Electronic Supplementary Information

A one-pot reduction route to bimetallic manganese 1,8-naphthyridine complexes

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Characterisation data for [MnBr(CO)$_3$(^{Me}L)] (1)

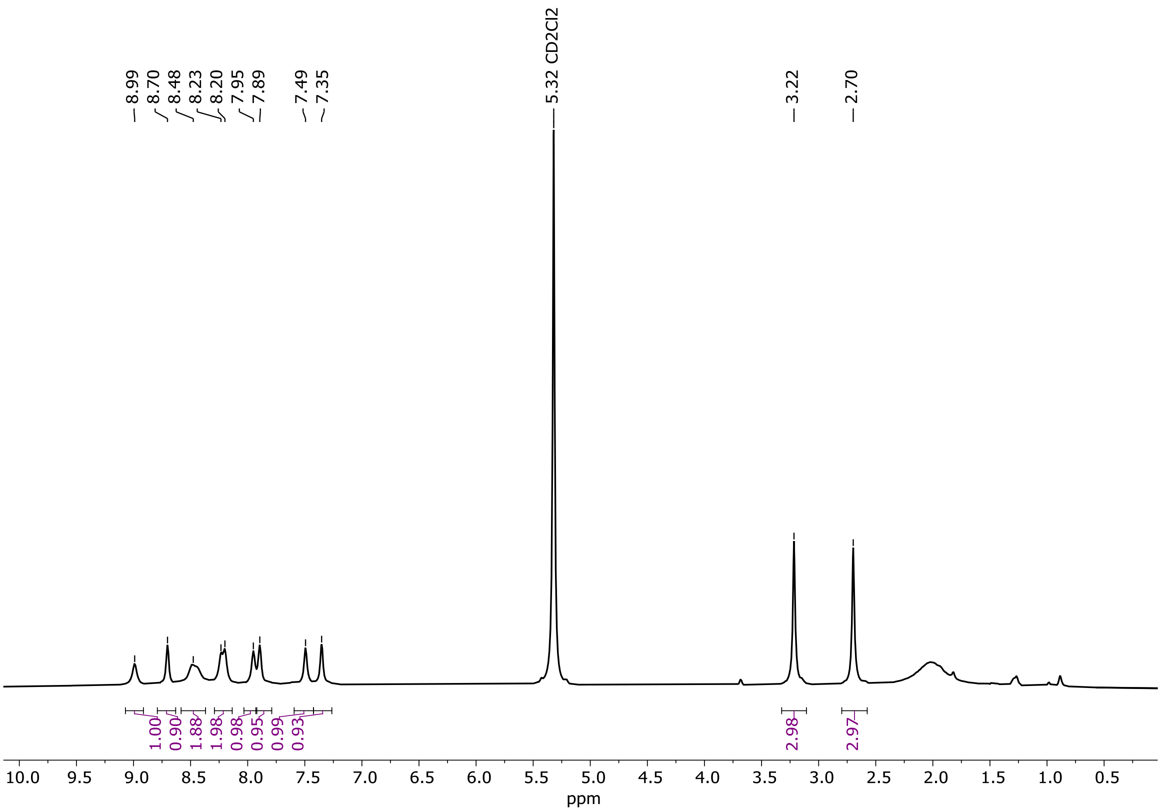

Figure S1. ^{1}H NMR spectrum of 1 in CD_2Cl_2.

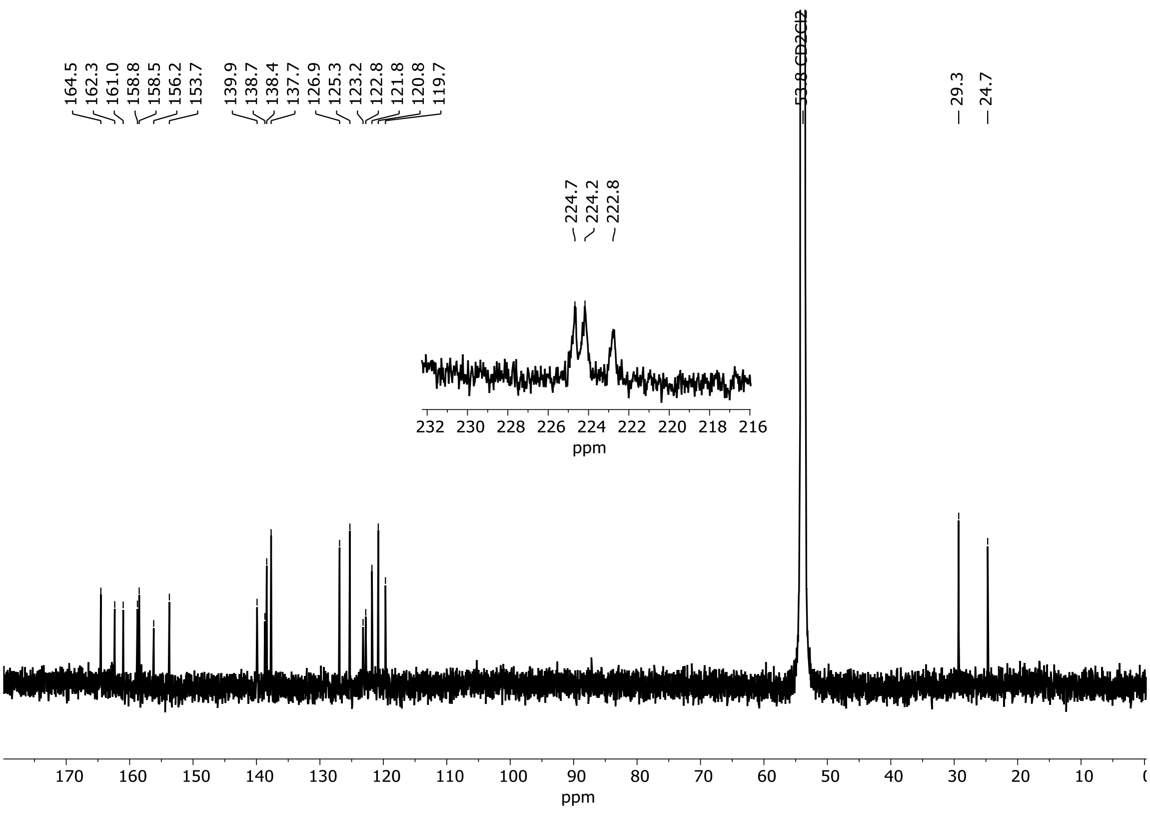

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in CD_2Cl_2. Insert: Carbonyl region of the $^{13}C\{^{1}H\}$ NMR spectrum.

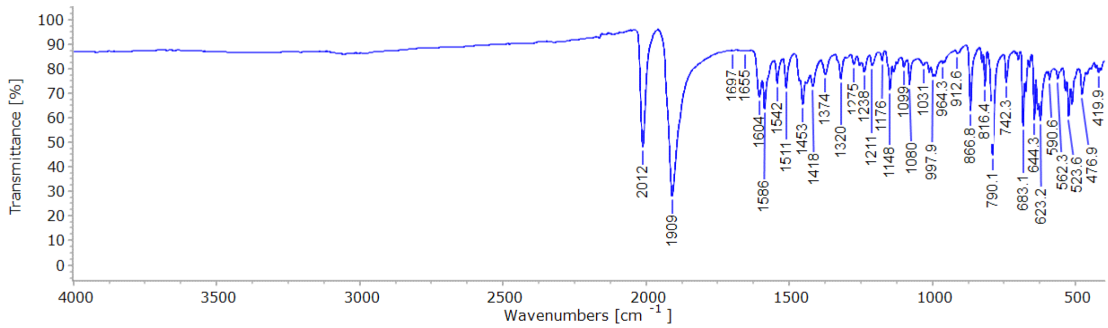

Figure S3. Solid-state IR spectrum of **1**.

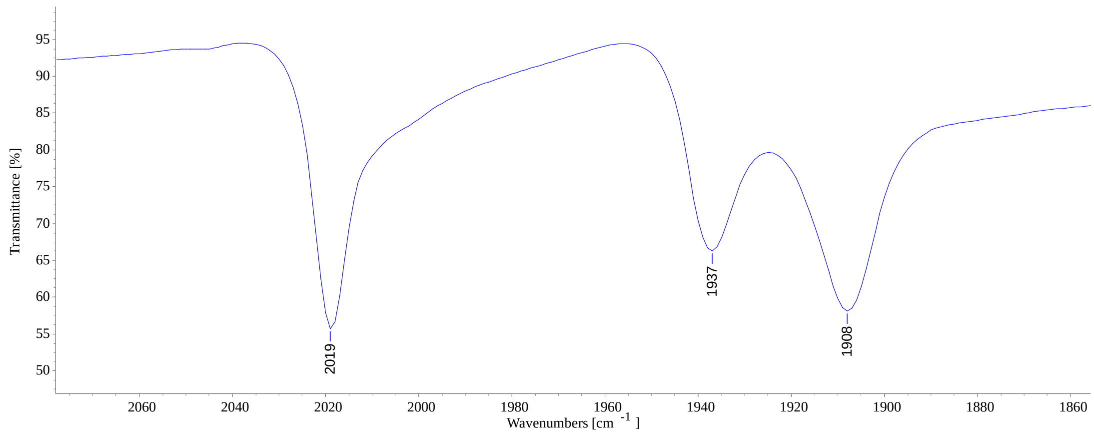

Figure S4. Solution-state IR spectrum of **1** in THF.

