-0.00089200
N	-1.93588200	1.39550600	-0.00142600
H	-3.90264200	-0.00200500	-1.16488500
H	-2.41355100	-2.28915400	0.01093700
H	-2.42136300	2.28621100	-0.01075000
Mn	0.00249600	-1.51370400	-0.00131300
Mn	-0.00248500	1.51378800	0.00048300
Si	-2.92244300	-0.00256500	0.00103300
Si	2.92243800	0.00248800	0.00001400
H	-3.89786800	-0.00638500	1.17098100
H	3.90156200	0.00225400	1.16684400

Zero-point correction= 0.092462 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1010.688915

M2A. $[Mn_2(HN\text{-}SiH_2\text{-}NH)_2]^{-}$ (Ms=2) (*ipso* coordinated)

Mn	0.01663700	0.84351100	0.08040000
Mn	-0.01663700	-0.84351100	0.08040000
N	-1.09357600	-2.25910400	-0.63462200
N	1.09357600	2.25910400	-0.63462200
N	-1.09357600	2.27756900	0.67538500
N	1.09357600	-2.27756900	0.67538500
Si	0.07474700	-3.42054000	-0.11955000
Si	-0.07474700	3.42054000	-0.11955000
H	-0.45927400	-4.50123400	0.78489200
H	0.45927400	4.50123400	0.78489200
H	0.72439300	-4.19535700	-1.23884200
H	-0.72439300	4.19535700	-1.23884200
H	-1.79219300	-2.37146000	-1.35154100
H	1.94683900	-2.44130800	1.18384900
H	1.79219300	2.37146000	-1.35154100
H	-1.94683900	2.44130800	1.18384900

Zero-point correction= 0.094865 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1010.635418

$[Mn_2(HN\text{-}SiH_2\text{-}NH)_2]^{-}$ (Ms=4)

Mn	0.00008300	0.90828700	0.00048000
Mn	-0.00008300	-0.90828700	0.00048000
N	-1.27624300	-2.29792800	0.29387400
N	1.27624300	2.29792800	0.29387400
N	-1.27624300	2.29701300	-0.29450600
N	1.27624300	-2.29701300	-0.29450600
Si	0.00044600	-3.43813600	-0.00054800
Si	-0.00044600	3.43813600	-0.00054800
H	0.23864000	-4.36089200	1.16221900
H	-0.23864000	4.36089200	1.16221900
H	-0.23743600	-4.36022600	-1.16388300
H	0.23743600	4.36022600	-1.16388300
H	-1.99949600	-2.43344900	0.98663300
H	2.00184100	-2.43193300	-0.98487400

H	1.99949600	2.43344900	0.98663300
H	-2.00184100	2.43193300	-0.98487400

Zero-point correction= 0.095369 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1010.644421

$[Mn_2(HN\text{-}SiH_2\text{-}NH)_2]^-$ (Ms=6)

Mn	-0.10196700	1.12041500	0.68461400
Mn	0.10196700	-1.12041500	0.68461400
N	-0.10196700	-1.88678000	-1.03669600
N	0.10196700	1.88678000	-1.03669600
N	-1.62502400	2.30751400	0.83040300
N	1.62502400	-2.30751400	0.83040300
Si	1.44533100	-2.65664700	-0.86226800
Si	-1.44533100	2.65664700	-0.86226800
H	1.39672600	-4.12490800	-1.16762800
H	-1.39672600	4.12490800	-1.16762800
H	2.54025700	-2.13123100	-1.75217900
H	-2.54025700	2.13123100	-1.75217900
H	-0.35465600	-1.32413000	-1.83949600
H	2.51459400	-1.94848200	1.15975300
H	0.35465600	1.32413000	-1.83949600
H	-2.51459400	1.94848200	1.15975300

Zero-point correction= 0.095392 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1010.660499

M2B. $[Mn_2(HN\text{-}SiH_2\text{-}NH)_2]^-$ (Ms=2) (digonal type)

N	-1.91943000	-1.28906000	0.00087300
N	-1.91314800	1.49439800	-0.00134100
H	-3.88549300	0.10788200	-1.17243100
H	-2.41023500	-2.17949600	0.00223200
H	-2.37994400	2.39270100	-0.00213900
N	1.90736100	1.49594300	0.00103500
N	1.92530200	-1.28821800	-0.00125000
H	3.88481300	0.11910500	-1.17253400
H	2.37175700	2.39556900	0.00244700
H	2.41944000	-2.17666300	-0.00300700
Mn	-0.00278500	1.19101000	-0.00015400
Mn	0.00304900	-1.45556000	-0.00000300
Si	2.92862400	0.10405500	0.00024800
Si	-2.92914200	0.09851800	0.00023100
H	3.88410300	0.11765000	1.17363400
H	-3.88438300	0.10952700	1.17379700

Zero-point correction= 0.093169 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1010.784766

$[Mn_2(HN\text{-}SiH_2\text{-}NH)_2]^-$ (Ms=4)

N	-1.91610200	-1.39807200	0.00010600
N	-1.86513300	1.34650600	-0.00064000
H	-3.88281000	0.01795900	-1.17375100
H	-2.35554100	-2.31007000	0.00060300
H	-2.30748500	2.26343500	-0.00020700
N	1.86407500	1.34645900	0.00031300
N	1.91726500	-1.39786200	-0.00040700
H	3.88257800	0.02039200	-1.17386100
H	2.30592700	2.26366200	0.00079600
H	2.35707700	-2.30964700	-0.00129300
Mn	-0.00052200	1.20080600	-0.00024700
Mn	0.00050400	-1.15269600	0.00014300
Si	2.92856400	-0.01616100	0.00019500
Si	-2.92858500	-0.01715600	0.00016300
H	3.88196900	0.01997100	1.17476200
H	-3.88171600	0.01876000	1.17494300

Zero-point correction= 0.094751 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1010.728521

$[Mn_2(HN\text{-}SiH_2\text{-}NH)_2]^-$ (Ms=6)

N	-1.93964500	-1.44628300	-0.17429900
N	-1.86921900	1.33804800	0.18511600
H	-3.80792200	0.09149300	-1.23643700
H	-2.38066300	-2.23381500	-0.63429200
H	-2.28813400	2.08680500	0.73126400
N	1.89858300	1.32524300	-0.22071100
N	1.90242000	-1.45254500	0.16612300
H	3.86161500	-0.15210100	-1.17829300
H	2.36776200	2.12353800	-0.63715000
H	2.34961500	-2.26587100	0.57211700
Mn	0.02023800	1.38983100	0.01853100
Mn	-0.01985600	-1.25793300	0.02484700
Si	2.90025600	-0.06437100	-0.01407300
Si	-2.90105800	-0.02759500	-0.03388200
H	3.84079500	0.05332000	1.16345100
H	-3.88636600	-0.06452300	1.11267700

Zero-point correction= 0.094986 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1010.727515

M3A. $Mn_2(HN{=}CH\text{-}CH{=}CH\text{-}NH)_2$ (Ms=1) (*ipso* coordinated)

Mn	1.33049600	0.00161900	0.00423900
Mn	-1.33063000	0.00123100	0.00021000
N	-2.79854200	1.03917900	1.01033300
N	2.79451000	1.02018800	-1.02969900
N	2.79760200	-1.01523300	1.03377500
N	-2.79342000	-1.04605200	-1.00457200
H	-2.57956500	1.74704300	1.70296400
H	2.57127300	1.71838400	-1.73085000
H	2.57744200	-1.71095400	1.73805400
C	-4.10251300	-0.89553900	-0.86667800
C	-4.10662000	0.89338600	0.86056600
C	4.10351400	0.87315500	-0.88781400
C	4.10584000	-0.87487000	0.88058500
C	-4.74467900	0.00072000	-0.00664100
C	4.74501700	-0.00338600	-0.00670600
H	-4.76033400	-1.52464300	-1.47686000
H	-5.82870800	0.00203300	-0.01012800
H	-4.76801300	1.52139200	1.46818000
H	4.76602800	-1.49156100	1.50085500
H	5.82898200	-0.00671300	-0.01139300
H	4.76225100	1.48733800	-1.51219500
H	-2.57040100	-1.76094200	-1.68859700

Zero-point correction= 0.166769 (Hartree/Particle)
Sum of electronic and zero-point Energies= -661.428143

$Mn_2(HN{=}CH\text{-}CH{=}CH\text{-}NH)_2$ (Ms=3)

Mn	0.84852000	-0.00024400	0.00001100
Mn	-0.84848500	-0.00029900	-0.00007700
N	-2.04946500	-1.39680900	0.53876800
N	2.04885500	1.39675800	0.53894400
N	2.04943800	-1.39674300	-0.53893500
N	-2.04887000	1.39666700	-0.53902300
H	-1.83416700	-2.30651100	0.92624800
H	1.83312200	2.30645300	0.92619600
H	1.83415300	-2.30637700	-0.92657900
C	-3.36552200	1.16899600	-0.46268700
C	-3.36601300	-1.16841700	0.46273400
C	3.36549900	1.16899700	0.46278800
C	3.36599000	-1.16845000	-0.46259100
C	-3.98040200	0.00046600	0.00013800

C	3.98036600	0.00036000	0.00020000
H	-4.03315900	1.96836100	-0.79459100
H	-5.06515500	0.00075100	0.00031300
H	-4.03400800	-1.96745300	0.79471300
H	4.03399500	-1.96750300	-0.79450700
H	5.06511900	0.00055100	0.00028400
H	4.03315300	1.96836900	0.79464000
H	-1.83314300	2.30613400	-0.92681800

Zero-point correction= 0.167799 (Hartree/Particle)
Sum of electronic and zero-point Energies= -661.342811

$Mn_2(HN=CH-CH=CH-NH)_2$ (Ms=5)

Mn	-1.29560700	-0.04322600	-0.07084400
Mn	1.06627300	-0.02531400	-0.03540400
N	2.44579000	0.73317700	1.26981600
N	-2.35627900	-1.37327100	0.68426600
N	-2.33790800	1.35367700	-0.71987700
N	2.55909100	-0.72039900	-1.24759600
H	2.18588200	1.22404500	2.11817300
H	-2.14572200	-2.25982400	1.12582200
H	-2.11459100	2.22509800	-1.18468700
C	3.85824900	-0.58879400	-1.02102900
C	3.76120900	0.65519600	1.13155000
C	-3.67557400	-1.09363500	0.63134100
C	-3.66029200	1.16360500	-0.52968100
C	4.44748600	0.04560900	0.07687900
C	-4.26201400	0.05502700	0.08196300
H	4.55210600	-1.01205800	-1.75554600
H	5.53056300	0.06757300	0.11304000
H	4.38630300	1.10668400	1.90967400
H	-4.32881900	1.94891500	-0.88702500
H	-5.34529700	0.09149400	0.13849200
H	-4.35506500	-1.83369900	1.05779200
H	2.37874600	-1.21906600	-2.11191400

Zero-point correction= 0.163331 (Hartree/Particle)
Sum of electronic and zero-point Energies= -661.350661

M3B. $Mn_2(HN=CH-CH=CH-NH)_2$ (Ms=1) (digonal type)

N	-1.94768900	1.54615700	-0.33883700
N	-0.88191600	-1.82085100	1.33123500
N	0.97287600	-0.93945500	-1.53627500
N	1.66935000	1.58631000	0.24540400
Mn	-0.09564700	-0.63742000	0.02547800
Mn	-0.14076200	1.15157400	0.23791700
C	1.92641200	-1.36280500	-0.65702300
C	2.78734200	0.83625100	0.28036700
C	-2.53015100	0.47822300	-0.90379900
C	-1.80386800	-0.87754500	0.99921600
C	2.84080900	-0.52734900	0.03534900
C	-2.23124000	-0.80114300	-0.39160800
H	0.62241700	-1.72511800	-2.08091000
H	2.15975900	-2.43215800	-0.59596200
H	3.72795300	-1.03399100	0.41270900
H	3.71110400	1.32657000	0.59379800
H	1.88582200	2.56897400	0.38939900
H	-2.27256100	2.42976400	-0.71290900
H	-3.15668300	0.59687200	-1.79091300
H	-2.55049900	-1.69413100	-0.92380200
H	-2.17190300	-0.13354800	1.71392900
H	-0.66934100	-1.83601000	2.32407800

Zero-point correction= 0.165993 (Hartree/Particle)
Sum of electronic and zero-point Energies= -661.310648

$Mn_2(HN=CH-CH=CH-NH)_2$ (Ms=3)

N	-2.84856300	-1.03921400	0.09882900
N	1.72319000	-2.00919200	-0.79642200
N	2.64240200	0.88043800	-0.28502500
N	-1.26242900	2.37657800	-0.52920000
Mn	1.08709100	-0.34524800	0.02687000
Mn	-1.55711300	0.46396100	-0.04194500
C	2.01141100	1.23384700	0.86879900
C	0.06048500	2.10795000	-0.47018300
C	-1.66857400	-1.53480100	0.58024500
C	0.69709900	-2.28980600	0.05867400
C	0.66204800	1.70366000	0.75263200
C	-0.57116600	-1.73691300	-0.33233200
H	3.57547600	0.52699000	-0.08796700
H	2.46816300	1.17587200	1.86098000
H	0.08816400	1.86612800	1.66619200
H	0.71890700	2.19684200	-1.34140400
H	-1.53806100	2.73393200	-1.43842300
H	-3.56353100	-1.00205300	0.81988000
H	-1.53301900	-1.83102000	1.62767400
H	-0.80106200	-1.72000800	-1.40119700
H	0.80314800	-2.87105100	0.98248400
H	2.60235000	-2.40734900	-0.47563700

Zero-point correction= 0.162483 (Hartree/Particle)
Sum of electronic and zero-point Energies= -661.379553

$Mn_2(HN{=}CH{-}CH{=}CH{-}NH)_2$ (Ms=5)

N	-2.89506400	-0.79132100	0.29647400
N	1.51009100	-2.04131400	-0.88788700
N	2.68551700	0.59108900	-0.19331500
N	-1.00104100	2.44604600	-0.58597600
Mn	0.97503700	-0.37958300	0.03611200
Mn	-1.44478500	0.57831600	-0.11593400
C	2.08140500	1.01716600	0.94896700
C	0.28488700	2.00617100	-0.47872000
C	-1.77880000	-1.46251800	0.63200600
C	0.49769000	-2.28768700	-0.01979200
C	0.81100600	1.64916500	0.80158500
C	-0.76394500	-1.68131100	-0.35719500
H	3.54001200	0.08372200	0.02228000
H	2.50032000	0.88310900	1.95025100
H	0.24179400	1.92925600	1.68617800
H	0.98016700	2.01357300	-1.32281700
H	-1.19987200	2.76762500	-1.52916300
H	-3.53796700	-0.69661800	1.07654600
H	-1.58435200	-1.81656200	1.65355000
H	-1.05662800	-1.63340600	-1.40894600
H	0.59427800	-2.89157900	0.89231600
H	2.37595500	-2.48487700	-0.59083900

Zero-point correction= 0.165364 (Hartree/Particle)
Sum of electronic and zero-point Energies= -661.361064

M4. $Mn_2(CO)_{10}$ (Ms=1)

Mn	-1.45060900	-0.00026200	0.00004100
Mn	1.45043600	0.00016000	0.00005600
C	1.31052100	1.65916800	-0.80463600
C	1.30931700	-0.80537200	-1.65844700
C	3.24101000	0.00016500	-0.00079900
C	1.31112600	-1.65852400	0.80535700
C	1.31051800	0.80513600	1.65878800
C	-1.31040000	0.60021600	-1.74290700
C	-1.31187800	1.74311000	0.59961100
C	-3.24165400	-0.00030300	-0.00070800
C	-1.31189200	-0.60004300	1.74350400
C	-1.31118900	-1.74359600	-0.59964700

O	-1.24992700	2.83328500	0.97391000
O	-1.25049100	-0.97439000	2.83365900
O	1.25031100	2.69705900	-1.30631300
O	1.25072900	1.30745900	2.69638700
O	1.25169900	-2.69634100	1.30724800
O	4.39817800	-0.00038200	-0.00119500
O	1.24785700	-1.30826000	-2.69568700
O	-1.24709200	0.97540000	-2.83267600
O	-1.24854400	-2.83351500	-0.97456500
O	-4.39878800	0.00003600	-0.00116000

Zero-point correction= 0.087409 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1341.300245

$Mn_2(CO)_{10}$ (Ms=3)

Mn	-1.93091400	-0.00037100	0.00026000
Mn	1.93463400	0.00041300	-0.00030700
C	1.68723100	0.75882300	-1.66900400
C	1.68805600	-1.66863400	-0.75812300
C	3.74498600	0.00059600	-0.00205800
C	1.69099400	-0.75844500	1.66868500
C	1.68922200	1.66912300	0.75878900
C	-1.68843800	-0.67510400	-1.70551700
C	-1.68953900	1.70540800	-0.67470300
C	-3.74095700	-0.00185400	0.00008900
C	-1.68992300	0.67558200	1.70580800
C	-1.68651100	-1.70570600	0.67565900
O	-1.51099100	2.76750500	-1.09125700
O	-1.51193000	1.09314400	2.76759900
O	1.50215300	1.23152100	-2.70632300
O	1.50536600	2.70622000	1.23246000
O	1.50835600	-1.23183300	2.70613100
O	4.90181800	0.00071800	-0.00295900
O	1.50329100	-2.70634700	-1.23010200
O	-1.50948700	-1.09139000	-2.76764300
O	-1.50619400	-2.76727800	1.09277400
O	-4.89785000	-0.00223200	-0.00025300

Zero-point correction= 0.085097 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1341.243227

$Mn_2(CO)_{10}$ (Ms=5)

Mn	-1.51285700	-0.11879200	0.02262200
Mn	1.16430700	0.17450700	-0.03322100
C	1.55157600	-1.35023100	1.41879300
C	1.25645500	1.65922900	1.51853200
C	3.93545900	0.21372000	-0.04652600
C	1.17677000	1.75222300	-1.48855100
C	1.48544700	-1.25967800	-1.58904700
C	-1.24259500	-0.14531200	1.84002900
C	-1.10231800	-1.90951800	-0.03892200
C	-3.30578400	-0.30561000	0.06625900
C	-1.34034200	-0.04781000	-1.80522800
C	-1.47723600	1.71665300	0.06952400
O	-0.86453700	-3.04421900	-0.08134000
O	-1.25508700	-0.00616000	-2.96152500
O	1.42321600	-2.20074100	2.18071400
O	1.33509600	-2.05860700	-2.40089200
O	0.87618000	2.56176900	-2.24486000
O	4.90983900	-0.36800200	0.05652500
O	0.99164200	2.41436500	2.34157500
O	-1.09510900	-0.16563800	2.99065700
O	-1.47829100	2.87654000	0.09950500
O	-4.45680500	-0.42616500	0.09411900

Zero-point correction= 0.076547 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1341.179808

M5. $Mn_2(CO)_{10}$ (Ms=1)

C	-2.79126300	0.98768200	-0.71158300
C	-2.78407200	-0.36006000	-1.15873400
C	-2.78914500	-1.20392700	-0.01233100
C	-2.79885900	-0.37584500	1.14229100
C	-2.80005800	0.97884300	0.71100400
C	2.78755100	0.76630600	-0.94383900
C	2.79474100	-0.65168200	-1.02595800
C	2.79937400	-1.16799500	0.29928400
C	2.79681200	-0.06743600	1.20024600
C	2.78993500	1.12761800	0.43308800
Mn	1.07384400	-0.00549200	-0.00262200
Mn	-1.07376300	0.00762900	0.00362300
C	-0.00032400	-0.38787800	1.55507500
C	0.00276200	1.53791600	-0.43725000
C	-0.00341800	-1.15919400	-1.10021500
O	-0.03191500	-2.02710000	-1.90554800
O	0.02291400	2.67874700	-0.75545500
O	0.00498100	-0.68073400	2.70261800
H	2.73857600	-1.23926800	-1.93267200
H	2.74165500	-2.21316200	0.57346300
H	2.71926500	1.45534900	-1.77549200
H	2.72220700	2.13610100	0.81987900
H	2.74199800	-0.13378600	2.27869700
H	-2.72061400	-2.28386200	-0.02419500
H	-2.74680300	-0.71377000	2.16881700
H	-2.71438900	-0.69374900	-2.18578000
H	-2.73126900	1.86867600	-1.33664700
H	-2.74471200	1.85065600	1.34952200

Zero-point correction= 0.196190 (Hartree/Particle)
Sum of electronic and zero-point Energies= -934.858428

$Mn_2(CO)_{10}$ (Ms=3)

C	-2.89736900	0.12247300	-1.15527700
C	-2.63690700	-1.20093700	-0.70618300
C	-2.66436200	-1.18517900	0.71448800
C	-2.94432000	0.14020800	1.13935800
C	-3.09037700	0.95771900	-0.01910300
C	2.93662100	0.27396300	-1.14126300
C	3.04048700	-1.03562800	-0.60238600
C	2.94631000	-0.91700200	0.81847700
C	2.86903600	0.47513400	1.13834300
C	2.85057300	1.20882300	-0.06392400
Mn	1.15431000	-0.18945200	-0.04669600
Mn	-1.11483400	0.13973600	0.03491600
C	-0.34217300	1.20935700	1.22830900
C	-0.30237500	0.99982100	-1.31046700
C	0.19907500	-1.70358500	0.07255900
O	-0.11151600	-2.84206000	0.14635500
O	-0.03743900	1.65222600	-2.25449500
O	0.00415300	1.97790200	2.04540000
H	3.11130600	-1.95853600	-1.16106200
H	2.97155800	-1.73335800	1.52771000
H	2.88674700	0.52703900	-2.19344300
H	2.72616100	2.27971100	-0.16097600
H	2.73174400	0.88669000	2.13061700
H	-2.43931900	-2.02717400	1.35583500
H	-2.99950500	0.47949000	2.16520600
H	-2.40913900	-2.05776300	-1.32534800
H	-2.90621000	0.45064400	-2.18645700
H	-3.28713800	2.02061800	-0.03324100

Zero-point correction= 0.194444 (Hartree/Particle)
Sum of electronic and zero-point Energies= -934.832167

$Mn_2(CO)_{10}$ (Ms=5)

C	-3.02761200	0.07335200	-1.18214200
C	-2.73608700	-1.23920700	-0.73797400
C	-2.76244400	-1.23714000	0.68913500
C	-3.07627900	0.07859300	1.11504300
C	-3.22877500	0.90036000	-0.03746300
C	3.22898500	-0.09349400	-1.20974500
C	3.19565400	-1.24621900	-0.37904400
C	3.21276600	-0.81054900	0.97399200
C	3.25091500	0.60648900	0.98113900
C	3.25320700	1.05409300	-0.36872100
Mn	1.27640400	-0.02471400	-0.03812000
Mn	-1.24221300	0.11662900	0.00767200
C	-0.51573900	1.00417400	1.36823000
C	-0.49869300	1.15215600	-1.23486300
C	-0.06158100	-1.46901200	-0.03977000
O	-0.14530700	-2.65430000	-0.05507900
O	-0.14709200	1.88914200	-2.07844300
O	-0.16523000	1.63325500	2.29392400
H	3.14694200	-2.27476600	-0.71304100
H	3.17916100	-1.45163100	1.84587300
H	3.22235300	-0.08680100	-2.29290200
H	3.27436000	2.08541200	-0.69862600
H	3.24846500	1.23962900	1.85986500
H	-2.54449000	-2.08432400	1.32462400
H	-3.14042300	0.41338800	2.14196100
H	-2.48929700	-2.08793900	-1.36066100
H	-3.05042500	0.40355800	-2.21216100
H	-3.44628900	1.95923300	-0.04383700

Zero-point correction= 0.193126 (Hartree/Particle)
Sum of electronic and zero-point Energies= -934.845284

1A. $Mn_2(HNCHNH)_2$ (Ms=1)

C	2.60072500	0.00030100	-0.00055400
N	1.98209700	-1.17087900	-0.00144900
N	1.98181800	1.17131100	0.00113500
H	3.69886700	0.00041300	-0.00121900
H	2.64317800	-1.93762300	-0.00277700
H	2.64276900	1.93817700	0.00129800
C	-2.60070000	-0.00035600	-0.00049800
N	-1.98217600	1.17092500	-0.00148500
N	-1.98175200	-1.17131400	0.00101300
H	-3.69884100	-0.00052600	-0.00102500
H	-2.64348700	1.93748200	-0.00309900
H	-2.64266700	-1.93821000	0.00184900
Mn	-0.00028400	1.41966100	0.00035000
Mn	0.00028900	-1.41964900	0.00032200

Zero-point correction= 0.098920 (Hartree/Particle)
Sum of electronic and zero-point Energies= -506.684037

$Mn_2(HNCHNH)_2$ (Ms=3)

C	2.63459700	-0.00778300	-0.00111100
N	1.98033600	-1.16795100	-0.02171900
N	1.97820900	1.13751200	0.02787600
H	3.73295600	-0.01386600	-0.01213800
H	2.60164300	-1.96582900	-0.04992000
H	2.60412100	1.93484600	0.03749200
C	-2.63458300	-0.00794200	0.00070200
N	-1.97820400	1.13744900	-0.02818200
N	-1.98033200	-1.16804000	0.02126300
H	-3.73295200	-0.01383900	0.01166400
H	-2.60426200	1.93467800	-0.03720200

H	-2.60155800	-1.96598800	0.04903500
Mn	-0.00009100	1.12119200	0.00011000
Mn	0.00008700	-1.09672900	0.00024400

Zero-point correction= 0.099614 (Hartree/Particle)
Sum of electronic and zero-point Energies= -506.652103

$Mn_2(HNCHNH)_2$ (Ms=5)

C	-2.65086800	-0.00001400	0.00034500
N	-1.98819900	1.14571700	0.00015000
N	-1.98817800	-1.14573500	0.00006700
H	-3.75014700	-0.00002600	0.00064000
H	-2.58280400	1.96259800	0.00026100
H	-2.58277000	-1.96262600	0.00021000
C	2.65086700	0.00000500	0.00020400
N	1.98819200	-1.14572600	0.00030600
N	1.98817300	1.14572500	0.00022700
H	3.75014500	0.00001600	0.00011700
H	2.58279400	-1.96261100	0.00029500
H	2.58276100	1.96262100	0.00010100
Mn	0.00000900	-0.95310100	-0.00020900
Mn	-0.00000500	0.95310900	-0.00019800

Zero-point correction= 0.099863 (Hartree/Particle)
Sum of electronic and zero-point Energies= -506.623120

1B. $Mn_2(HNCHNH)_2$ (Ms=1)