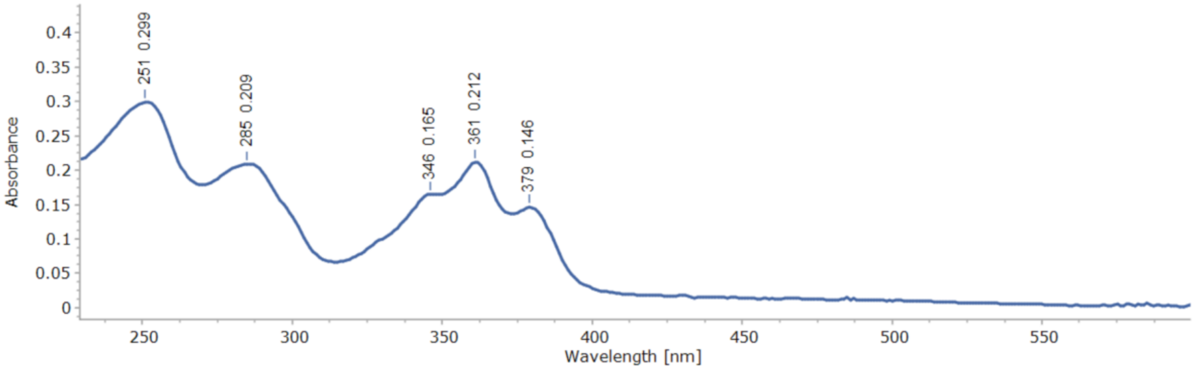

Figure S5. UV-Vis spectrum of **1** in DCM (0.01 mM).

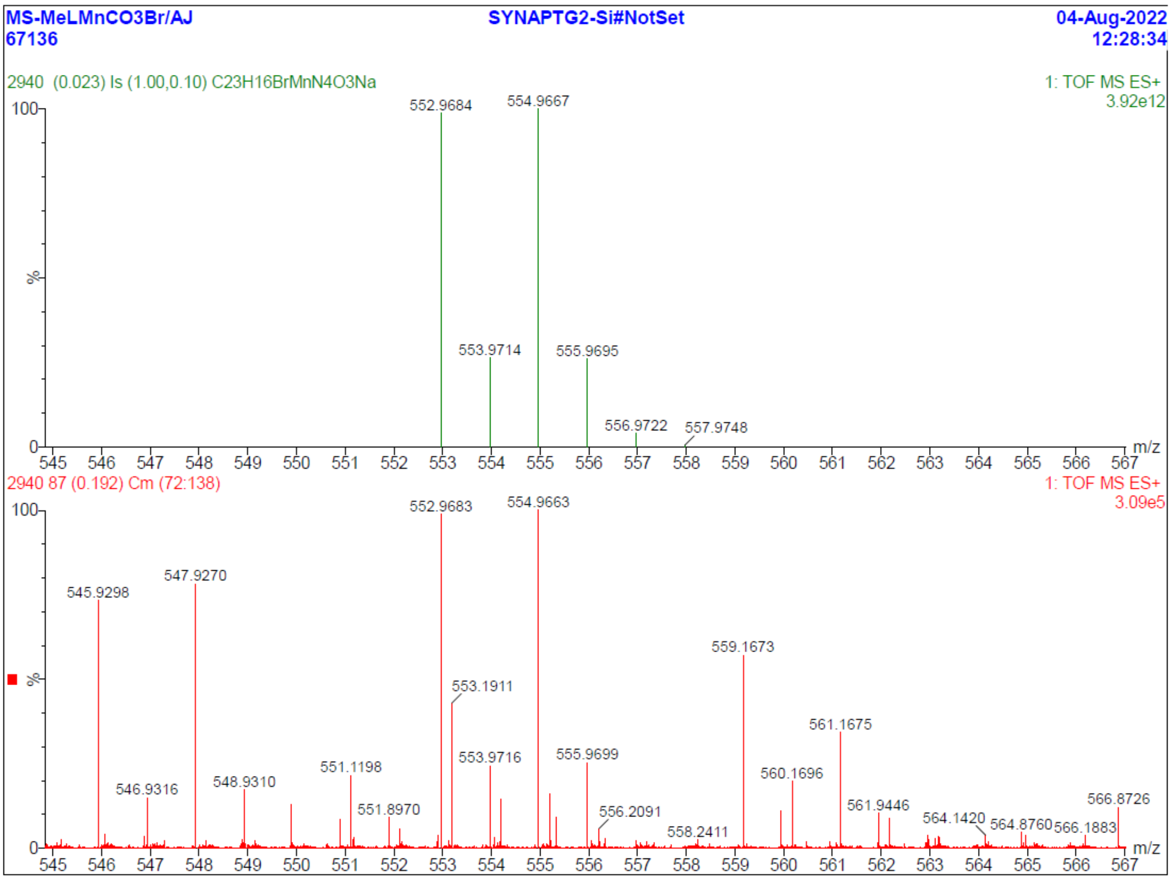

Figure S6. High resolution ESI mass spectrum of **1** (bottom) and simulated isotope pattern for [**1** + Na]$^+$ (top).

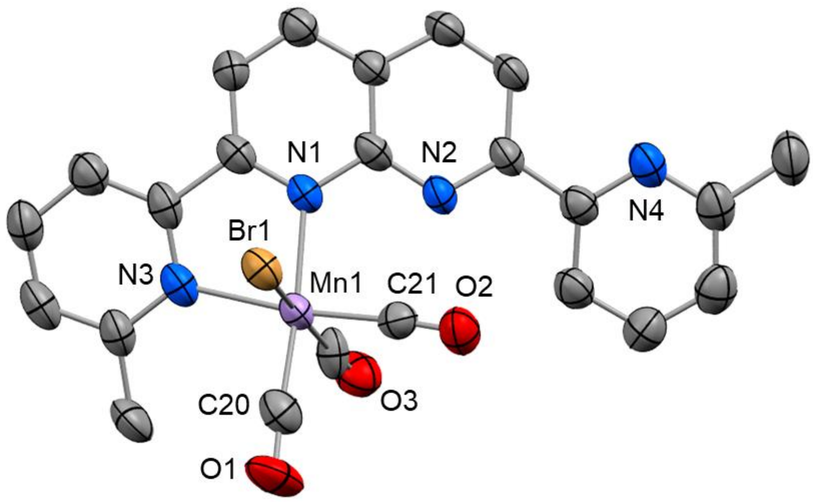

Figure S7. X-ray crystal structure of **1**·THF (50% displacement ellipsoids, hydrogen atoms and solvent omitted). Selected bond lengths (Å) and angles (°): Mn1–N1 2.055(6), Mn1–N3 2.092(5), Mn1–Br1 2.536(1), Mn–CO 1.814(9) – 1.830(7), N1–Mn1–N3 78.0(2).

Characterisation data for [$Mn_2(CO)_6(^{Me}L)$] (2)

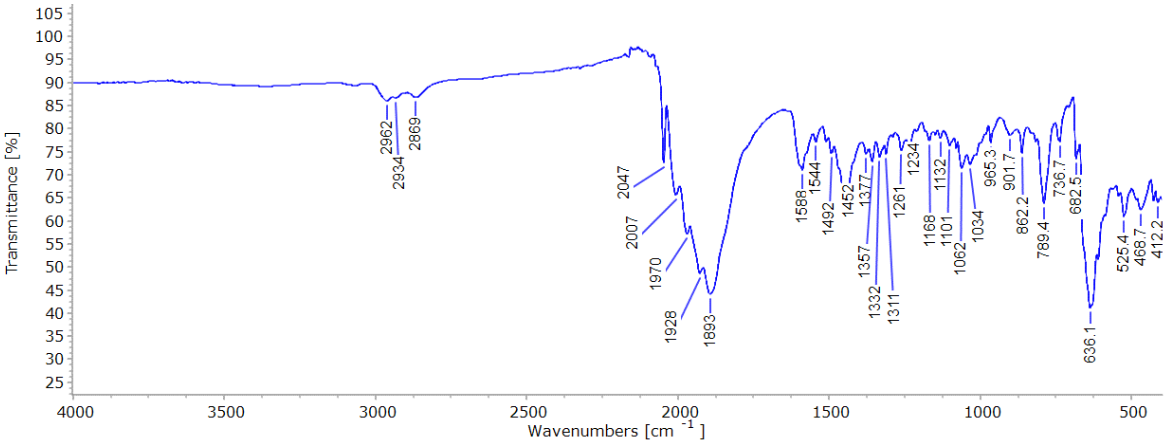

Figure S8. Solid-state IR spectrum of **2**.

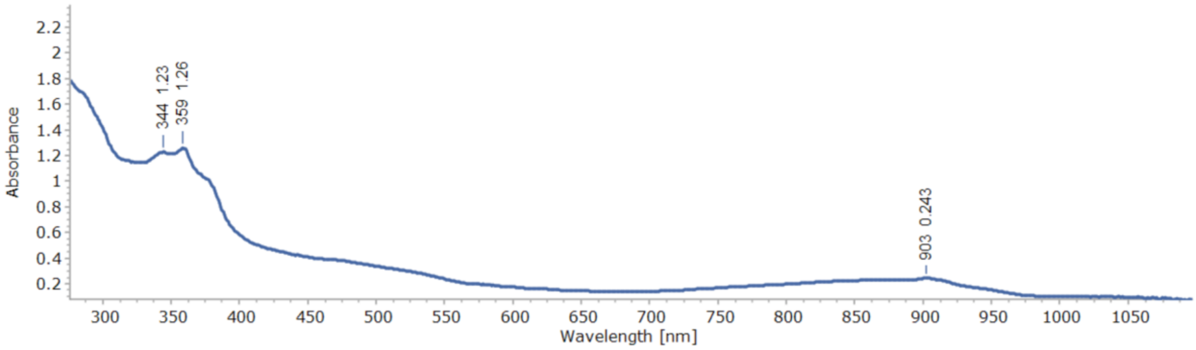

Figure S9. UV-Vis spectrum of **2** in THF (0.15 mM).