Mn	0.72407200	-0.47984300	-0.45393600
Mn	-0.72407200	0.47984300	-0.45393600
N	-0.72407200	2.28663900	-0.22308200
N	0.72407200	-2.28663900	-0.22308200
N	2.17218900	-0.76465400	0.65093700
N	-2.17218900	0.76465400	0.65093700
H	-1.48996500	2.46866500	1.77782900
H	1.48996500	-2.46866500	1.77782900
H	-2.66239200	2.84095000	0.47734000
H	2.66239200	-2.84095000	0.47734000
C	-1.81822900	2.18932300	0.76106300
C	1.81822900	-2.18932300	0.76106300
H	-0.01378300	2.96971700	0.01234000
H	-2.47699700	0.34201900	1.51954400
H	0.01378300	-2.96971700	0.01234000
H	2.47699700	-0.34201900	1.51954400

Zero-point correction= 0.118499 (Hartree/Particle)
Sum of electronic and zero-point Energies= -507.646248

$Mn_2(HNCHNH)_3$ (Ms=3)

Mn	0.46594100	-0.85568700	-0.76407000
Mn	-0.46594100	0.85568700	-0.76407000
N	0.46594100	2.06029000	0.21293500
N	-0.46594100	-2.06029000	0.21293500
N	1.60792100	-1.14508700	0.65063500
N	-1.60792100	1.14508700	0.65063500
H	-0.98896200	3.03509700	1.42898300
H	0.98896200	-3.03509700	1.42898300
H	-0.20369600	1.63372300	2.21619400
H	0.20369600	-1.63372300	2.21619400
C	-0.58093600	2.02861300	1.25802400
C	0.58093600	-2.02861300	1.25802400
H	1.40734600	2.00061400	0.58906400
H	-1.79789000	0.36059900	1.27437600
H	-1.40734600	-2.00061400	0.58906400
H	1.79789000	-0.36059900	1.27437600

Zero-point correction= 0.121880 (Hartree/Particle)

Sum of electronic and zero-point Energies= -507.645652

$Mn_2(HNCHNH)_4$ (Ms=5)

Mn	0.96864300	-0.44018200	-0.70108500
Mn	-0.96864300	0.44018200	-0.70108500
N	-0.96864300	2.19208500	-0.17321100
N	0.96864300	-2.19208500	-0.17321100
N	1.69357400	-0.31480600	0.98680500
N	-1.69357400	0.31480600	0.98680500
H	-0.80775400	2.01907400	1.96658200
H	0.80775400	-2.01907400	1.96658200
H	-2.46207800	2.26823200	1.34323800
H	2.46207800	-2.26823200	1.34323800
C	-1.49953100	1.77598100	1.14574500
C	1.49953100	-1.77598100	1.14574500
H	-0.12183900	2.74280000	-0.05976900
H	-1.17367300	-0.18346200	1.70743800
H	0.12183900	-2.74280000	-0.05976900
H	1.17367300	0.18346200	1.70743800

Zero-point correction= 0.118404 (Hartree/Particle)
Sum of electronic and zero-point Energies= -507.684999

2. $Mn_2(HNCHNH)_2.H_2O$ (Ms=1)

N	-1.07518200	-2.03114600	0.12590000
N	1.23640700	-1.97838400	-0.11232800
N	-1.23670200	1.97831200	0.11458400
N	1.07481800	2.03103800	-0.12375600
C	0.09083300	-2.63659200	-0.00482000
H	0.11384400	-3.73587100	-0.02674300
C	-0.09106200	2.63652700	0.00763000
H	-0.11394500	3.73578400	0.03061200
H	1.84132200	2.68981900	-0.18807900
H	-2.01476600	2.61590100	0.23083200
H	2.01450800	-2.61606000	-0.22790000
H	-1.84152900	-2.69004800	0.19075300
O	3.64439200	0.16996700	0.26067500
H	4.10745300	-0.20525900	-0.49903900
O	-3.64278300	-0.16940300	-0.26546900
H	-4.11299700	0.21219700	0.48649800
H	3.91872300	-0.34838200	1.02713600
H	-3.91103500	0.34142800	-1.03912600
Mn	-1.34874100	-0.03812200	0.20621200
Mn	1.34840300	0.03802700	-0.20598300

Zero-point correction= 0.145296 (Hartree/Particle)
Sum of electronic and zero-point Energies= -689.498582

$Mn_2(HNCHNH)_2.H_2O$ (Ms=3)

N	-1.51185100	-1.93262900	-0.33208800
N	-2.20845300	0.27817100	-0.28361500
N	2.29015500	-0.72950000	-0.48432300
N	1.57480000	1.47439900	-0.37973600
C	-2.47315800	-1.01619900	-0.36940700
H	-3.51645700	-1.34940400	-0.46582900
C	2.52982000	0.57672700	-0.56738000
H	3.55315500	0.91419000	-0.78731500
H	1.93829700	2.41771700	-0.48515900
H	3.11613000	-1.27984900	-0.68267500
H	-3.05941400	0.82955500	-0.34803800
H	-1.87736100	-2.87332800	-0.40450600
O	-0.97620600	2.95650100	0.50377000
H	-1.70036900	2.73218000	1.10178500
O	0.64694100	-1.07532800	2.17133400
H	1.57277700	-0.80672400	2.24081600
H	-0.25168800	3.21542700	1.08668700

H	0.18120400	-0.21732300	1.94616600
Mn	0.38802100	-1.32221600	-0.12933000
Mn	-0.33500900	0.93709200	-0.21561800

Zero-point correction= 0.147044 (Hartree/Particle)
Sum of electronic and zero-point Energies= -659.485729

$Mn_2(HNCHNH)_2.H_2O$ (Ms=5)

N	-1.14447300	-1.98944300	0.06181900
N	1.14321000	-1.99010400	0.06124300
N	-1.13712000	2.00069100	0.09750900
N	1.13828700	2.00000900	0.09719600
C	-0.00079600	-2.65682100	0.13227400
H	-0.00109100	-3.75240000	0.22791700
C	0.00078600	2.67704800	0.09019200
H	0.00111400	3.77671800	0.08637300
H	1.97288500	2.57026900	0.07366800
H	-1.97138400	2.57144100	0.07408800
H	1.95025100	-2.59714300	0.13240700
H	-1.95178800	-2.59604600	0.13365800
O	3.39384200	0.05008700	-0.28101000
H	3.45598300	-0.49665500	-1.07258400
O	-3.39398400	0.05146100	-0.28170900
H	-3.83029400	-0.45420000	0.41201300
H	3.83002200	-0.45605400	0.41244700
H	-3.45430500	-0.49667300	-1.07246500
Mn	-0.98719700	0.01728500	0.03086400
Mn	0.98721600	0.01667200	0.03053800

Zero-point correction= 0.146454 (Hartree/Particle)
Sum of electronic and zero-point Energies= -659.439906

3. $Mn_2(HNCHNH)_3$ (Ms=2)

N	1.83680800	-0.76160300	-1.13842000
N	1.83685200	-0.76201200	1.13812900
N	0.00040900	1.78525700	-1.13687900
N	0.00041000	1.78493200	1.13740100
N	-1.83714000	-0.76099100	-1.13841600
N	-1.83717500	-0.76142400	1.13813500
C	2.47094700	-1.03346200	-0.00020400
H	3.47528000	-1.47289700	-0.00030600
C	0.00060500	2.46821500	0.00036400
H	0.00090700	3.56483300	0.00050800
C	-2.47133600	-1.03272300	-0.00019900
H	-3.47577100	-1.47192300	-0.00030300
H	2.37959800	-0.96980600	1.96700600
H	2.37951300	-0.96910900	-1.96739700
H	0.00059100	2.36193800	1.96885200
H	0.00057300	2.36248900	-1.96817200
H	-2.37995300	-0.96915800	1.96700500
H	-2.37989000	-0.96839300	-1.96738800
Mn	-0.00006400	-0.15116800	0.99892300
Mn	-0.00006700	-0.15080200	-0.99889200

Zero-point correction= 0.148369 (Hartree/Particle)
Sum of electronic and zero-point Energies= -656.020207

$Mn_2(HNCHNH)_3$ (Ms=4)

N	1.84703100	-0.79554500	-1.13815400
N	1.84703200	-0.79535100	1.13826300
N	0.00005700	1.83483400	-1.13640100
N	0.00006000	1.83497200	1.13616400
N	-1.84705800	-0.79547500	-1.13816400
N	-1.84710000	-0.79524400	1.13825200
C	2.45773000	-1.10118900	0.00008100
H	3.44074000	-1.58942200	0.00012200

C	0.00009200	2.52001800	-0.00015900
H	0.00014500	3.61781100	-0.00022100
C	-2.45779300	-1.10107100	0.00006300
H	-3.44082600	-1.58925800	0.00009300
H	2.37119700	-1.05169000	1.96471700
H	2.37119700	-1.05202600	-1.96456300
H	0.00010100	2.41071400	1.96798600
H	0.00008400	2.41048500	-1.96828600
H	-2.37129700	-1.05153800	1.96469900
H	-2.37121600	-1.05194600	-1.96458200
Mn	-0.00001500	-0.12747200	0.96619200
Mn	-0.00000300	-0.12760900	-0.96617500

Zero-point correction= 0.147958 (Hartree/Particle)
Sum of electronic and zero-point Energies= -656.040233

$Mn_2(HNCHNH)_3$ (Ms=6)

N	1.90393700	-0.81933600	-1.14527300
N	1.90398800	-0.81973500	1.14502800
N	0.00061400	1.82099700	-1.14983200
N	0.00063300	1.82072500	1.15032800
N	-1.90441700	-0.81851900	-1.14528700
N	-1.90439400	-0.81888000	1.14508900
C	2.56141800	-0.91629400	-0.00015100
H	3.64861600	-1.08005100	-0.00019900
C	0.00052300	2.47451500	0.00032600
H	0.00040300	3.57638500	0.00045100
C	-2.56177400	-0.91562900	-0.00010300
H	-3.64894000	-1.07964400	-0.00011100
H	2.51147100	-0.87353800	1.95354400
H	2.51137700	-0.87289900	-1.95383700
H	0.00040700	2.42711000	1.95970700
H	0.00039300	2.42757100	-1.95906800
H	-2.51190600	-0.87310900	1.95355100
H	-2.51194400	-0.87255600	-1.95375000
Mn	-0.00005100	-0.18397900	1.04335600
Mn	-0.00008500	-0.18368400	-1.04339900

Zero-point correction= 0.149046 (Hartree/Particle)
Sum of electronic and zero-point Energies= -656.061904

4. $Mn_2(HNCHNH)_3.2H_2O$ (Ms=2)

C	0.49513100	-1.30383400	-2.19217900
C	-1.08106100	2.67266400	-0.11463600
C	0.52249800	-1.04961700	2.31828200
N	-0.73417300	-1.37530600	-1.69484100
N	0.22975300	2.52743300	-0.11370600
N	-0.70351500	-1.18938800	1.82747100
H	0.76947600	-1.56612200	3.25797400
H	-1.26078200	-1.80687900	2.40517200
H	-1.29500000	-2.05094600	-2.19942300
H	0.74231800	-1.92690600	-3.06465900
H	-1.49889800	3.68947800	-0.15850000
H	0.70517000	3.42049500	-0.15598100
Mn	-1.26651500	-0.33315500	0.02044800
Mn	1.20110700	0.72567000	-0.04602700
O	4.10252500	-0.69713700	0.00797700
H	3.27384300	-1.19160800	0.06454000
O	-3.49779400	-1.16717100	0.04683400
H	-4.05846100	-0.92968600	0.79242200
H	3.79154800	0.22276400	-0.03019500
H	-4.02833500	-1.00900400	-0.74083700
N	1.43162200	-0.52447300	-1.68530100
N	-1.92297900	1.64587500	-0.06552400
N	1.45586400	-0.32628800	1.72893600
H	2.30321400	-0.60399500	-2.19693400
H	2.32174800	-0.33271500	2.25591900

H	-2.88390000	1.96645800	-0.07656300

Zero-point correction= 0.193933 (Hartree/Particle)
Sum of electronic and zero-point Energies= -808.943433

$Mn_2(HNCHNH)_3.2H_2O$ (Ms=4)

C	0.21999300	-2.47311000	-1.03716100
C	-0.43555600	2.54034000	-1.03775600
C	0.12807200	0.07775000	2.57275000
N	-0.95833200	-2.03720300	-0.61585600
N	0.80169500	2.06839800	-1.06722500
N	-1.04052600	-0.11169000	1.99473100
H	0.18088200	0.12067800	3.67208200
H	-1.79732900	-0.21237400	2.66050500
H	-1.63965600	-2.79079600	-0.61046600
H	0.30642300	-3.50890400	-1.40243500
H	-0.61830900	3.56944900	-1.38492100
H	1.45148600	2.74193400	-1.45234400
Mn	-1.19030400	-0.10882400	-0.02782900
Mn	1.20166200	0.22103700	-0.24100100
O	3.63446200	-0.14538900	-0.10709600
H	3.43453000	-0.93670300	0.40985700
O	-3.47100400	-0.42975100	-0.10206100
H	-3.87263700	0.30334100	-0.57965900
H	4.10425900	0.43748000	0.49753500
H	-3.65888000	-1.20855300	-0.63625100
N	1.29861300	-1.70316800	-1.03096200
N	-1.46092500	1.81862200	-0.60557800
N	1.24914400	0.22107800	1.86921800
H	2.09113900	-2.16318100	-1.46376500
H	2.03407600	0.40631900	2.48321400
H	-2.31033400	2.37497300	-0.59665400

Zero-point correction= 0.196794 (Hartree/Particle)
Sum of electronic and zero-point Energies= -808.896006

$Mn_2(HNCHNH)_3.2H_2O$ (Ms=6)