Characterisation data for [$MnCl_2(^{Me}L)$] (3)

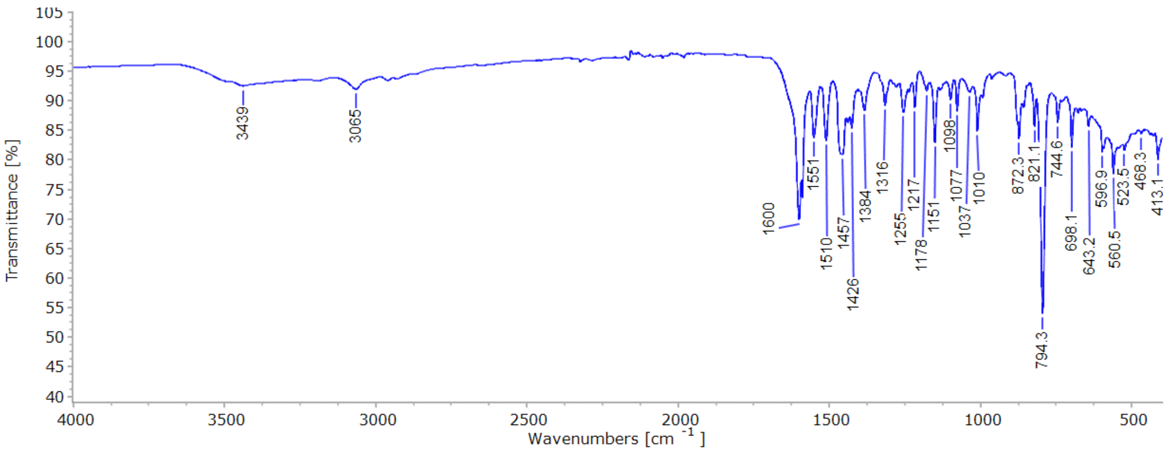

Figure S10. Solid-state IR spectrum of **3**.

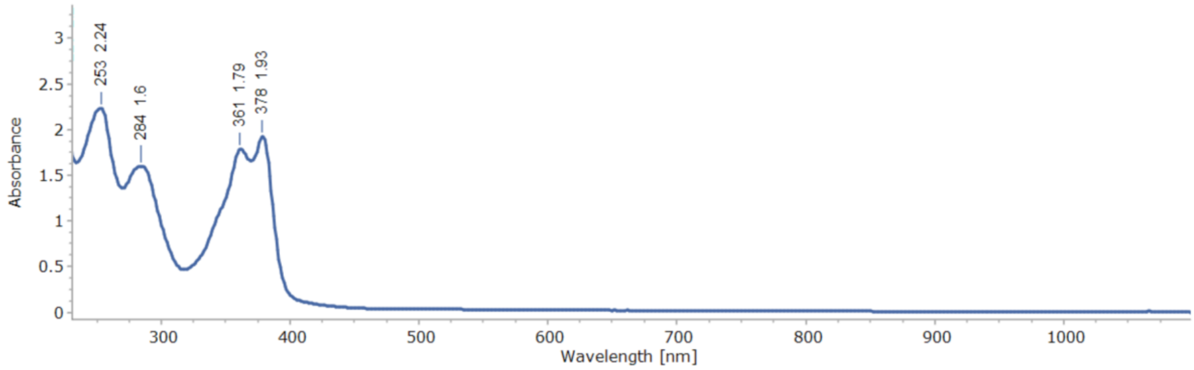

Figure S11. UV-Vis spectrum of **3** in DCM (0.1 mM).

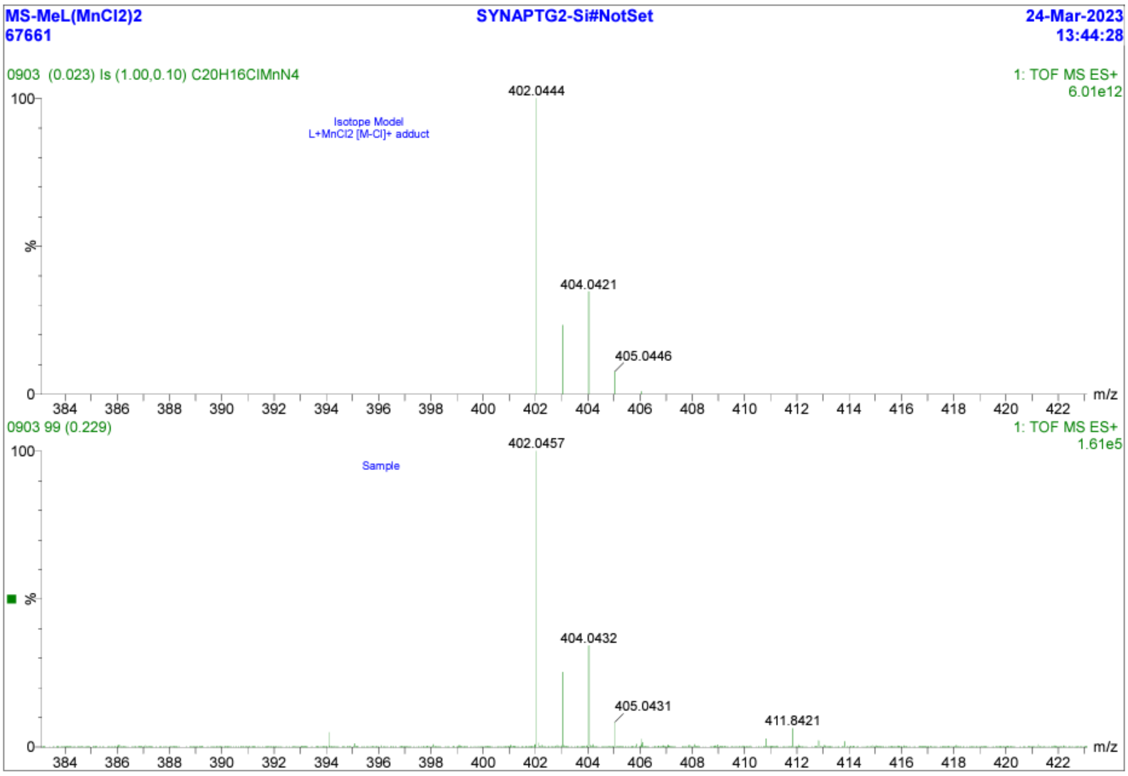

Figure S12. High resolution ESI mass spectrum of **3** (bottom) and simulated isotope pattern for [**3** − Cl]$^+$ (top).

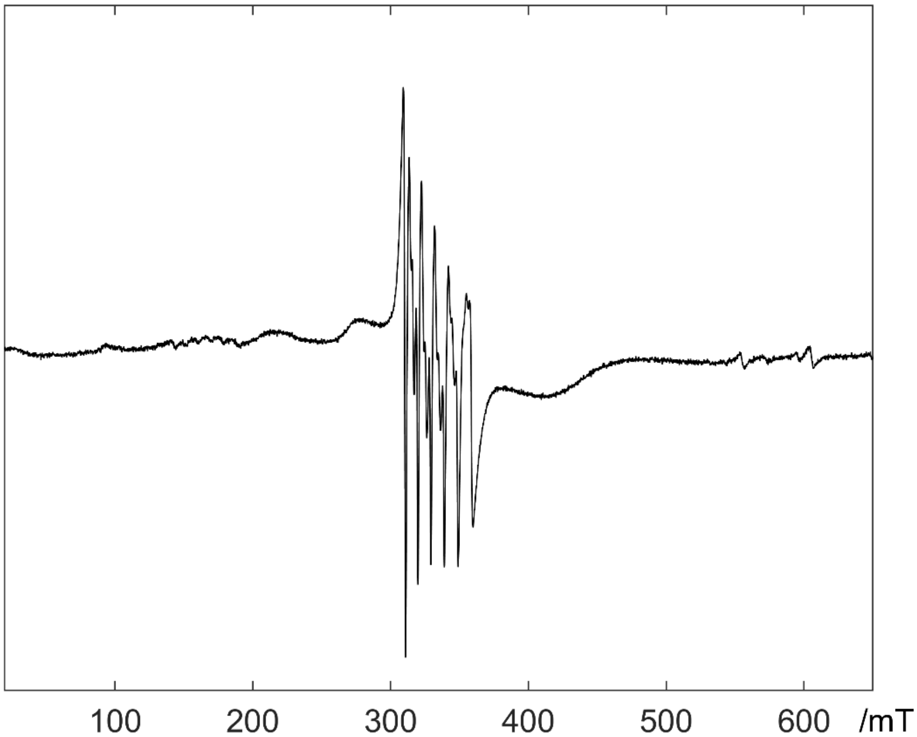

Figure S13. The X-band CW EPR spectrum of **3** in 2-methyl-THF at 50 K. The spectrum was acquired under non-saturating conditions with a microwave power of 0.0006325 mW and a modulation amplitude of 0.5 mT. The central six-line splitting pattern arises from hyperfine interactions to a single ^{55}Mn nucleus (I = 5/2, 100% natural abundance), suggesting compound **3** retains its monometallic nature in solution.