C	-0.15465000	2.54733900	-0.82972100
C	0.61304500	-2.58190100	-0.55857300
C	0.19414800	0.20459500	2.64972200
N	0.97609600	2.15271700	-0.27822000
N	-0.54829800	-2.04679700	-0.93484000
N	1.32254100	0.29297000	1.96898700
H	0.23331000	0.28437300	3.74803100
H	2.13339600	0.43131500	2.56090400
H	1.60257000	2.91926000	-0.06261200
H	-0.31644800	3.61768700	-1.03260100
H	0.77496900	-3.66661200	-0.65836900
H	-1.19671900	-2.75279200	-1.26522800
Mn	1.27746200	0.17481000	0.00196500
Mn	-0.94801800	-0.16038800	-0.03965400
O	-3.33189100	-0.42723500	-0.12801900
H	-3.69302300	0.36734100	0.27909000
O	1.20716500	0.06662600	-2.15766600
H	0.76429400	-0.79494900	-2.24531000
H	-3.59406700	-1.15074200	0.45048800
H	0.47795600	0.69868600	-2.29843600
N	-1.08995800	1.65693100	-1.16490500
N	1.58227800	-1.81908700	-0.08956100
N	-0.97420800	0.02270100	2.05081000
H	-1.90133200	2.10518100	-1.57660600
H	-1.72792200	-0.02729300	2.72633400
H	2.41029800	-2.34337200	0.16754300

Zero-point correction= 0.197754 (Hartree/Particle)
Sum of electronic and zero-point Energies= -808.903111

5. $Mn_2(HNCHNH)_4$ (Ms=1)

N	0.72370800	-1.84221500	1.13925500
N	0.72365400	-1.84358500	-1.13764700
N	-0.72244200	1.84405400	1.13774100
N	-0.72490300	1.84170900	-1.13916600
N	1.84503100	0.72396300	1.13885800
N	1.84353500	0.72321800	-1.14098600
C	0.96769200	-2.46481000	0.00117200
H	1.36974100	-3.48674600	0.00178200
C	-0.96760500	2.46481500	-0.00109200
H	-1.36954300	3.48679700	-0.00172600
C	2.46371100	0.96698400	-0.00154900
H	3.48595900	1.36857500	-0.00235800
N	-1.84456500	-0.72511900	-1.13894800
N	-1.84399400	-0.72202700	1.14089500
C	-2.46374900	-0.96687100	0.00145900
H	-3.48605700	-1.36830500	0.00227100
H	-2.39394800	-0.94275100	-1.96031200
H	-0.94113900	2.38864000	-1.96278300
H	-0.93596400	2.39304400	1.96068100
H	-2.39330700	-0.93661000	1.96310900
H	2.39242000	0.93881700	-1.96322000
H	2.39469200	0.94084400	1.96023300
H	0.93826400	-2.39212500	-1.96060900
H	0.93923400	-2.38943100	1.96286600
Mn	0.00050200	0.00081800	1.06687600
Mn	-0.00053500	-0.00087600	-1.06687100

Zero-point correction= 0.198927 (Hartree/Particle)
Sum of electronic and zero-point Energies= -805.435213

$Mn_2(HNCHNH)_4$ (Ms=3)

N	1.44279500	1.35717200	1.14006400
N	1.44412200	1.35757800	-1.13845200
N	-1.44491800	-1.35678200	1.13863500
N	-1.44178400	-1.35814000	-1.13986100
N	-1.35818700	1.44397400	1.13821500
N	-1.35693500	1.44281000	-1.14027700
C	1.92935500	1.81425800	0.00117600
H	2.72964800	2.56623500	0.00177000
C	-1.92922800	-1.81433600	-0.00101600
H	-2.72952600	-2.56630600	-0.00169800
C	-1.81452900	1.92922600	-0.00154400
H	-2.56674500	2.72929000	-0.00238600
N	1.35898600	-1.44297600	-1.13837900
N	1.35583600	-1.44353000	1.14015100
C	1.81431200	-1.92913300	0.00140100
H	2.56627100	-2.72943400	0.00225900
H	1.76436200	-1.87171900	-1.96058400
H	-1.86949400	-1.76285400	-1.96293800
H	-1.87575200	-1.75969200	1.96095300
H	1.75816500	-1.87341000	1.96327400
H	-1.75999000	1.87179700	-1.96349900
H	-1.76291300	1.87308400	1.96054300
H	1.87411300	1.76127000	-1.96083700
H	1.87094400	1.76144600	1.96312100
Mn	-0.00098800	0.00018900	1.06496200
Mn	0.00107000	-0.00021000	-1.06499200

Zero-point correction= 0.198334 (Hartree/Particle)
Sum of electronic and zero-point Energies= -805.457412

$Mn_2(HNCHNH)_4$ (Ms=5)

N	1.45542500	1.39442900	1.14713800

N	1.45595100	1.39521500	-1.14605000
N	-1.45699200	-1.39413800	1.14608900
N	-1.45437000	-1.39549000	-1.14710000
N	-1.39504200	1.45621900	1.14594900
N	-1.39459200	1.45512800	-1.14723900
C	1.92516800	1.84405700	0.00080500
H	2.72066700	2.60397700	0.00126100
C	-1.92523600	-1.84396900	-0.00077800
H	-2.72085500	-2.60376300	-0.00125700
C	-1.84404300	1.92516100	-0.00095800
H	-2.60395500	2.72066700	-0.00150000
N	1.39615000	-1.45519100	-1.14597600
N	1.39352200	-1.45616600	1.14721200
C	1.84400000	-1.92522600	0.00093400
H	2.60381100	-2.72082800	0.00148400
H	1.81161300	-1.88775900	-1.95986700
H	-1.88632400	-1.81054300	-1.96153400
H	-1.89146200	-1.80753900	1.96002100
H	1.80652700	-1.89000300	1.96168900
H	-1.80849000	1.88811400	-1.96171400
H	-1.80980200	1.88944600	1.95985000
H	1.88954100	1.80950700	-1.95999800
H	1.88800300	1.80884400	1.96156500
Mn	-0.00065800	0.00007200	1.08399500
Mn	0.00069900	-0.00008500	-1.08400200

Zero-point correction= 0.197346 (Hartree/Particle)
Sum of electronic and zero-point Energies= -805.482302

6. $Mn_2(HNCHNH)_4.2H_2O$ (Ms=1)

N	-0.75799800	-1.59634000	1.51909600
N	1.52423400	-1.32821100	1.20455700
N	-1.31318700	1.57299100	-0.94790100
N	0.80660000	1.24377500	-1.82557700
N	-0.80322300	1.23676000	1.83093700
N	1.31661900	1.56788200	0.95424300
C	0.49228200	-1.93853400	1.76263200
H	0.68043300	-2.77371400	2.45397100
C	-0.34694200	1.87848900	-1.80223200
H	-0.51672200	2.70360900	-2.51215800
C	0.35093800	1.87038200	1.81029000
H	0.52169600	2.69195400	2.52409000
N	0.75461200	-1.59025300	-1.52538300
N	-1.52736900	-1.32192100	-1.20891000
C	-0.49603100	-1.93000600	-1.77053800
H	-0.68494300	-2.76128500	-2.46636500
H	1.42869000	-2.15797500	-2.02177300
H	1.39213100	1.52385800	-2.60358200
H	-2.03889800	2.28065600	-0.94143000
H	-2.40445000	-1.77476500	-1.44353700
H	2.04256500	2.27532600	0.95018500
H	-1.38808400	1.51342300	2.61066300
H	2.40101700	-1.78235100	1.43775300
H	-1.43284900	-2.16738500	2.01057600
O	3.70995900	0.13270700	-0.15562900
H	3.46556000	0.32203100	0.76132300
O	-3.71015500	0.13729800	0.15419700
H	-4.03425700	0.97304100	0.50365500
H	4.03081900	0.96915600	-0.50642300
H	-3.46387500	0.32647800	-0.76229900
Mn	-1.23152800	-0.04182100	0.33072300
Mn	1.23149700	-0.04205400	-0.33038500

Zero-point correction= 0.246406 (Hartree/Particle)
Sum of electronic and zero-point Energies= -958.300886

$Mn_2(HNCHNH)_4.2H_2O$ (Ms=3)

N	1.26125700	-1.21175700	1.59326900
N	-1.01048100	-1.55660200	1.47574300
N	0.97184800	1.33871600	-1.57829500
N	-1.28673200	1.49847200	-1.13374400
N	1.20096000	-1.57032400	-1.25585500
N	-1.09523600	-1.37746900	-1.35244300
C	0.17550300	-1.83613600	1.99720100
H	0.24169400	-2.60752200	2.77803200
C	-0.18647300	1.93052100	-1.74799400
H	-0.26560800	2.80487000	-2.41156200
C	0.02785800	-1.99670900	-1.68079400
H	-0.02908700	-2.88426100	-2.32811000
N	-1.12754500	1.26156600	1.68072100
N	1.09091900	1.66239400	1.23958500
C	-0.00442900	1.92900100	1.91419600
H	-0.00497800	2.71716200	2.68133300
H	-1.87483200	1.46380100	2.33044000
H	-2.01216100	2.20647000	-1.12055400
H	1.70704400	1.77217400	-2.12628500
H	1.86115000	2.28304200	1.45662700
H	-1.92491700	-1.87520800	-1.65333700
H	1.94435700	-2.20248300	-1.53168000
H	-1.76727900	-2.13668900	1.81094000
H	2.08486800	-1.49501900	2.11035700
O	-3.59853400	-0.23793100	-0.68555000
H	-4.22812100	0.44365300	-0.43314700
O	3.48387000	0.16335300	-0.64000000
H	3.10449300	-0.13519800	-1.47915200
H	-3.07136700	0.15652100	-1.39977500
H	3.89323200	-0.62458700	-0.26775900
Mn	1.18788600	0.06457800	0.00499200
Mn	-1.14192100	-0.05518300	0.17938800

Zero-point correction= 0.245242 (Hartree/Particle)
Sum of electronic and zero-point Energies= -958.295967

$Mn_2(HNCHNH)_4.2H_2O$ (Ms=5)

N	1.25326300	-1.12253800	1.63910400
N	-0.93384200	-1.69647700	1.27154100
N	0.96898800	1.34071600	-1.57388600
N	-1.28947900	1.50654800	-1.20121500
N	1.28650400	-1.50937300	-1.20081300
N	-0.97292000	-1.34462900	-1.56799000
C	0.19048300	-1.84697000	1.94047500
H	0.24665100	-2.58427300	2.75664500
C	-0.18366300	1.94199700	-1.78010000
H	-0.22905800	2.82116400	-2.44157500
C	0.17930500	-1.94620100	-1.77590800
H	0.22308700	-2.82675600	-2.43563900
N	-1.24915200	1.12665300	1.63933700
N	0.93703000	1.69961400	1.26489700
C	-0.18567400	1.85192900	1.93614600
H	-0.23988400	2.59147100	2.75042100
H	-2.02871200	1.26848200	2.26866200
H	-2.06661500	2.14423300	-1.32843000
H	1.74490700	1.80635200	-2.02963400
H	1.69313300	2.30295600	1.56151600
H	-1.75011400	-1.81177200	-2.02001000
H	2.06380900	-2.14648700	-1.32982800
H	-1.68920100	-2.29905400	1.57157700
H	2.03411600	-1.26244500	2.26727600
O	-3.51042400	-0.27613100	-0.33752800
H	-3.80882400	0.50988400	0.13234000
O	3.50873800	0.27472900	-0.34109100

H	3.22528600	-0.05810800	-1.20418200
H	-3.22356800	0.05631900	-1.19971900
H	3.80556600	-0.51104000	0.13022200
Mn	1.07895400	0.11186600	0.04164300
Mn	-1.07865600	-0.11177900	0.04471000

Zero-point correction= 0.244758 (Hartree/Particle)
Sum of electronic and zero-point Energies= -958.302948

7A. $Mn_2[HNC(NH)_2NH]_2$ (Ms=1)

C	-2.62410100	0.00000000	-0.00534100
C	2.62409700	-0.00000400	-0.00536100
N	-1.97719700	1.16574600	0.00284300
N	-1.97719400	-1.16575800	0.00359400
N	1.97719300	-1.16577300	0.00265700
N	1.97719100	1.16573100	0.00370400
H	2.61119100	1.95451700	-0.02943600
H	2.61127800	-1.95442800	-0.03186300
H	-2.61125600	-1.95448500	-0.02963900
H	-2.61121200	1.95446200	-0.03164400
N	4.01161500	0.00000000	-0.07919500
N	-4.01161400	0.00002800	-0.07922700
H	4.47054400	0.83744600	0.24408600
H	4.47054400	-0.83735800	0.24431600
H	-4.47052600	0.83743500	0.24418400
H	-4.47059200	-0.83737100	0.24410200
Mn	0.00001500	1.40521900	0.00454500
Mn	-0.00001200	-1.40521900	0.00463400

Zero-point correction= 0.139942 (Hartree/Particle)
Sum of electronic and zero-point Energies= -617.382992

$Mn_2[HNC(NH)_2NH]_2$ (Ms=3)

C	-2.65720200	-0.04177600	-0.00254800
C	2.65717800	-0.04171700	-0.00194200
N	-1.98656600	1.10363300	0.00391000
N	-2.00146000	-1.20966600	0.00687500
N	2.00177000	-1.20975200	0.00790400
N	1.98629400	1.10354400	0.00628600
H	2.59104400	1.91556900	-0.01230500
H	2.62024500	-2.00898500	-0.04449800
H	-2.61969700	-2.00913000	-0.04481300
H	-2.59161800	1.91545800	-0.01310900
N	4.04675100	-0.04102200	-0.07762200
N	-4.04688800	-0.04141600	-0.07620800
H	4.49641800	0.80687700	0.23259100
H	4.50073600	-0.86335300	0.28958100
H	-4.49627200	0.80643200	0.23455300
H	-4.49999400	-0.86371400	0.29213400
Mn	-0.00011200	1.22675000	-0.00017400
Mn	0.00011100	-1.11216800	-0.00003500