Characterisation data for [$Mn_2(^{Me}L)_2$] (4)

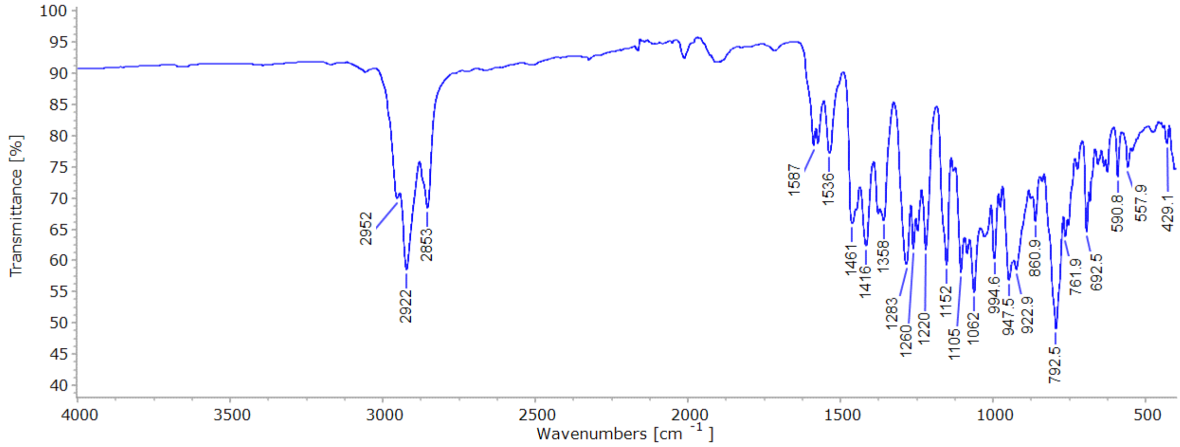

Figure S14. Solid-state (nujol) IR spectrum of **4**.

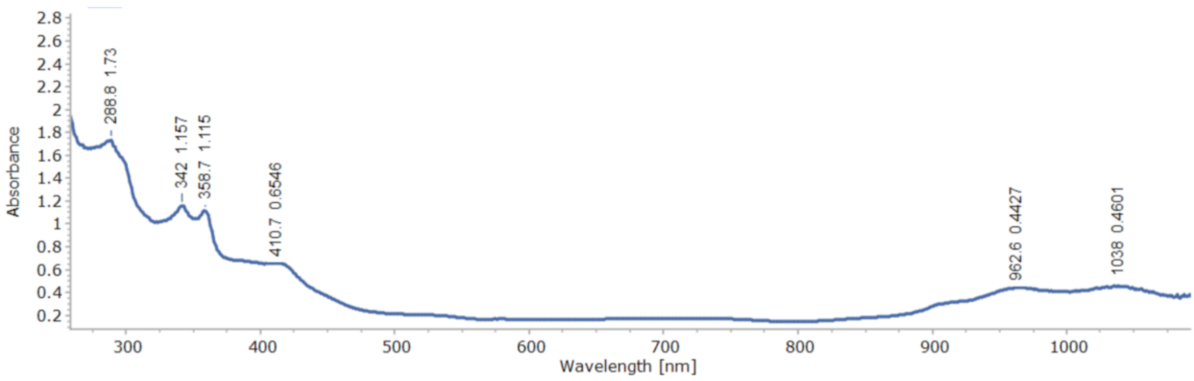

Figure S15. UV-Vis spectrum of **4** in THF (0.1 mM).

Crystallographic data

Table S1. Summary of the crystallographic data.

	[MnBr(CO)$_3$(^{Me}L)]·THF (1·THF)	**[Mn$_2$(CO)$_6$(^{Me}L)] (2)**	**[MnCl$_2$(^{Me}L)]$_2$·(CH$_2$Cl$_2$)$_2$ (3$_2$·(CH$_2$Cl$_2$)$_2$)**	**[Mn$_2$(^{Me}L)$_2$] (4)**
CCDC Number	2266510	2266511	2266512	2266513
Chemical formula	$C_{27}H_{24}BrMnN_4O_4$	$C_{26}H_{16}Mn_2N_4O_6$	$C_{42}H_{36}Cl_8Mn_2N_8$	$C_{100}H_{80}Mn_5N_{20}$
Formula mass	603.35	590.31	1046.27	1836.54
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic
a/Å	9.0809(7)	15.9780(4)	9.89580(10)	30.545(6)
b/Å	11.6416(8)	10.8779(2)	17.77790(10)	12.893(3)
c/Å	12.6776(11)	13.9502(3)	25.6158(2)	22.833(5)
α/°	78.587(7)	90	90	90
β/°	84.102(7)	96.032(2)	91.1170(10)	104.52(3)
γ/°	81.662(6)	90	90	90
Volume/Å^3	1296.05(18)	2411.22(9)	4505.64(6)	8705(3)
Temperature/K	150	150	150	100(2)
Space group	P-1	C2/c	P2$_1$/c	P2/c
Z	2	4	4	4
Radiation type	Cu Kα	Cu Kα	Cu Kα	Synchrotron – equivalent to Mo Kα
Absorption coefficient	6.289	8.969	9.260	0.767
No of reflections measured	7410	7442	64904	78241
No of independent reflections	4839	2424	9584	25666
R_{int}	0.0425	0.0206	0.0854	0.0691
Final R_1 values ($I > 2\sigma(I)$)	0.0683	0.0322	0.0682	0.0653
Final wR(F^2) values ($I > 2\sigma(I)$)	0.1744	0.0853	0.1882	0.1979
Goodness of fit on F^2	1.026	1.058	1.040	1.042

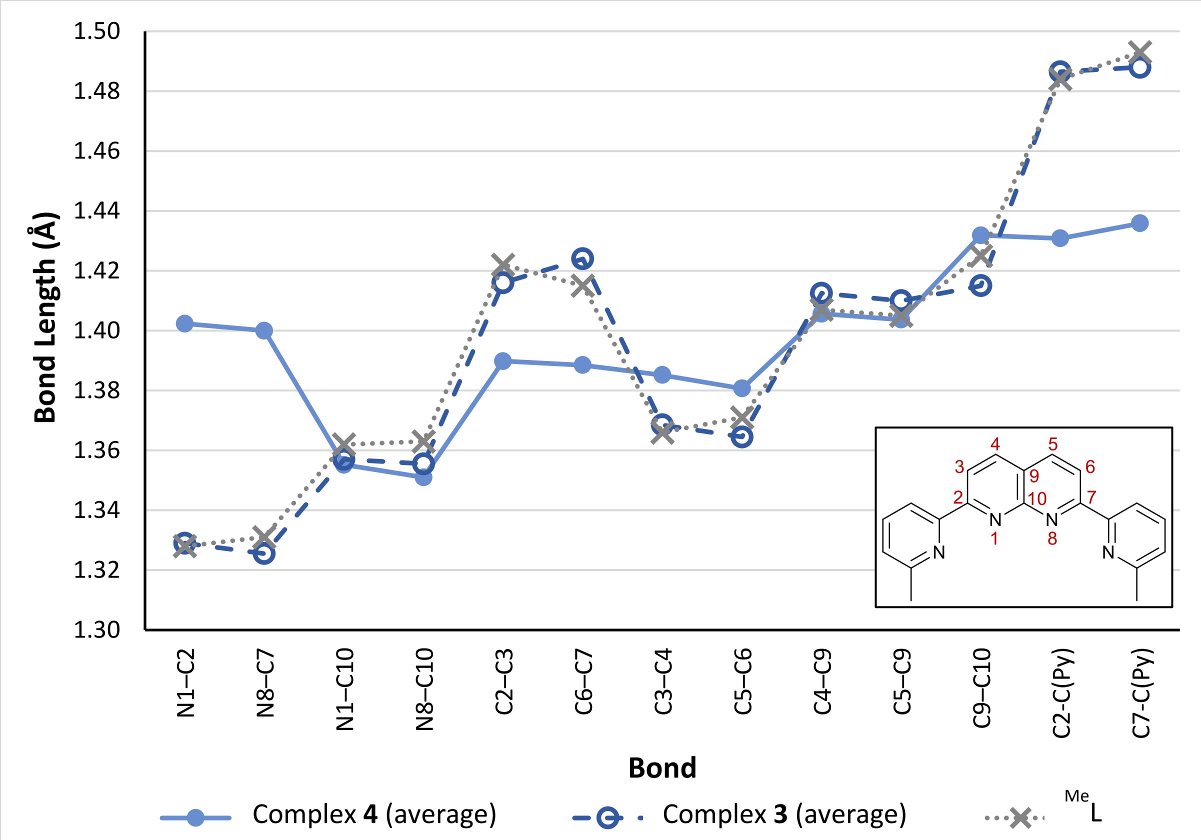

Figure S16. Comparison of naphthyridyl N–C and C–C bond lengths from X-ray crystallographic data for complex **4** (average of three independent **4** molecules in the unit cell), complex **3** (average of the two **^{Me}L** ligands in the **3**$_2$ structure) and ^{Me}L.[1] Insert: Atom numbering scheme.