Zero-point correction= 0.133056 (Hartree/Particle)
Sum of electronic and zero-point Energies= -617.364677

$Mn_2[HNC(NH)_2NH]_2$ (Ms=5)

C	-2.66322400	-0.00001900	0.00219500
C	2.66323900	0.00002700	0.00232200
N	-1.97608200	1.13999400	-0.00923900
N	-1.97616900	-1.14004100	-0.00982300
N	1.97606200	-1.13998600	-0.00903700
N	1.97615500	1.14004200	-0.00939700
H	2.55311900	1.97065900	0.02742700
H	2.55295900	-1.97055300	0.03009700
H	-2.55313400	-1.97060300	0.02826400
H	-2.55300600	1.97057400	0.02900600

N	4.04858000	-0.00011200	0.08028000
N	-4.04856600	0.00000600	0.08058600
H	4.50638000	0.83762000	-0.24437800
H	4.50615600	-0.83775500	-0.24493000
H	-4.50624800	0.83776800	-0.24416100
H	-4.50635000	-0.83756200	-0.24454000
Mn	0.00000500	0.98459600	-0.00052300
Mn	0.00000100	-0.98457700	-0.00057600

Zero-point correction= 0.133814 (Hartree/Particle)
Sum of electronic and zero-point Energies= -617.323893

7B. $Mn_2[HNC(NH)_2NH]_2$ (Ms=1)

Mn	-1.33367100	-0.01048700	-0.00718100
Mn	1.33361600	-0.00730600	0.00682700
N	3.11838600	-0.92704800	-0.61567600
N	-3.11163900	0.61907600	-0.93322400
N	-3.11667500	-0.65652900	0.89961800
N	3.10986900	0.90607000	0.65961600
C	3.84576500	0.00644100	0.00254900
C	-3.84581200	0.00516900	-0.00219600
H	3.62319700	-1.61306100	-1.15754600
H	3.60746100	1.65373500	1.12053500
H	-3.61019300	1.16444900	-1.62100500
H	-3.61961700	-1.11373700	1.64599000
N	-5.22312800	0.09665600	0.05763800
N	5.22350400	0.07069600	-0.08036100
H	5.68970400	0.59557500	0.64327700
H	5.69677700	-0.78741600	-0.31721000
H	-5.69224500	0.33694600	-0.80175200
H	-5.69565500	-0.62378400	0.58118100

Zero-point correction= 0.129776 (Hartree/Particle)
Sum of electronic and zero-point Energies= -617.362699

$Mn_2[HNC(NH)_2NH]_3$ (Ms=3)

Mn	-1.33366700	0.62933600	-0.48269800
Mn	1.17896300	0.35477600	-0.30844700
N	2.72819300	-1.01144600	-0.53593300
N	-3.11527000	0.84189100	0.66459800
N	-2.43692000	-1.02973100	-0.35965500
N	2.93809800	0.76591600	0.79632500
C	3.52607000	-0.31152100	0.27670400
C	-3.40513300	-0.41092900	0.33002500
H	3.12469600	-1.82351200	-0.98468400
H	3.50480700	1.35131500	1.39229200
H	-3.85178300	1.35228600	1.13178200
H	-2.62437200	-1.95792900	-0.70738700
N	-4.62246900	-1.01905500	0.59475800
N	4.84807400	-0.64327800	0.50452700
H	5.26265400	-0.26617700	1.34259200
H	5.10258700	-1.60376000	0.33367300
H	-5.14444000	-0.62303700	1.36152800
H	-4.61010600	-2.02736600	0.61611300

Zero-point correction= 0.130081 (Hartree/Particle)
Sum of electronic and zero-point Energies= -617.313448

$Mn_2[HNC(NH)_2NH]_4$ (Ms=5)

Mn	-1.06812200	-0.89324900	0.10170500
Mn	0.95922500	-0.69103900	-0.15083400
N	2.92866500	-0.66134300	0.44266300
N	-2.83307900	-0.44566500	-0.77526100
N	-2.07101800	0.49047600	1.08431900
N	1.80468200	1.08008600	-0.34954200
C	3.00243500	0.58832000	-0.00637500

C	-2.93968100	0.57972600	0.06923800
H	3.79660200	-1.13466000	0.64732900
H	1.75915400	1.97888200	-0.80433800
H	-3.33073000	-0.37334600	-1.65140500
H	-1.92172200	1.31685700	1.64514600
N	-3.78361300	1.65410600	-0.11977300
N	4.18012000	1.29148500	-0.16428400
H	4.09511100	2.29568100	-0.19483500
H	4.95904100	0.97778200	0.39391200
H	-4.57869400	1.48817000	-0.71760700
H	-4.01316500	2.18554900	0.70599200

Zero-point correction= 0.130765 (Hartree/Particle)
Sum of electronic and zero-point Energies= -617.245233

8. $Mn_2[HNC(NH)_2NH]_2.2H_2O$ (Ms=1)

C	-2.61497200	-0.37403400	-0.08240300
C	2.69964400	-0.02983000	-0.11891900
N	-2.04460900	0.78370600	0.26977900
N	-1.89016000	-1.39868500	-0.51902100
N	2.10800800	-1.12933100	-0.57563600
N	1.98843100	0.98465400	0.38398300
H	2.58790800	1.70722300	0.76583500
H	2.77086300	-1.81450600	-0.91704900
H	-2.45879800	-2.19907100	-0.76792300
H	-2.71336700	1.40736500	0.71085100
N	4.09121100	0.03931000	-0.08643200
N	-3.99024500	-0.52317200	0.07705800
H	4.47813500	0.97053600	-0.11192100
H	4.57150100	-0.58561000	-0.71598900
H	-4.53057600	0.32712800	0.03137400
H	-4.41570200	-1.27496800	-0.44351800
O	0.24596100	-1.34872000	1.92754600
O	-0.73423700	3.30126600	-0.57630700
H	-1.40317900	2.82071800	-1.08823900
H	-0.11970600	3.64500600	-1.23417600
H	-0.50880100	-0.78083400	2.15027900
H	1.00070700	-0.74183900	1.99447900
Mn	0.12298000	-1.48446200	-0.52064500
Mn	-0.03095100	1.16551300	0.24768100

Zero-point correction= 0.181877 (Hartree/Particle)
Sum of electronic and zero-point Energies= -770.199703

$Mn_2[HNC(NH)_2NH]_2.2H_2O$ (Ms=3)

C	-2.62705000	-0.13217900	0.42137400
C	2.65574900	-0.26441500	0.35653400
N	-1.93825400	0.99163900	0.23993300
N	-2.00768400	-1.31607500	0.35387900
N	1.97202200	-1.41201100	0.28808500
N	2.01493500	0.89692500	0.27783000
H	2.64171000	1.69390500	0.34541900
H	2.57169700	-2.22738600	0.29672400
H	-2.63490500	-2.09479500	0.51421200
H	-2.54277500	1.80833400	0.28751700
N	4.04569700	-0.30077600	0.44549400
N	-4.00856200	-0.08811400	0.60695500
H	4.47298800	0.54274200	0.79771100
H	4.42945800	-1.12558200	0.88147200
H	-4.40710200	-0.88765000	1.07570300
H	-4.35892800	0.77842700	0.98770900
O	-0.32981400	-1.14797400	-2.26297300
O	0.26840300	3.15523200	-0.52746300
H	-0.57941600	3.54206600	-0.77636100
H	0.57967800	2.71124500	-1.34448000
H	-1.29376200	-1.07063600	-2.28510200
H	-0.04121800	-0.20432900	-2.10453900

Mn	-0.01161200	-1.35149300	0.02016600
Mn	0.04899500	1.00965500	0.11962700

Zero-point correction= 0.181300 (Hartree/Particle)
Sum of electronic and zero-point Energies= -707.183488

$Mn_2[HNC(NH)_2NH]_2.2H_2O$ (Ms=5)

C	-2.68511300	0.00224100	0.00189200
C	2.68361500	-0.00589800	-0.00000300
N	-1.99607700	1.07196600	0.39168700
N	-2.00008500	-1.06113700	-0.40876900
N	1.99406100	-1.06413300	-0.41508500
N	1.99942400	1.06850600	0.38710800
H	2.57053100	1.77707100	0.83399600
H	2.56658500	-1.81125700	-0.79125900
H	-2.57578800	-1.80397900	-0.78855100
H	-2.56464800	1.78873400	0.82835000
N	4.07032400	-0.03512500	0.08371600
N	-4.07249600	-0.01829200	0.07795300
H	4.52868500	0.86143700	0.02641400
H	4.52967700	-0.73704300	-0.47604500
H	-4.52470800	0.88128800	0.01908200
H	-4.53302300	-0.71632200	-0.48568600
O	-0.00708100	-3.07591400	0.50495200
O	0.01618900	3.09023400	-0.48577600
H	-0.74012300	2.85526400	-1.04214400
H	0.78961200	2.84014300	-1.01185000
H	-0.77523700	-2.85215200	1.04928000
H	0.75417700	-2.85508600	1.05989300
Mn	-0.00258300	-0.93217800	-0.38666100
Mn	0.00035600	0.93004900	0.37856200

Zero-point correction= 0.182616 (Hartree/Particle)
Sum of electronic and zero-point Energies= -707.149693

9. $Mn_2[HNC(NH)_2NH]_3$ (Ms=2)

C	-2.22930300	-1.55424500	0.04451400
C	-0.23322800	2.70380100	0.04280600
C	2.46432600	-1.14421200	0.04228600
N	-0.16490600	2.05402000	1.20717600
N	-0.20285800	2.04922600	-1.11154200
N	1.86129700	-0.89297100	1.20665000
N	1.87061100	-0.86618400	-1.11201600
N	-1.69708700	-1.17459200	1.20835200
N	-1.67955000	-1.19881800	-1.11017600
N	-0.28061300	4.10182800	0.04925800
N	3.76605700	-1.65683700	0.04774700
N	-3.41973000	-2.29034500	0.05076700
H	-3.56726000	-2.84810900	0.87899700
H	-3.58887700	-2.82765800	-0.78664500
H	-0.69538100	4.50718200	0.87523700
H	-0.65600600	4.51665200	-0.79060500
H	4.00826200	-2.18830100	0.87068200
H	4.03097000	-2.14571700	-0.79449100
H	2.46133700	-1.09081500	-1.90438400
H	2.44781800	-1.11986400	1.99973000
H	-2.20141000	-1.55488200	-1.90280000
H	-2.25107900	-1.47685300	1.99977300
H	-0.13848300	2.68608700	1.99726100
H	-0.26469200	2.67721500	-1.90456700
Mn	0.00119400	-0.00145300	1.18904500
Mn	0.00006600	-0.00031900	-1.36381900

Zero-point correction= 0.197461 (Hartree/Particle)
Sum of electronic and zero-point Energies= -822.167228

$Mn_2[HNC(NH)_2NH]_3$ (Ms=4)

C	-2.61631300	0.92818100	-0.06029700
C	2.33335600	1.41712400	-0.03742200
C	0.34094900	-2.53205000	0.15899100
N	1.69960800	1.35360200	1.13387200
N	1.79214900	0.90493900	-1.13990700
N	0.09721000	-1.79886700	1.24625600
N	0.35702600	-1.98019300	-1.04931800
N	-1.98470000	1.01182900	1.10878800
N	-1.99777000	0.45992400	-1.14410500
N	3.60998900	1.98382600	-0.10495400
N	0.63720200	-3.89360700	0.29614100
N	-3.92946200	1.39454000	-0.16229600
H	-4.47415900	1.31979000	0.68373200
H	-4.44284000	1.06353300	-0.96512700
H	3.83654400	2.61542700	0.64856100
H	3.84727200	2.38152000	-1.00199600
H	0.31725900	-4.31166900	1.15729900
H	0.38491900	-4.45892300	-0.50115700
H	0.65644700	-2.62918100	-1.76774300
H	0.06866300	-2.36388300	2.08635700
H	-2.62027800	0.39777400	-1.94121300
H	-2.53832200	1.48911800	1.80928500
H	2.20538200	1.82202900	1.87462900
H	2.43291400	0.94126700	-1.92512400
Mn	-0.05478400	0.26861800	1.20255500
Mn	-0.02483700	0.00345100	-1.27521400

Zero-point correction= 0.198873 (Hartree/Particle)
Sum of electronic and zero-point Energies= -822.122778

$Mn_2[HNC(NH)_2NH]_3$ (Ms=6)

C	0.34727400	2.34180000	0.00001700
C	2.45582500	-1.20479700	-0.00016500
C	-2.71698300	-0.74816300	0.00015400
N	1.78816900	-1.06441000	1.14176900
N	1.78802600	-1.06438000	-1.14201200
N	-2.03492900	-0.71370800	1.14172500
N	-2.03506600	-0.71368300	-1.14149700
N	0.16542000	1.69608600	1.14903200
N	0.16527400	1.69612500	-1.14899500
N	3.80596300	-1.55702800	-0.00025600
N	-4.10552000	-0.88463400	0.00023800
N	0.76952100	3.67540100	0.00000900
H	0.52461900	4.19095400	0.83296600
H	0.52450900	4.19098400	-0.83289800
H	4.31323400	-1.30310100	0.83407200
H	4.31313600	-1.30304800	-0.83462800
H	-4.56747800	-0.55675600	0.83506600
H	-4.56758100	-0.55674300	-0.83452700
H	-2.62540500	-0.72432100	-1.96471400
H	-2.62516900	-0.72437800	1.96501200
H	0.38490400	2.25362100	-1.96525900
H	0.38513500	2.25355800	1.96528900
H	2.37090000	-1.16253900	1.96478800
H	2.37064800	-1.16251900	-1.96510700
Mn	-0.06926100	-0.30436000	1.03515400
Mn	-0.06938500	-0.30432600	-1.03516200

Zero-point correction= 0.199815 (Hartree/Particle)
Sum of electronic and zero-point Energies= -822.108217

10. $Mn_2[HNC(NH)_2NH]_3.2H_2O$ (Ms=2)

C	-1.34376200	2.00486400	-0.56179400

C	-1.22490500	-2.20523600	0.46451100
C	3.03733500	-0.10260400	-0.41149400
N	-1.15461500	-1.70782400	-0.77212800
N	-0.55533100	-1.63075000	1.46299200
N	2.30037200	-0.51183400	-1.43814300
N	2.46363400	0.31430300	0.71753800
N	-0.68855600	1.51923100	-1.60097100
N	-1.00521400	1.67551400	0.69281700
N	-1.98287000	-3.34861900	0.70747300
N	4.43082400	-0.16385000	-0.49655600
N	-2.48606100	2.80530400	-0.74733800
H	-2.58577300	3.19179500	-1.67555200
H	-2.61791600	3.51528200	-0.04017100
H	-2.71220400	-3.51978100	0.03071300
H	-2.33751100	-3.42541900	1.64936900
H	4.80285300	-0.06732600	-1.42975000
H	4.92474900	0.42054900	0.16086400
H	3.13281000	0.63270200	1.40860500
H	2.86488500	-0.87963000	-2.19438100
H	-1.78937800	1.84593200	1.31790700
H	-0.98315400	1.93997500	-2.47568300
H	-1.70889800	-2.25162900	-1.42617900
H	-0.64632400	-2.14332400	2.33152800
Mn	0.26077500	-0.36410700	-1.51709100
Mn	0.43531800	0.14058500	1.05435900
O	0.72320800	1.52032000	3.03223200
H	0.30035500	2.22917700	2.52257500
O	-3.70339000	-0.09559800	-0.29793000
H	-3.66170800	0.85146600	-0.48092300
H	0.18208900	1.40818600	3.81974700
H	-2.79306000	-0.40017000	-0.45193300

Zero-point correction= 0.248279 (Hartree/Particle)
Sum of electronic and zero-point Energies= -974.988749

$Mn_2[HNC(NH)_2NH]_3.2H_2O$ (Ms=4)

C	-0.64727600	2.31631800	-0.86028100
C	2.52244500	-1.13457900	-0.37348200
C	-2.13595900	-1.21703000	1.31124000
N	2.27511100	-0.52119600	0.79316200
N	1.61578300	-1.12751000	-1.34185400
N	-1.22333800	-0.65938300	2.10583000
N	-1.98368500	-1.19699900	-0.01212700
N	-0.34974300	2.13995700	0.42683200
N	-0.58088500	1.29282400	-1.70804500
N	3.72514100	-1.82540600	-0.52767800
N	-3.22957300	-1.87882300	1.87595600
N	-0.96472000	3.58743800	-1.34758000
H	-1.14880300	4.28987000	-0.64767500
H	-1.64515300	3.60341100	-2.09268300
H	4.51141500	-1.43329000	-0.03139500
H	3.96284700	-2.07471800	-1.47598300
H	-3.50710600	-1.54218300	2.78582200
H	-4.02326900	-1.98803400	1.26248500
H	-2.73927100	-1.67459600	-0.49415000
H	-1.42731600	-0.79724200	3.08770100
H	-0.52148100	1.61745600	-2.66944800
H	-0.70752700	2.89335000	1.00684800
H	2.92985000	-0.82618500	1.50733100
H	1.96587400	-1.54810500	-2.19743100
Mn	0.37746500	0.28584800	1.21559600
Mn	-0.27927800	-0.58982800	-0.89771500
O	-1.42597900	-1.27007400	-2.94502200
H	-1.81637900	-0.41637700	-2.70024100
O	2.04874200	2.03134800	2.08427000
H	1.55697200	2.56043000	1.43738200
H	-0.83358700	-1.06687500	-3.67518500
H	2.58228200	1.44784300	1.51926600

Zero-point correction= 0.247563 (Hartree/Particle)
Sum of electronic and zero-point Energies= -974.940643

$Mn_2[HNC(NH)_2NH]_3.2H_2O$ (Ms=6)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.14005308
C	4.27201031	0.00000000	1.21435243
N	0.36298067	-1.15607840	3.58461221
N	0.51020410	1.13720126	3.66648992
N	3.76062295	-1.15705372	1.61240977
N	3.53321106	1.10970743	1.30376163
N	0.64414390	-1.12304312	0.24041171
N	0.37177804	1.14096329	0.60064737
N	-0.87331816	0.01441887	5.22340929
N	5.59265422	0.08437164	0.77276168
N	-1.15262087	0.02524356	-0.80897707
H	-1.23042479	-0.75905698	-1.44145989
H	-1.29027287	0.89699204	-1.30277157
H	-1.50726626	-0.77133779	5.25179567
H	-1.37717625	0.88169219	5.33901809
H	5.98683512	-0.77911909	0.43135784
H	5.78682784	0.85555159	0.15183772
H	4.04474519	1.94864030	1.04736715
H	4.39511199	-1.93653181	1.49195787
H	-0.38941035	1.81534660	0.59827970
H	0.31431575	-1.89635366	-0.32677724
H	-0.03750783	-1.95792465	4.05843835
H	0.15320991	1.95452963	4.15170839
Mn	1.76422131	-1.12559543	2.07759032
Mn	1.70807296	1.12005589	2.08267395
O	1.79821028	3.45731051	1.73003163
H	1.57162168	3.27235142	0.80832727
O	-2.27084406	-0.81182652	2.02454633
H	-2.26076949	-0.52437203	1.10283970
H	1.04285072	3.93567239	2.08659134
H	-1.33103079	-0.93671119	2.23623512

Zero-point correction= 0.248282 (Hartree/Particle)
Sum of electronic and zero-point Energies= -974.936109

11. $Mn_2[HNC(NH)_2NH]_4$ (Ms=1)

N	1.62099300	-1.20348700	1.08967400
N	-1.62154800	1.20240800	1.08938500
N	1.20292000	1.62141900	1.08748500
N	-1.20365300	-1.62172100	1.08719400
C	1.85693300	-1.92771700	0.00124400
C	-1.85674000	1.92754000	0.00128200
N	1.67259000	1.13315600	-1.08508600
C	1.92852100	1.85588100	-0.00028900
N	1.13304300	-1.67310200	-1.08314500
N	-1.67261800	-1.13226400	-1.08518300
C	-1.92786900	-1.85672800	-0.00132400
N	-1.13242400	1.67343600	-1.08305900
H	2.40290000	-1.10566300	1.72616700
H	1.02076000	-2.45831600	-1.71292700
H	2.45845500	1.01788600	-1.71367600
H	1.10780400	2.40195200	1.72599600
H	-1.01930500	2.45909100	-1.71219200
H	-2.40342700	1.10482200	1.72601200
H	-1.10823700	-2.40264600	1.72532900
H	-2.45801000	-1.01708000	-1.71424600
N	-2.78679900	2.97121800	-0.00223400
N	2.97225400	2.78591000	-0.00445600
N	2.78748400	-2.97093700	-0.00256100
N	-2.97342200	-2.78464700	-0.00518400

H	-3.03818400	-3.33848900	-0.84685600
H	3.35123200	-3.03780000	0.83167200
H	3.03839000	3.35083700	0.82890900
H	-3.35142600	3.03729600	0.83146500
H	3.34182800	-3.03408100	-0.84389800
H	3.03559100	3.33968200	-0.84624000
H	-3.34034900	3.03520400	-0.84403500
H	-3.04105100	-3.34903700	0.82841100
Mn	-0.00014900	-0.00050300	0.89162000
Mn	0.00039800	0.00021300	-0.89222700

Zero-point correction= 0.265903 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1026.825651

$Mn_2[HNC(NH)_2NH]_4$ (Ms=3)

N	-1.57924000	1.25201200	1.10190500
N	1.57924700	-1.25193200	1.10205700
N	-1.25197100	-1.57917400	1.10210100
N	1.25197700	1.57931100	1.10186400
C	-1.82260800	1.93636400	-0.00267000
C	1.82260200	-1.93638900	-0.00245500
N	-1.61484400	-1.17910900	-1.12176300
C	-1.93638300	-1.82258900	-0.00243000
N	-1.17907700	1.61477300	-1.12196000
N	1.61481800	1.17904200	-1.12197300
C	1.93637300	1.82261600	-0.00269300
N	1.17907500	-1.61488800	-1.12177900
H	-2.21152500	1.45804500	1.86634200
H	-1.20178400	2.33306300	-1.83393500
H	-2.33316300	-1.20185800	-1.83370900
H	-1.45795400	-2.21143400	1.86657200
H	1.20175900	-2.33325500	-1.83367800
H	2.21152500	-1.45791400	1.86651400
H	1.45802100	2.21160600	1.86629000
H	2.33315300	1.20169300	-1.83390400
N	2.70142200	-3.02862900	-0.00937800
N	-3.02861600	-2.70141900	-0.00934500
N	-2.70145200	3.02859200	-0.00968900
N	3.02861500	2.70144700	-0.00972000
H	3.10598300	3.24554700	-0.85726900
H	-3.29192700	3.08936200	0.80706100
H	-3.08937600	-3.29184000	0.80744500
H	3.29187600	-3.08937500	0.80738800
H	-3.24558000	3.10595200	-0.85722100
H	-3.10605800	-3.24557800	-0.85684700
H	3.24554100	-3.10610100	-0.85690300
H	3.08935700	3.29196000	0.80700600
Mn	0.00000500	0.00004600	1.11939000
Mn	0.00001900	-0.00004900	-1.08122600

Zero-point correction= 0.265379 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1026.867453

$Mn_2[HNC(NH)_2NH]_4$ (Ms=5)

N	-1.94850200	0.51861300	1.09609600
N	1.94842000	-0.51888100	1.09644100
N	-0.51866100	-1.94837100	1.09630900
N	0.51871700	1.94852100	1.09618400
C	-2.43717700	1.07657500	-0.00031300
C	2.43694400	-1.07685200	0.00004000
N	-1.07594900	-1.69968400	-1.10285200
C	-1.07660500	-2.43699100	-0.00009000
N	-1.69968700	1.07600400	-1.10299300
N	1.07605400	1.69966200	-1.10286900
C	1.07674500	2.43719000	-0.00019300
N	1.69967500	-1.07603600	-1.10272500
H	-2.61442900	0.39932800	1.84853200

H	-2.01713500	1.71557300	-1.82013100
H	-1.71561400	-2.01721200	-1.81987100
H	-0.39933700	-2.61430100	1.84873000
H	2.01708800	-1.71581300	-1.81969200
H	2.61444700	-0.39951000	1.84876900
H	0.39956600	2.61448100	1.84861200
H	1.71571600	2.01693600	-1.81999700
N	3.68627100	-1.70929700	0.00114200
N	-1.70881600	-3.68640600	0.00099900
N	-3.68651800	1.70849500	0.00088500
N	1.70881600	3.68631200	0.00120500
H	1.61444800	4.19386400	-0.86655800
H	-4.26928100	1.48138600	0.79331500
H	-1.48089500	-4.26895200	0.79340300
H	4.26876000	-1.48156200	0.79365000
H	-4.19413700	1.61281200	-0.86674000
H	-1.61122200	-4.19427900	-0.86631800
H	4.19425800	-1.61137800	-0.86607200
H	1.48255800	4.26919400	0.79375600
Mn	-0.00008300	0.00019400	1.07387500
Mn	-0.00003600	0.00010100	-1.06046700

Zero-point correction= 0.265793 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1026.877263

12. $Mn_2[HNC(NH)_2NH]_4.2H_2O$ (Ms=1)

C	1.33761400	2.12145800	0.68082300
C	1.79695700	-1.61087800	0.75605500
C	-1.45935700	-2.09522300	-0.86755400
N	1.06506900	-0.98529700	1.65971300
N	1.62464800	-1.37834000	-0.55792900
N	-1.37290600	-1.80792600	0.44258200
N	-0.95011200	-1.28620900	-1.77457200
N	0.29268300	1.74768300	1.41327800
N	1.66776700	1.45246200	-0.41392500
N	2.80418900	-2.48270700	1.16268400
N	-2.04165200	-3.31524400	-1.22996400
N	2.05166700	3.26789400	1.05088200
H	2.15274800	3.38167500	2.04937400
H	2.94006000	3.36718000	0.58089300
H	2.61208200	-3.04818300	1.97457600
H	3.30135700	-2.96965300	0.43405400
H	-2.85296800	-3.56539100	-0.68302800
H	-2.20391400	-3.43232000	-2.21961800
N	-0.92520000	1.55625900	-1.61521500
N	-2.17420300	0.94333800	0.22400700
C	-2.00436200	1.69857700	-0.85323900
N	-3.00030300	2.61415400	-1.21465500
H	-2.71339300	3.30312700	-1.89390100
H	-3.46870100	3.04541100	-0.43098100
H	-0.01200900	2.44505500	2.08016300
H	2.56369600	1.71683400	-0.81113100
H	-3.06515600	1.09999500	0.68433500
H	-0.78961600	2.30259000	-2.28409100
H	-1.29586500	-2.65644900	0.99567900
H	-1.25605200	-1.48938700	-2.72039700
H	1.46385900	-1.03422600	2.59145700
H	1.82659700	-2.19657400	-1.12337000
O	4.06892300	0.07893000	-1.50687200
H	3.26673500	-0.31340100	-1.10820300
O	-2.53045800	-0.47735200	2.73017100
H	-2.65183300	-0.99354700	1.91208900
H	4.14070600	-0.33939500	-2.36788000
H	-2.22353600	-1.11736000	3.37862200
Mn	-0.61628500	-0.00515300	1.06974900
Mn	0.40191900	0.11376600	-1.19573800