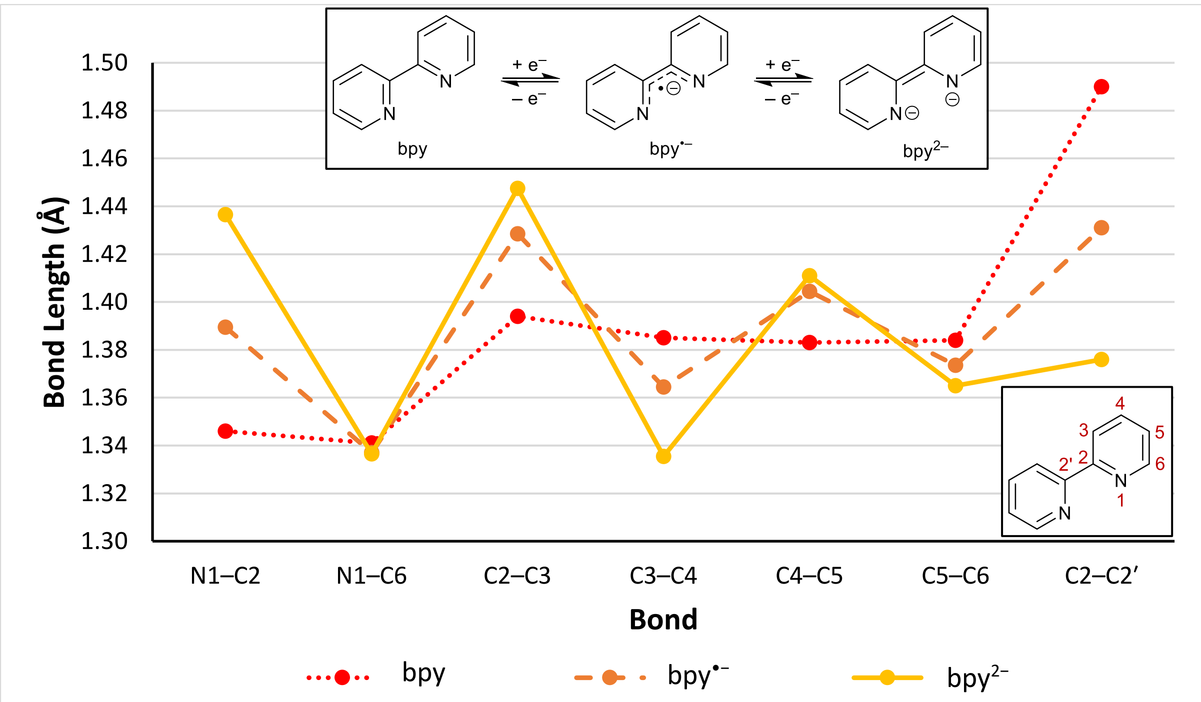

Figure S17. Comparison of 2,2′-bipyridine (bpy) average N–C and C–C bond lengths from X-ray crystallographic data for different bpy oxidation states.[2–6] Insert: bpy oxidation states (top), atom numbering scheme (bottom).

Supplementary EPR data and discussion

1) Spin Hamiltonian Formalism: The basis set that describes the Mn-dimer spin manifold can be built from the product of the eigenstates of the interacting spins:

$$|S_a \quad S_b \quad M_a \quad M_b \quad I_a \quad I_b \quad m_a \quad m_b\rangle \qquad \textbf{(Eq. S1)}$$

Here S_a refers to spin fragment a, S_B to spin fragment b. For a high spin Mn^{II} both takes the value 5/2. For a high spin Mn^0 both take the vale 3/2. M_a and M_b refers to the electronic magnetic sub-level, $-S_i$, $1-S_i$, …, S_i-1, S_i; I_i takes the value 5/2; and the corresponding m_i terms the values $-I_i$, $1-I_i$, ..., I_i-1, I_i.

The full spin Hamiltonian that describes the spin manifold is:

$$\hat{H} = -2J\vec{S}_a \cdot \vec{S}_b + \vec{S}_a \cdot \mathbf{d_{ab}} \cdot \vec{S}_b + \vec{S}_a \cdot \mathbf{d_a} \cdot \vec{S}_a + \vec{S}_b \cdot \mathbf{d_b} \cdot \vec{S}_b + \beta\vec{B}_0 \cdot \mathbf{g_a} \cdot \vec{S}_a + \beta\vec{B}_0 \cdot \mathbf{g_b} \cdot \vec{S}_b$$
$$-g_n\beta_n\vec{B}_0 \cdot \vec{I}_a - g_n\beta_n\vec{B}_0 \cdot \vec{I}_b + \vec{S}_a \cdot \mathbf{a_a} \cdot \vec{I}_a + \vec{S}_b \cdot \mathbf{a_b} \cdot \vec{I}_b \qquad \textbf{(Eq. S2)}$$

It contains: i) a magnetic exchange coupling term, parameterized in terms of J; ii) an electronic dipolar coupling term, parameterized in terms of d_{ab}, which itself is constrained by the distance between the two Mn ions; iii) second order zero field splitting terms, describing splitting of energy levels of each spin fragment (a and b) at zero-field; iv) the electron Zeeman terms describing the electron spin interaction of each spin fragment (a and b) with the applied magnetic field; v) the set of nuclear Zeeman terms, describing the interaction of each ^{55}Mn nucleus with the applied magnetic field and; vi) the set of hyperfine terms describing the interaction between the electron spin fragment *a or b* and each ^{55}Mn nucleus I_i.

Owing to the symmetry of the system we used the following approximations. We also assume that dipolar coupling between the two Mn sites (d_{ab}) is significantly smaller than that of the exchange coupling or the zero-field splitting of each site i.e. for a distance of 3.17 Å the electron-electron dipolar coupling is 1600 MHz and thus set to be zero.

$$\mathbf{d} = \mathbf{d_a} = \mathbf{d_b}$$
$$\mathbf{g} = \mathbf{g_a} = \mathbf{g_b}$$
$$\mathbf{a} = \mathbf{a_a} = \mathbf{a_b}$$
$$\mathbf{d_{ab}} = 0$$

(Eqs. S3)

Note too that the zero field splitting term of each spin fragment can be expressed in terms of two parameters (d_a and e_a):

$$\vec{S}_a \cdot \mathbf{d_a} \cdot \vec{S}_a = d_a\left[\vec{S}_{a,z}^2 - \frac{1}{3}S_a(S_a+1) + \frac{e_a}{d_a}\left(\vec{S}_{a,x}^2 - \vec{S}_{a,y}^2\right)\right] \qquad \textbf{(Eq. S4)}$$

In the instance where the first term of the spin Hamiltonian is large (strong exchange limit), the spin manifold can be described in terms of a set of spin sub-manifolds which each having a net (effective) spin.

$$\hat{H} = -2J\vec{S}_a \cdot \vec{S}_b \qquad \textbf{(Eq. S5)}$$

The effective spin states for a $S_a = S_b = 3/2$ dimer are:

$$S = |S_a + S_b|, |S_a + S_b - 1| \dots\dots\dots |S_a - S_b| = 3, 2, 1 \text{ and } 0$$

And the energy levels of the spin ladder are determined by:

$$E(S) = -JS(S+1) \qquad \textbf{(Eq. S6)}$$

The sign of J determines which of the effective spin states is the lowest in energy. For an antiferromagnetic interaction between the two sites (negative J), the S = 0 spin state is the lowest in energy, whereas for a ferromagnetic interaction between the two sites (positive J), the S = 3 state is the lowest in energy.

The basis set that describes each spin sub-manifold product of the effective spin eigenstate with that of the two nuclear spin eigenstates:

$$|S \quad M_S \quad I_a \quad I_b \quad m_a \quad m_b\rangle \qquad \textbf{(Eq. S7)}$$

And the effective spin Hamiltonian that describes each spin sub-manifold is:

$$\hat{H}_S = \vec{S}\cdot\mathbf{D}\cdot\vec{S} + \beta\vec{B}_0\cdot\mathbf{G}\cdot\vec{S} + \sum_{i=a,b}(-g_n\beta_n\vec{B}_0\cdot\vec{I}_i + \vec{S}\cdot\mathbf{A}\cdot\vec{I}_i) \qquad \textbf{(Eq. S8)}$$

It contains: i) a second order zero field splitting terms, describing splitting of energy levels of the spin sub-manifold at zero-field; ii) the electron Zeeman terms describing the interaction of the effective electron spin with the applied magnetic field; iii) the set of nuclear Zeeman terms, describing the nuclear spins interaction with the applied magnetic field and; iv) the set of hyperfine term describing the interaction between the effective electron spin and each nuclear spins I_i.

The spin Hamiltonian tensors **D**, **G** and **A** that describe the system in the strong exchange limit are a weighted sum of the spin Hamiltonian parameters of the individual spin fragments a and b. For an exchange coupled dimer **D**, **G** and **A** are equal to:

$$\mathbf{D} = \kappa_a\mathbf{d_a} + \kappa_b\mathbf{d_b} + \kappa_{ab}\mathbf{d_{ab}} = 2\kappa_a\mathbf{d}$$

$$\mathbf{G} = c_a\mathbf{g_a} + c_b\mathbf{g_b} = 2c_a\mathbf{g}$$

$$\mathbf{A} = c_a\mathbf{a_a} + c_b\mathbf{a_b} = 2c_a\mathbf{a}$$

(Eqs. S9)

Table S2 lists set of weights (spin projection factors) for a $Mn^{II}Mn^{II}$ dimer (S_a = 5/2, S_b = 5/2) and for a Mn^0Mn^0 dimer (S_a = 3/2, S_b = 3/2).

Table S2. Spin projection coefficients for homovalent exchange coupled dimers.[7]

S_1, S_2		S_T = 1	S_T = 2	S_T = 3	S_T = 4	S_T = 5
3/2, 3/2	c_a, c_b	0.5	**0.5**	0.5	-	-
	κ_a, κ_b	-1.2	**0.0**	0.2	-	-
	κ_{ab}	1.7	**0.5**	0.3	-	-
5/2, 5/2	c_a, c_b	0.5	0.5	**0.5**	0.5	0.5
	κ_a, κ_b	3.2	0.48	**0.02**	0.14	0.22
	κ_{ab}	3.7	0.98	**0.52**	1.25	0.28

2) Simulating the EPR spectrum. As briefly described in the main text, the Mn dimer species (**4**) displays two EPR signals:

- A multiline signal, centred at g = 2 with resolved ^{55}Mn hyperfine structure – at least 19 peaks are observed
- A broader EPR signal with two intense turning points at g = 5.1 and 2.0.