Zero-point correction= 0.315992 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1179.69212

$Mn_2[HNC(NH)_2NH]_4.2H_2O$ (Ms=3)

C	-0.03218700	-2.63632500	-0.29861500
C	2.64202700	-0.20815200	0.32466700
C	0.14912100	2.67721800	0.38038900
N	2.13823000	-0.20022200	-0.91601400
N	1.81689800	0.03377400	1.32220200
N	0.50403600	2.14904500	-0.79435300
N	-0.36162100	1.87257200	1.29435000
N	-0.19803900	-1.81300900	-1.31383500
N	-0.01684300	-2.12070300	0.94237400
N	3.98850800	-0.52899500	0.52639900
N	0.25622000	4.04914900	0.62148500
N	0.18586800	-4.00473200	-0.47190800
H	0.02980900	-4.35108000	-1.40662300
H	-0.24952900	-4.58800800	0.22780900
H	4.61192000	-0.15762400	-0.17574600
H	4.33183000	-0.35855500	1.46017400
H	0.73453000	4.57251200	-0.09565100
H	0.56857200	4.29536500	1.54928800
N	-2.19252100	-0.30058400	0.76424500
N	-1.82770900	0.55506200	-1.30242700
C	-2.68504100	0.11352200	-0.40408400
N	-4.06188900	0.13570900	-0.65046900
H	-4.62326700	-0.33489900	0.04315700
H	-4.32540600	-0.12458400	-1.58966100
H	-0.35560800	-2.24109100	-2.21815500
H	0.60399900	-2.64256700	1.55307500
H	-2.24187200	1.06254500	-2.07522700
H	-2.77785500	-0.99743700	1.21405000
H	1.25909500	2.66095700	-1.23928700
H	-0.83941600	2.33747800	2.05622100
H	2.63652000	-0.83712200	-1.53007400
H	2.24148700	0.17354500	2.23146200
O	-0.91924800	-0.60477900	3.36390700
H	-0.99184300	-1.43531400	2.86912500
O	0.69605300	0.71720600	-3.31071000
H	0.24863600	1.54911500	-3.10705200
H	-1.64799600	-0.07620700	3.00976000
H	1.54745500	0.79715300	-2.85311400
Mn	0.12211500	0.15058000	-0.96970600
Mn	-0.16359500	-0.09740500	0.94900300

Zero-point correction= 0.316800 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1179.661561

$Mn_2[HNC(NH)_2NH]_4.2H_2O$ (Ms=5)

C	-1.92460200	-1.74786400	0.43780400
C	-1.92406900	1.74844600	-0.43778500
C	1.88311200	1.87223100	-0.50529400
N	-1.58946200	1.46899200	0.82750900
N	-1.15911700	1.30683700	-1.41903700
N	1.23664500	1.88541300	0.65976600
N	1.67673700	0.86953600	-1.34054100
N	-1.15950500	-1.30647700	1.41904400
N	-1.58993000	-1.46850800	-0.82749300
N	-3.09956900	2.45567100	-0.69169100
N	2.81058400	2.86772100	-0.81889300
N	-3.10030300	-2.45474400	0.69173100
H	-3.20285100	-2.80286100	1.63305800
H	-3.33211100	-3.15118900	-0.00100000
H	-3.33114900	3.15219600	0.00103600
H	-3.20203300	2.80380900	-1.63301900
H	2.79561100	3.67705400	-0.21729500
H	2.85133100	3.11818500	-1.79555500
N	1.23604400	-1.88579900	-0.65976900

N	1.67649000	-0.87005400	1.34052500
C	1.88254500	-1.87281200	0.50527300
N	2.80972500	-2.86857900	0.81885300
H	2.79449900	-3.67790800	0.21725500
H	2.85041800	-3.11905500	1.79551400
H	-1.41508000	-1.63384800	2.34373200
H	-2.39754800	-1.46536700	-1.44211000
H	2.32494900	-0.83249700	2.11776500
H	1.18448500	-2.81162700	-1.07135200
H	1.18534900	2.81126300	1.07133300
H	2.32516600	0.83179000	-2.11779700
H	-2.39707800	1.46606400	1.44213000
H	-1.41460800	1.63429000	-2.34371900
O	0.07706300	-1.39380900	-3.33322500
H	-0.44207300	-1.94180600	-2.72405900
O	0.07755000	1.39384000	3.33324800
H	0.98757700	1.53500500	3.04115800
H	0.98706300	-1.53531600	-3.04122200
H	-0.44144200	1.94195400	2.72406500
Mn	0.04629400	0.26517600	1.03116700
Mn	0.04619900	-0.26519500	-1.03117200

Zero-point correction= 0.315416 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1179.696579

13a. $Mn_2(OCHO)_2$ (Ms=1)

C	2.52113300	0.00058900	0.00026500
C	-2.52111100	-0.00068700	0.00040200
O	-1.96396700	1.13366000	0.00050300
O	-1.96311200	-1.13460200	-0.00032400
O	1.96297900	1.13445200	-0.00011300
O	1.96418800	-1.13383100	0.00057000
H	3.62183800	0.00120500	0.00032800
H	-3.62180900	-0.00109500	0.00095900
Mn	-0.00049400	1.40329100	-0.00022600
Mn	0.00045900	-1.40316900	-0.00018900

Zero-point correction= 0.048977 (Hartree/Particle)
Sum of electronic and zero-point Energies= -586.239379

$Mn_2(OCHO)_2$ (Ms=3)

C	2.55189300	-0.00191700	-0.02493000
C	-2.55200100	-0.00197300	-0.02437800
O	-1.98177800	1.12192200	-0.02134000
O	-1.96223000	-1.13222500	-0.00149200
O	1.98153100	1.12191300	-0.02031700
O	1.96214600	-1.13223500	-0.00139800
H	3.65013100	-0.01991000	-0.05219100
H	-3.65031400	-0.02003600	-0.04962600
Mn	0.00007700	1.10194800	0.02130700
Mn	0.00006200	-1.09281600	0.00885400

Zero-point correction= 0.049671 (Hartree/Particle)
Sum of electronic and zero-point Energies= -586.214114

$Mn_2(OCHO)_2$ (Ms=5)

C	2.54689200	0.00015500	0.00057800
C	-2.54674000	-0.00020600	0.00028400
O	-1.96135600	1.12228100	0.00003700
O	-1.96086300	-1.12251100	0.00214600
O	1.96086700	1.12237100	0.00236800
O	1.96172800	-1.12237700	-0.00064600
H	3.64603100	0.00074300	0.00036800
H	-3.64586500	-0.00045800	-0.00038200
Mn	-0.00010700	0.97974100	-0.00089400
Mn	-0.00005600	-0.97966500	-0.00056200

Zero-point correction= 0.050433 (Hartree/Particle)
Sum of electronic and zero-point Energies= -586.185908

13b. $Mn_2(OCHO)_2$ (Ms=1)

Mn	-0.41442800	0.83522800	-0.69065400
Mn	0.41442800	-0.83522800	-0.69065400
H	-0.08551100	-2.97195700	1.47050900
H	0.08551100	2.97195700	1.47050900
H	-1.00442500	-1.45893500	1.87728800
H	1.00442500	1.45893500	1.87728800
C	-0.31571500	-1.93947700	1.16770600
C	0.31571500	1.93947700	1.16770600
O	0.87433600	1.94670700	-0.15068700
O	-0.87433600	1.19234200	1.01472800
O	-0.87433600	-1.94670700	-0.15068700
O	0.87433600	-1.19234200	1.01472800

Zero-point correction= 0.072033 (Hartree/Particle)
Sum of electronic and zero-point Energies= -587.204821

$Mn_2(OCHO)_3$ (Ms=3)

Mn	-0.30233600	0.93373500	-0.70185400
Mn	0.30233600	-0.93373500	-0.70185400
H	-0.04840300	-3.17010800	1.36744100
H	0.04840300	3.17010800	1.36744100
H	-0.69712300	-1.61669900	2.04402700
H	0.69712300	1.61669900	2.04402700
C	-0.21557200	-2.09906700	1.18012100
C	0.21557200	2.09906700	1.18012100
O	1.00896000	1.92582400	0.01246100
O	-1.00896000	1.45864100	0.86930800
O	-1.00896000	-1.92582400	0.01246100
O	1.00896000	-1.45864100	0.86930800

Zero-point correction= 0.071109 (Hartree/Particle)
Sum of electronic and zero-point Energies= -587.205087

$Mn_2(OCHO)_4$ (Ms=5)

Mn	0.40964300	0.99425300	-0.66672400
Mn	-0.40964300	-0.99425300	-0.66672400
H	0.97903700	-1.75434400	1.86850800
H	-0.97903700	1.75434400	1.86850800
H	0.05121200	-3.23527400	1.38164700
H	-0.05121200	3.23527400	1.38164700
C	0.30022100	-2.19542800	1.12420000
C	-0.30022100	2.19542800	1.12420000
O	0.88038700	1.42038900	1.00647900
O	-0.88038700	2.13774600	-0.17238500
O	-0.88038700	-1.42038900	1.00647900
O	0.88038700	-2.13774600	-0.17238500

Zero-point correction= 0.071380 (Hartree/Particle)
Sum of electronic and zero-point Energies= -587.245607

14. $Mn_2(OCHO)_2.2H_2O$ (Ms=1)

C	0.78006700	-2.48537400	-0.04006800
C	-0.77943500	2.48502300	0.04072600
O	-1.68492900	1.60347400	0.10997300
O	0.46322600	2.27793600	-0.04023000
O	-0.46263900	-2.27851800	0.04083000
O	1.68538000	-1.60372100	-0.11017900
O	3.35278700	0.53353300	0.24747200
O	-3.35336000	-0.53081900	-0.24687900

H	3.53059200	-0.38843900	0.47951100
H	3.62297600	1.06571600	1.00252300
H	-3.62517000	-1.06097600	-1.00276900
H	-3.52827000	0.39214000	-0.47744800
H	-1.10715200	3.53829500	0.05339300
H	1.10801200	-3.53858600	-0.05183500
Mn	-1.19247900	-0.40218900	0.33757700
Mn	1.19214000	0.40134400	-0.33818600

Zero-point correction= 0.097979 (Hartree/Particle)
Sum of electronic and zero-point Energies= -739.077012

$Mn_2(OCHO)_2.2H_2O$ (Ms=3)

C	0.00438300	-2.56872600	0.03604700
C	-0.00668000	2.56888600	0.03621100
O	-1.08816900	1.96308500	0.30699400
O	1.07201100	1.96501000	-0.24940800
O	-1.07972900	-1.96770000	0.30679500
O	1.08051900	-1.96009100	-0.24929600
O	3.06762700	0.00507400	0.09833000
O	-3.02193700	-0.00594500	-0.31846000
H	3.34287500	-0.77095700	0.59862300
H	3.34266500	0.78047600	0.59967200
H	-3.24696600	-0.78084900	-0.84468400
H	-3.24962800	0.77033200	-0.84153300
H	-0.00432900	3.66734500	0.04889700
H	0.01152400	-3.66716800	0.04843600
Mn	-0.87260800	-0.00177700	0.24674400
Mn	0.85561000	0.00195300	-0.21484800

Zero-point correction= 0.100019 (Hartree/Particle)
Sum of electronic and zero-point Energies= -739.015462

$Mn_2(OCHO)_2.2H_2O$ (Ms=5)

C	-0.52519600	-2.52087600	0.00243400
C	0.52533100	2.52079700	-0.00251500
O	-0.65629900	2.17415700	0.27970300
O	1.46802500	1.73404300	-0.30723000
O	-1.46799100	-1.73416400	0.30692600
O	0.65642500	-2.17415600	-0.27976100
O	3.00468700	-0.50961400	0.28644200
O	-3.00462400	0.50975600	-0.28554100
H	3.13013800	-1.20634300	0.93986500
H	3.33935600	0.30734700	0.67539300
H	-3.34071200	-0.30622900	-0.67527000
H	-3.13241400	1.20820900	-0.93665500
H	0.75304600	3.59925900	0.01224800
H	-0.75277100	-3.59936700	-0.01214000
Mn	-0.93220700	0.19718300	0.29996400
Mn	0.93223800	-0.19728600	-0.30025500

Zero-point correction= 0.099258 (Hartree/Particle)
Sum of electronic and zero-point Energies= -739.024743

15. $Mn_2(OCHO)_3$ (Ms=2)

O	0.00842600	2.00879200	-1.17940100
O	0.00868400	2.01003200	1.07941800
O	1.78007500	-0.97430900	1.08732600
O	1.77408700	-1.00816000	-1.17114500
O	-1.78622200	-0.96144700	1.08863100
C	0.01120000	2.57704200	-0.04531900
C	2.27781500	-1.26002100	-0.03481400
C	-2.28823200	-1.24161100	-0.03301500
O	-1.78405200	-0.99294500	-1.16986400
H	-3.26252700	-1.75470000	-0.03024200
H	0.01618100	3.67860900	-0.05105800