The lineshape of both are indicative of a coupled dimer. A detailed explanation of this is given below. All EPR simulations reported use the Easyspin package[8] implemented in MATLAB.

2.1) The multiline EPR signal. The multiline EPR signal observed is reminiscent of that seen for a $Mn^{II}Mn^{II}$ dimer.[9–11] For such dimers, the exchange coupling between the two metal ions is typically much larger than that of the zero-field splitting (ZFS) of each Mn ion, as high spin Mn^{II} characteristically exhibits small ZFSs (*d* < 1 GHz, 0.03 cm^{-1}). As such, the EPR signals of exchange coupled $Mn^{II}Mn^{II}$ dimers are described in terms of effective spin states and their EPR spectra simulated using an effective spin Hamiltonian (Eq. S8) – see the left-hand side of Figure S19.

For an $Mn^{II}Mn^{II}$ dimer, the multiline signal is predominately associated with the S = 3 spin-submanifold. For this effective spin sub-manifold, the spin projection factors the site zero field splitting of the two Mn ions are approximately zero, leading to this submanifold resolving a narrow EPR signal centered at g = 2. The ^{55}Mn hyperfine coupling observed for the coupled spin system is approximately half that seen for a monomeric species. This is because the spin projection factor for each Mn ion is ½, regardless of the effective spin state (see spin Hamiltonian formalism section, Table S2). This leads to a 11-line multiline pattern with a peak-to-peak splitting of approximately 4.5 mT. For a corresponding Mn^0Mn^0 dimer there also exists an effective spin submanifold with similar properties to that of the S = 3 sub-manifold of the $Mn^{II}Mn^{II}$ dimer. It is the S = 2 spin submanifold (see Table S2). It too will have spin projection factors the site zero field splitting of the two Mn ions are zero, leading to narrow EPR signal centered at g = 2.

2.2) The broad EPR spectrum. The broad EPR spectrum resembles that of S = 3/2 species in the weak field regime i.e. (d > gβH ≈ 0.3 cm^{-1}), resolving an intense absorptive feature at g=5 and a derivate feature at g=2. The energy-levels of such a system can be described in term of two isolated Kramer's doublets, with the EPR signal arising from transition within these doublets. The position of the low field turning point and the presence of a second turning point in the g=2 region both constrain the d tensor to be rhombic (e/d = 0.33). A simulation of the spectrum assuming a single (isolated) S=3/2 spin system is shown in the main text.

While most features of the broad spectrum are captured by the simulation assuming a single (isolated) S=3/2 spin system, there are a number of features that are not. These include:

- Low field signal 22 mT (g = 30)
- Additional peak at 200 mT (g = 3.35)
- High field signal at 770 mT (g =0.87)

All these features have exactly the same, near-curie temperature dependence as those of the more intense turning points characteristic of an isolated rhombic S=3/2 spin system, indicating that they all arise from the same spin system. These additional features are taken as evidence that the spectrum should be assign to a magnetically coupled S=3/2 dimer.

2.3) S_1=3/2, S_2=3/2 exchange coupled spin state ladder. The temperature dependence of the EPR signals allows an estimate of the magnitude and sign of the magnetic exchange coupling (*J*) to be made. As shown in the main text, the temperature dependence is near-curie (linear), with the small drop in EPR intensity at low temperatures. The small drop in EPR intensity at low temperatures, must arise from populating the EPR silent states (e.g. an effective S = 0 state). This requires the ground state to have the lowest total effective spin and that the coupling between the two Mn ions to be antiferromagnetic. The near-linear temperature dependence of all EPR turning points indicates that all effective spin states of the manifold, including higher effective spin state (S = 2, S = 3), are populated at all temperatures assayed, suggesting the magnitude of *J* is estimated to be only 0.5 cm^{-1} i.e. of the same order of magnitude as that of the site ZFS of each Mn ion.

As a consequence, the Mn dimer is best described as being in the intermediate exchange limit ($|J| \approx |d|$). This result is expected. **4** has no direct through bond (super-exchange) pathway between the two Mn ions, and as such, the interaction between the two Mn ions is expected to be small; Mn^{II} dimers with no direct through bond linkage have exchange coupling of 1 cm^{-1}.[9] In addition, unlike high spin Mn^{II}, high spin Mn^{0} is expected to displaying large site ZFS (cm^{-1}), as seen in the recently characterized Mn^{0} complex.[12] Note that the ZFS of a transition metal ion has two contributions which arise from the spin-orbit coupling (SOC), spin-spin (SS) coupling of its set of d-electrons. Of these, the SOC dominates. A high spin Mn^{0} has an orbitally degenerate ground electronic state (^{4}F) in the absence of crystal field splitting, and as such, low lying electronic excited state, leading to a large SOC contributing to its ZFS (d). In contrast, a Mn^{II} ion has an orbitally non-degenerate ground state (^{6}S) and thus non SOC contribution, with its ZFS coming about from only the SS term.

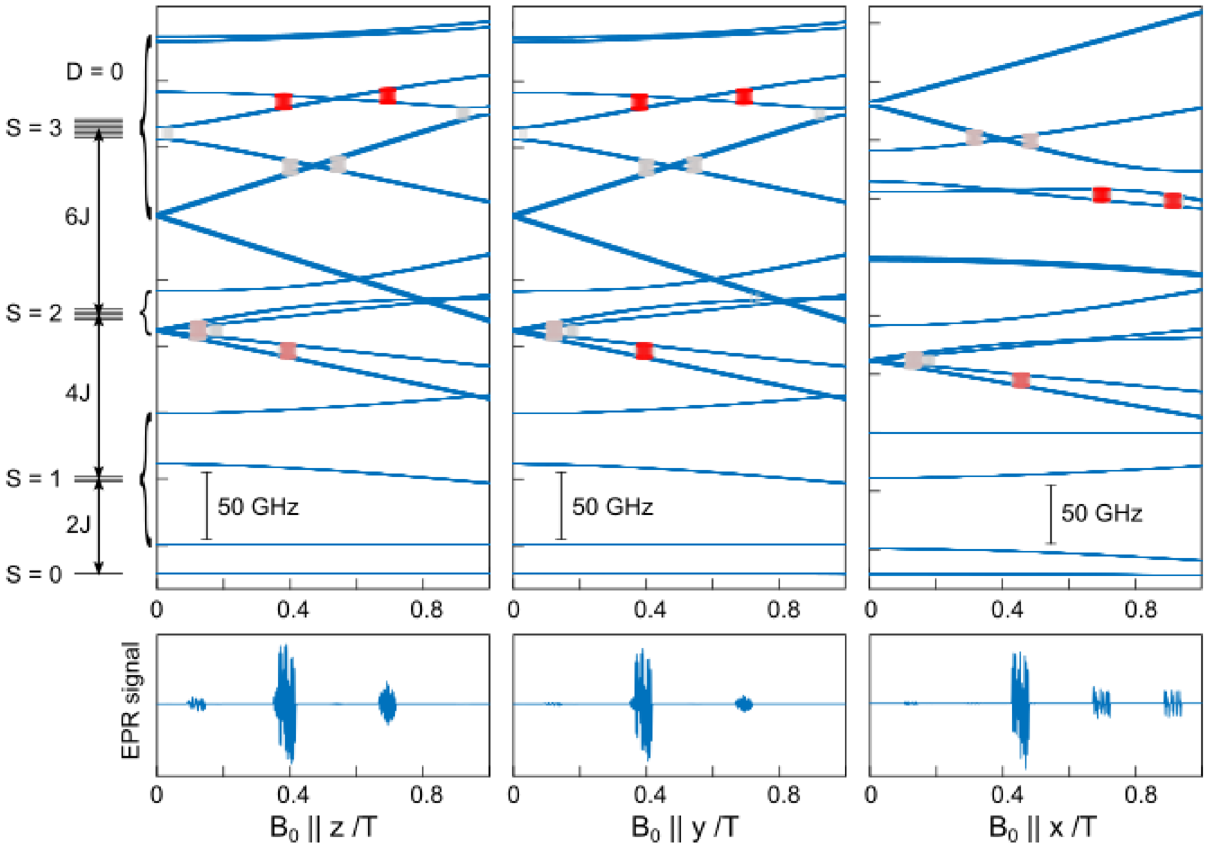

Figure S18. Top) Energy level diagrams for the $Mn^{0}Mn^{0}$ dimer complex simulation shown in the main text. Simulation parameters: S_1 = 3/2; S_2 =3/2; J = 0.85; d_1 = d_2 = -1.12 cm^{-1}; e_1/d_1 = e_2/d_2 = 0.26; g_1 = g_2 = 1.92. The three panels correspond to the B_0 field aligned along the three principal axes of the complex defined by the D-tensor: D_Z, D_Y and D_X. The red and grey vertical lines represent allowed transitions. The energy-level ladder on the left-hand side shows the energy-levels at zero-field in the absence of any ZFS. **Bottom)** Corresponding predicted single crystal EPR spectra at X-band.

Thus, describing the spin system in terms of effective spin state is strictly incorrect. That said, it is still useful to use this nomenclature, as it provides an explanation for how the two EPR signal observed come about. The exchange coupled spin state ladder of an S_1=3/2, S_2=3/2 is shown in Figure S18, solved along the three canonical axes. The lowest energy level is the effective S = 0 ground state, which has no magnetic field dependence. The next three levels derive from the effective S = 1 state, which has a large ZFS, as expected from the spin projection factors listed in Table S2. As such there is no EPR transitions between these levels as the resonance condition is not met.

It is instead the S =2, and to a lesser extent the S=3, effective spin states that describe the EPR signals observed. The S=2 effective spin state has a ZFS is small, which leads to transitions within this sub-manifold appearing at g = 2. Furthermore, along two axes, the same transition appears at the same resonance field(s), suggesting there are EPR transitions present that are intrinsically narrow. These would potentially allow ^{55}Mn hyperfine structure to be resolved, as seen earlier for Mn^{II} dimers (see Figure S18 and Figure S19, panel D) which shows an enlargement of the g = 2 region).

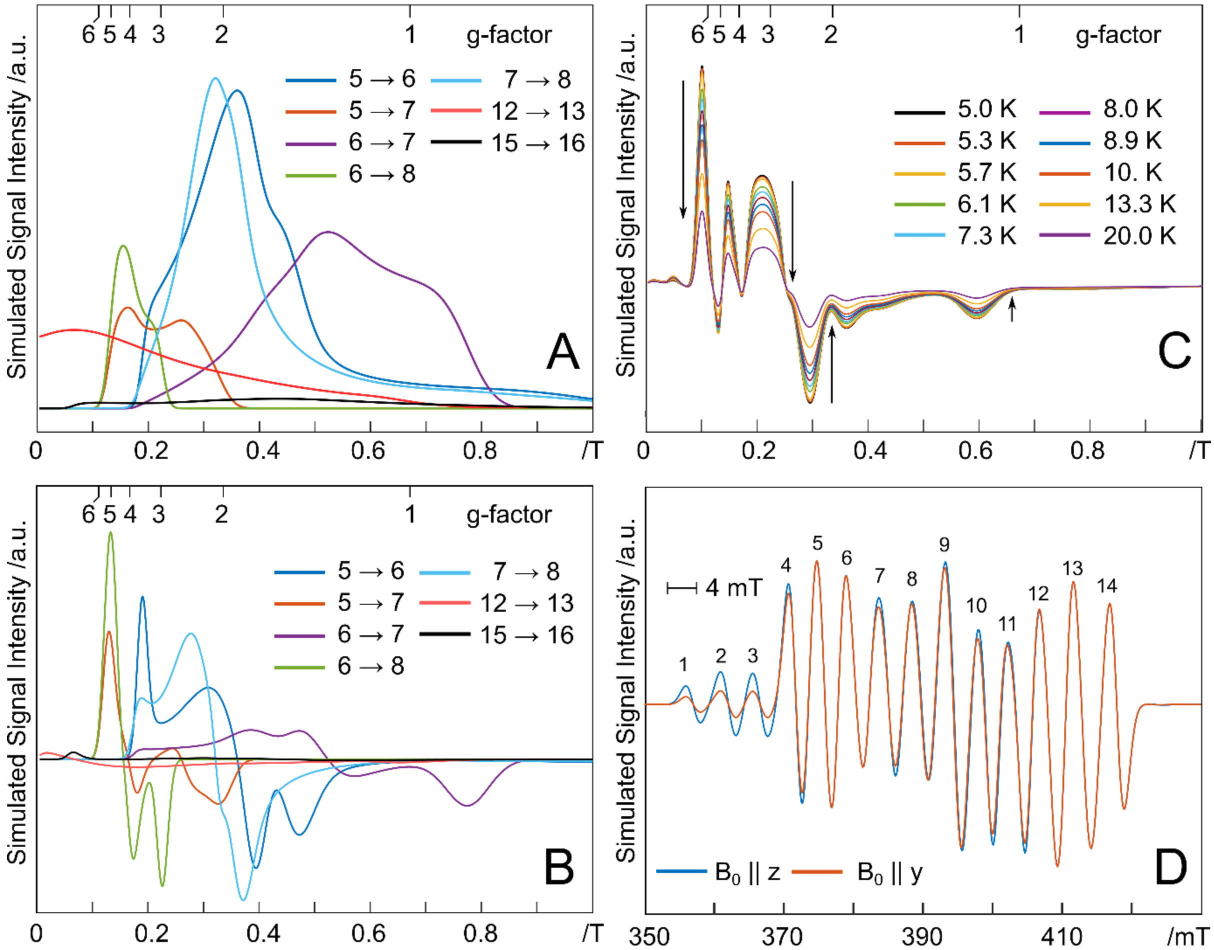

Figure S19. Decomposition of the Mn^0Mn^0 dimer complex simulation shown in the main text. Simulation parameters: S_1 = 3/2; S_2 =3/2; J = 0.85; d_1 = d_2 = -1.12 cm^{-1}; e_1/d_1 = e_2/d_2 = 0.26; g_1 = g_2 = 1.92. An isotropic linewidth of 20 mT was used. To capture linebroadening at higher magnetic fields, D strain was included i.e. d_{strain} = 0.24 cm^{-1} , e_{strain} = 0.168 cm^{-1}. **A)** Intense EPR transitions which make up the EPR spectrum. The energy levels 5 through 9 are derived from the effective S=2 spin sub-manifold. The energy levels 10 through 16 are derived from the effective S=3 spin sub-manifold. **B)** Corresponding first derivative of the EPR transitions shown in panel A. **C)** Calculated temperature dependence of the EPR signal over the 5-20 K temperature range. **D)** Calculated 14-line multiline spectrum assuming B_0 is aligned along the along the z and y principal axes of the complex defined by the D-tensor: D_Z, D_Y and D_X.

The same spin sub-manifold (S =2) also resolves transitions at low and high field, with these tuning points being dependent on the interplay of *J* and *D* i.e. the extent to which the S=2 submanifold mixes with S = 1 and S = 3 – or equally the extent to which the strong exchange limit breaks down.

The same observations can be made from decomposing the Mn^0 dimer simulation shown in the main text (Figure S19, panels A and B). In this simulation two identical interacting S=3/2 spin are assumed. This simulation reproduces all features seen in the experimental spectrum and its temperature dependence. All the intense transitions derive from the S=2 submanifold (energy-levels, 5 through 9), which goes to why the temperature dependence of all turning points are the same. Two transitions give rise to an axial signal whose main intensity is centred at g=2: the 5→6 and 7→8. The superposition of both likely give rise to the >11 peak multiline pattern observed.

As the shape of individual EPR transitions are dependent on the interplay of J and the fine structure parameters (d_1, d_2, e_1, e_2), we suspect the fitted values are correlated. That said, the reproduction of the temperature dependence (see Figure 5 main text and Figure S19, panel C), including the small deviation seen between the high and low field edges, suggests that the magnitude of both J and fine structure parameters (d_1, d_2) is well constrained, with both being approximately 1 cm^{-1} and the d must be negative.

We note that the ZFS is substantially smaller than for the for recently reported high spin, low coordinate Mn^0 complex (1 cm^{-1} vs. 3.1 cm^{-1}). In this previous study it was suggested that its oxidation state, while formally Mn^0, also had some Mn^{II} and Mn^{IV} character i.e. suggesting the ligand is partially reduced. We hypothesize that a decrease in magnitude of the ZFS seen for the Mn^0 site(s) of our complex reflects an increase in its Mn^{II} and Mn^{IV} character/more reduced ligand character – however we stress we can't quantify this increase. Note too that while each spin fragment of the dimer may have ligand character, the total spin of the spin fragment is well defined (S = 3/2).

2.4) Collapse of both the multiline and broad EPR signal at higher temperatures: It was seen that both the multiline and broad EPR signal were progressively lost at higher temperatures with the concomitant increase of a broad unstructured signal centred at g=2. This behaviour had not previously been seen for $Mn^{II}Mn^{II}$ dimers. We suspect that this is an example of exchange narrowing. Exchange narrowing can occur when the interaction between the two spin fragments is of the order of kT. Exchange narrowed spectra are characterized by a Lorentzian lineshape, is consistent with the signal observed.[13] Temperature induced exchange narrowing further supports the assignment of the two EPR signals to that of a weakly coupled dimer.

2.5) Inability to reproduce both EPR signals in a single simulation. In principle, the entire EPR lineshape (multiline + broad signal) should be reproduced by a single spin Hamiltonian simulation. We were not able to achieve this. This is because the apparent linewidth of the multiline signal and the broad signal are vastly different. It has previously been observed in Mn^{II} complexes that different spin sub-manifolds display different line broadening mechanisms. The linewidth of broader components of a Mn^{II} dimer signal are due to inhomogeneity of the ZFS tensor (D), which is composed of the site ZFS tensors (d_a and d_b). In contrast, the linewidth of the S =3 spin submanifold of Mn^{II} dimer signal is instead due to inhomogeneity of the d_{ab} tensor (i.e. small variations in the Mn-Mn distance). We suspect the same is the case here, for the Mn^0 dimer.