H	3.24756100	-1.78170500	-0.03302200
Mn	-0.00085800	-0.02572800	-1.22868600
Mn	0.00030200	-0.02428700	1.34522600

Zero-point correction= 0.072489 (Hartree/Particle)
Sum of electronic and zero-point Energies= -775.472814

$Mn_2(OCHO)_3$ (Ms=4)

O	-0.00024200	1.11931300	-1.58111500
O	0.00004300	-1.11934900	-1.58109300
O	-1.93930600	-1.12282300	0.52622700
O	-1.93932500	1.12276300	0.52659200
O	1.93938800	-1.12274500	0.52650100
C	-0.00016100	-0.00002400	-2.17907700
C	-2.52541100	-0.00005100	0.61302100
C	2.52548100	0.00007100	0.61286300
O	1.93936500	1.12284000	0.52609100
H	3.60962200	0.00011000	0.78196800
H	-0.00025900	-0.00003500	-3.27457800
H	-3.60954200	-0.00008500	0.78219600
Mn	-0.00001200	1.04353100	0.31766900
Mn	0.00006500	-1.04352900	0.31769000

Zero-point correction= 0.075326 (Hartree/Particle)
Sum of electronic and zero-point Energies= -775.380175

$Mn_2(OCHO)_3$ (Ms=6)

O	0.00001600	-2.11060200	-0.01987300
O	0.00000700	-0.99641600	1.93354500
O	-1.90668400	1.31216200	0.51398200
O	-1.91789600	-0.01894800	-1.30061700
O	1.90666700	1.31218300	0.51397400
C	0.00001600	-2.05182400	1.24569100
C	-2.47088800	0.76869400	-0.47882300
C	2.47087900	0.76871400	-0.47882700
O	1.91789400	-0.01893700	-1.30061800
H	3.53275100	1.00117500	-0.64655000
H	0.00002900	-3.01479700	1.77994400
H	-3.53276400	1.00114200	-0.64654300
Mn	0.00000000	-0.46079200	-1.09297300
Mn	-0.00000300	0.79133000	0.89544300

Zero-point correction= 0.072989 (Hartree/Particle)
Sum of electronic and zero-point Energies= -775.416930

16. $Mn_2(OCHO)_3.2H_2O$ (Ms=2)

O	-1.07372000	2.05005800	0.14911800
O	1.04615000	1.89005100	0.91288100
O	1.79474600	-0.52461300	-1.54755100
O	-0.32333400	-0.36957200	-2.30948800
O	0.52216000	-1.81744900	1.50444500
C	-0.02711100	2.51638300	0.66881800
C	0.91433500	-0.54986100	-2.45578700
C	-0.68700000	-2.17996300	1.40869400
O	-1.59025400	-1.63457500	0.72117200
H	-0.97440500	-3.06930200	1.99808200
H	-0.04158700	3.58659900	0.94614600
H	1.26575000	-0.74838200	-3.48280700
Mn	-1.30737800	0.04074500	-0.57498100
Mn	1.12677200	-0.17211300	0.42306100
O	-3.34685400	0.47780100	0.32258200
H	-3.45843900	-0.19163800	1.00886100
O	3.30934500	0.22660400	0.74928200
H	3.71175600	0.10093800	-0.11958900
H	-3.23481900	1.32376400	0.77370400
H	3.33963400	1.17642800	0.92372300

Zero-point correction= 0.121915 (Hartree/Particle)
Sum of electronic and zero-point Energies= -928.313681

$Mn_2(OCHO)_3.2H_2O$ (Ms=4)

O	1.08998900	-0.26474800	1.75202000
O	-1.08996600	0.26475000	1.75203800
O	-1.48279400	-1.69200600	-0.55710900
O	0.69238900	-2.17854500	-0.54958400
O	-0.69239100	2.17855400	-0.54955700
C	0.00001600	0.00000100	2.33866300
C	-0.52428300	-2.51646300	-0.64004600
C	0.52428000	2.51646800	-0.64005100
O	1.48279000	1.69200600	-0.55714300
H	0.75852200	3.57845200	-0.79755500
H	0.00002600	0.00000200	3.44183700
H	-0.75852500	-3.57844700	-0.79755200
Mn	0.90048800	-0.23316700	-0.29392500
Mn	-0.90049300	0.23317700	-0.29390600
O	3.16695600	-0.40596900	-0.28538300
H	3.39394700	0.53081300	-0.21870500
O	-3.16697000	0.40593300	-0.28539700
H	-3.39389500	-0.53086500	-0.21870600
H	3.34746700	-0.77463700	0.58800500
H	-3.34752200	0.77460800	0.58797900

Zero-point correction= 0.124195 (Hartree/Particle)
Sum of electronic and zero-point Energies= -928.219702

$Mn_2(OCHO)_3.2H_2O$ (Ms=6)

O	1.11915700	-0.15232900	1.83015700
O	-1.11910700	0.15230100	1.83020700
O	-1.38577000	-1.81213100	-0.57508700
O	0.83888100	-2.11605300	-0.58057000
O	-0.83890300	2.11606800	-0.58049300
C	0.00003400	-0.00004000	2.39989100
C	-0.34995600	-2.53865400	-0.62044000
C	0.34993300	2.53866700	-0.62041700
O	1.38574700	1.81214100	-0.57511000
H	0.49923500	3.62729500	-0.70395800
H	0.00005300	-0.00009000	3.50550900
H	-0.49925800	-3.62728300	-0.70397600
Mn	1.01862100	-0.14152700	-0.22130800
Mn	-1.01862900	0.14153200	-0.22126000
O	3.25859900	-0.27083800	-0.52084400
H	3.58350600	0.61467400	-0.31981100
O	-3.25859000	0.27084700	-0.52086100
H	-3.58350300	-0.61465900	-0.31981100
H	3.69565800	-0.86690500	0.09645500
H	-3.69567400	0.86693800	0.09639700

Zero-point correction= 0.122932 (Hartree/Particle)
Sum of electronic and zero-point Energies= -922.242791

17. $Mn_2(OCHO)_4$ (Ms=1)

O	-1.96047700	-0.00001000	1.11528600
O	-1.96035500	0.00020600	-1.11547100
O	1.96041200	-0.00028200	-1.11541900
O	1.96042800	0.00011900	1.11533500
O	0.00025000	1.95057200	-1.11495000
O	-0.00001700	-1.95051800	1.11510000
C	-2.55594300	0.00028900	-0.00012500
C	2.55595400	-0.00023700	-0.00005000
C	0.00021200	2.54878900	0.00003900
C	-0.00030900	-2.54880200	0.00013200

O	-0.00017100	-1.95067600	-1.11489700
O	-0.00008000	1.95058500	1.11504500
H	0.00031100	3.64532600	0.00002900
H	-3.65308900	0.00041700	-0.00019000
H	-0.00059400	-3.64534000	0.00022500
H	3.65309800	-0.00044000	-0.00005500
Mn	0.00003200	-0.00001700	-0.95704100
Mn	0.00000200	0.00001000	0.95703200

Zero-point correction= 0.101790 (Hartree/Particle)
Sum of electronic and zero-point Energies= -964.584298

$Mn_2(OCHO)_4$ (Ms=3)

O	0.00695600	1.94173200	1.11495100
O	0.00486200	1.94105400	-1.11568600
O	-0.00546000	-1.94177900	-1.11494000
O	-0.00629600	-1.94113700	1.11568800
O	1.95773700	-0.00707000	-1.11699000
O	-1.95776300	0.00602100	1.11700500
C	0.00805100	2.54090200	-0.00055400
C	-0.00793800	-2.54098000	0.00052200
C	2.55184300	-0.00748000	-0.00034500
C	-2.55186400	0.00766300	0.00033300
O	-1.95821500	0.00602400	-1.11655100
O	1.95820800	-0.00464800	1.11656600
H	3.64896800	-0.01110000	-0.00056500
H	0.01054100	3.63695700	-0.00088700
H	-3.64898700	0.01126100	0.00058800
H	-0.01028800	-3.63703400	0.00087400
Mn	-0.00020400	-0.00029800	-0.97947700
Mn	0.00016400	0.00020700	0.97947200

Zero-point correction= 0.101954 (Hartree/Particle)
Sum of electronic and zero-point Energies= -964.601144

$Mn_2(OCHO)_4$ (Ms=5)

O	-1.52690600	1.24021000	1.12541700
O	-1.47509200	1.30238500	-1.12409400
O	1.47522300	-1.30115400	-1.12504000
O	1.52684800	-1.24153200	1.12455100
O	1.30148100	1.47580400	-1.12423800
O	-1.24053400	-1.52754600	1.12460400
C	-1.94283100	1.64282200	0.00066500
C	1.94283300	-1.64290500	-0.00059600
C	1.64278100	1.94290800	0.00053200
C	-1.64296000	-1.94274500	-0.00046100
O	-1.30216200	-1.47442200	-1.12489000
O	1.24112300	1.52627800	1.12536200
H	2.35022000	2.78414600	0.00074600
H	-2.78401500	2.35032700	0.00095800
H	-2.35062000	-2.78379600	-0.00083500
H	2.78393900	-2.35050000	-0.00105000
Mn	-0.00005200	0.00039500	-1.05430500
Mn	0.00011900	-0.00042900	1.05374400

Zero-point correction= 0.100944 (Hartree/Particle)
Sum of electronic and zero-point Energies= -964.624714

18. $Mn_2(OCHO)_4.2H_2O$ (Ms=1)

H	-0.50081700	-2.80367400	-2.28523500
H	-0.64378700	2.34649100	-2.72685000
H	0.50097800	2.80364600	2.28528800
H	0.64364500	-2.34652300	2.72684100
O	-3.45627300	-0.02504100	0.34769900
H	-3.68295500	0.77602700	-0.14138100
O	3.45623800	0.02482300	-0.34776700

H	3.68285000	-0.77657900	0.14079900
H	3.69715300	0.75519300	0.23612300
H	-3.69715500	-0.75581200	-0.23569800
Mn	-1.22439200	-0.01394600	0.29487600
Mn	1.22438900	0.01400400	-0.29485700
O	1.46570000	-1.26635900	1.23400000
O	-0.73238100	-1.25722000	1.74152900
O	0.82390700	-1.53209100	-1.46018600
O	-1.38559600	-1.53110600	-0.99553300
O	0.73226100	1.25722900	-1.74152000
O	-1.46580500	1.26642600	-1.23391600
O	1.38572700	1.53115900	0.99548300
O	-0.82376200	1.53210800	1.46019700
C	0.46150100	-1.63187900	1.91039500
C	0.35478100	1.96539200	1.58800200
C	-0.46162700	1.63187300	-1.91038600
C	-0.35464800	-1.96533100	-1.58804700

Zero-point correction= 0.150158 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1117.425841

$Mn_2(OCHO)_4.2H_2O$ (Ms=3)

H	1.28660400	-1.90831300	2.83834600
H	-1.24267600	-3.07291000	-1.53855700
H	-1.28660400	1.90831300	-2.83834600
H	1.24267600	3.07291000	1.53855700
Mn	-0.97848700	0.14227600	0.52818700
Mn	0.97848700	-0.14227600	-0.52818700
O	1.64546100	1.51984900	0.31241900
O	-0.32688800	1.80993700	1.36148600
O	1.68732800	-1.18347700	0.99331000
O	-0.27328300	-0.88740600	2.06233600
O	0.32688800	-1.80993700	-1.36148600
O	-1.64546100	-1.51984900	-0.31241900
O	0.27328300	0.88740600	-2.06233600
O	-1.68732800	1.18347700	-0.99331000
C	0.86307700	2.14966400	1.07785200
C	-0.90455800	1.33565700	-1.98115200
C	-0.86307700	-2.14966400	-1.07785200
C	0.90455800	-1.33565700	1.98115200
O	2.82790700	-0.51040600	-1.49657600
O	-2.82790700	0.51040600	1.49657600
H	3.37431600	-0.89665400	-0.79887100
H	2.62680400	-1.23882200	-2.09944800
H	-2.62680400	1.23882200	2.09944800
H	-3.37431600	0.89665400	0.79887100

Zero-point correction= 0.152469 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1117.413328

$Mn_2(OCHO)_4.2H_2O$ (Ms=5)

H	0.50183200	2.59594700	-2.53656000
H	0.50181100	-2.59600500	-2.53650100
H	-0.50182800	-2.59593700	2.53656400
H	-0.50182000	2.59599500	2.53650800
O	3.33731300	-0.00000400	0.38794500
H	3.57379100	-0.76557500	-0.14940600
O	-3.33731600	0.00001700	-0.38793300
H	-3.57376500	0.76551300	0.14953800
H	-3.57378500	-0.76557200	0.14939500
H	3.57378300	0.76551000	-0.14949000
Mn	1.04669700	0.00000300	0.21286300
Mn	-1.04669600	0.00000200	-0.21286700
O	-1.38464500	1.40487800	1.16543700
O	0.82783800	1.41431600	1.58751900
O	-0.82782600	1.41428100	-1.58755700
O	1.38465500	1.40485600	-1.16546400

O	-0.82784400	-1.41432000	-1.58751900
O	1.38463900	-1.40488600	-1.16543400
O	-1.38464800	-1.40485900	1.16545600
O	0.82783100	-1.41427600	1.58755600
C	-0.35337200	1.81592100	1.77365800
C	-0.35337800	-1.81588100	1.77369500
C	0.35336700	-1.81592700	-1.77365400
C	0.35338400	1.81588500	-1.77369700

Zero-point correction= 0.150023 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1117.463784