Computational data

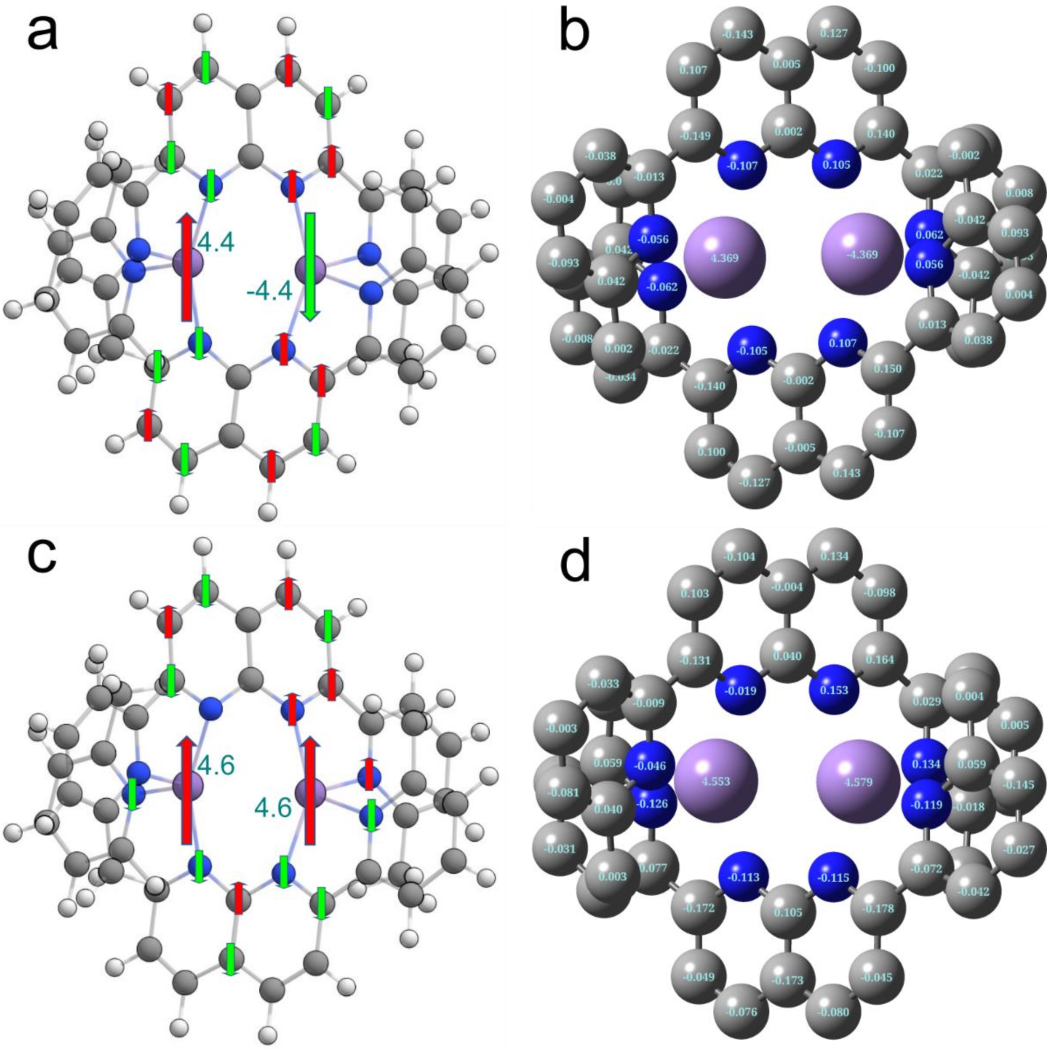

Figure S20. (a, c) Formal spin densities inducing local magnetic moments with their directions on Mn atoms, and the non-metallic atoms that have a significant contribution to the total magnetic moment of the open-shell singlet and nonet high spin states of **4**. **(b, d)** Formal spin density values of individual atoms in the open-shell singlet and nonet high spin states of **4**.

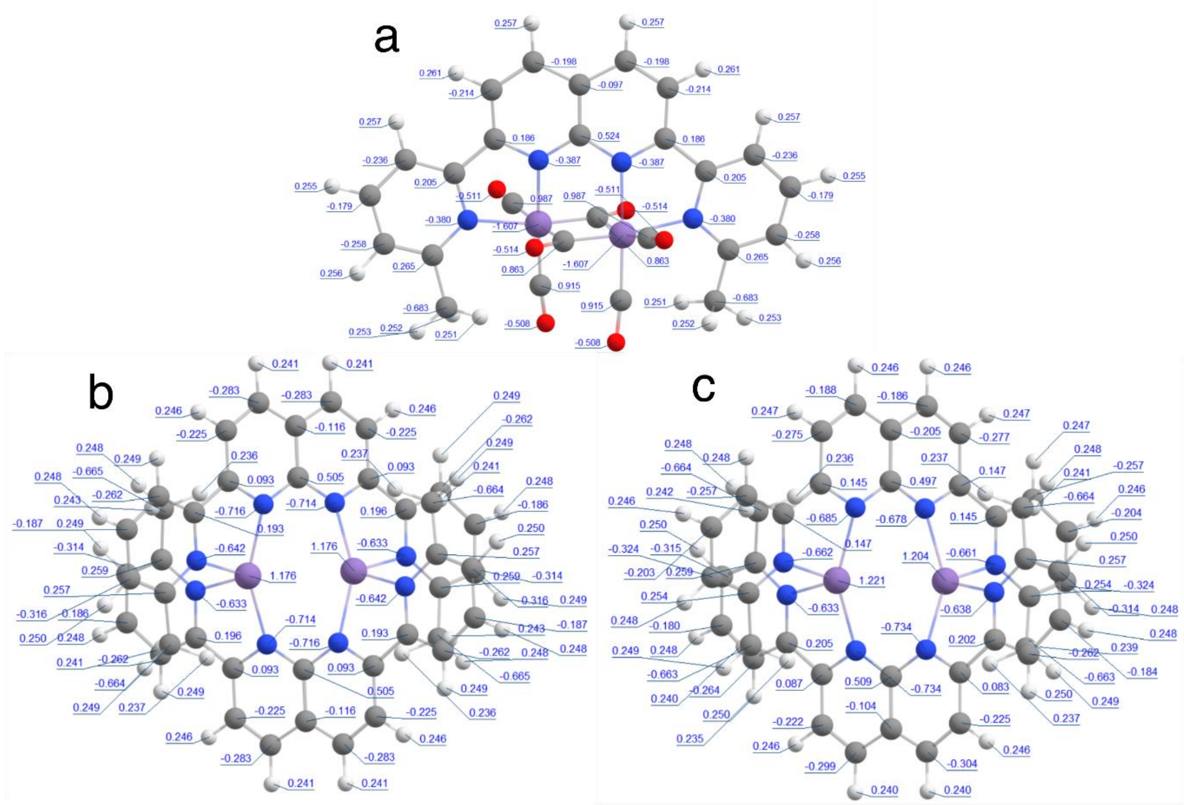

Figure S21. Charge of individual atoms obtained from NBO analysis of the singlet state of **2 (a)**, of the broken-symmetry singlet state of **4 (b)**, and the nonet state of **4 (c)**.

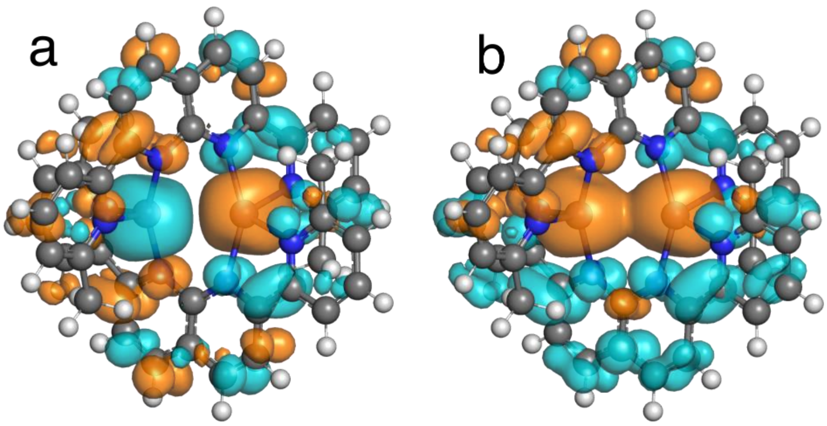

Figure S22. Spin densities of the open-shell singlet **(a)** and nonet **(b)** states of **4**.

Table S3. Relative Gibbs free energies (G, 298.15 K, THF) of the various spin states of **2** and **4**, and their calculated bond lengths, bond critical bond densities (ρ_{cp}), Laplacian of the electron density ($\nabla^2\rho_{cp}$), total energy density (H_{cp}) and metal-metal decomposed energy components of interactions between Mn and Mn.[a]

Species	Unpaired electrons	Relative G (kJ/mol)	M···M distance (Å)	BCP density ρ_{cp} (a.u.)	Laplacian $\nabla^2\rho_{cp}$ (a.u.)	Total energy density H_{cp} (a.u.)	$E_{covalent}$ (kcal/mol)
2-singlet	0	0	2.82	0.029	0.078	-0.001	-12.80
2-triplet	2	91.8	2.71	0.000	0.000	0.000	-
2-quintet	4	221.0	2.48	0.056	0.110	-0.014	-35.78
2-septet	6	287.4	3.44	0.000	0.000	0.000	-
2-nonet	8	228.2	3.41	0.000	0.000	0.000	-
4-singlet	0	443.0	2.91	0.023	0.030	-0.003	-29.05
4-singlet-BS	0	0	2.92	0.015	0.029	-0.003	-
4-triplet	2	463.6	2.89	0.022	0.034	-0.002	-
4-quintet	4	352.8	2.85	0.020	0.033	-0.002	-14.14
4-septet	6	185.4	2.91	0.019	0.027	-0.002	-16.09
4-nonet	8	41.6	2.97	0.012	0.030	0.006	-6.34
4-11et	10	70.8	2.98	0.013	0.028	0.004	-6.09

[a] Based on QTAIM calculations at the M062X/TZP//wB97XD/6-31G(d) level of theory unless noted otherwise. [b] Calculated with the wB97XD functional in conjunction with Def2TZVPD basis set for Mn and Def2SVPD for all non-metal atoms using wB97XD/6-31G(d) geometries, and SMD to model the THF solvent environment. BS indicates the spin broken symmetry state.

Table S4. Energy components (Hartree, 298.15 K) used to calculate Gibbs free energies of all species in Table S3.

Species	E [b]	E	ZPE	TC	TS	H	G
2-singlet	-3971.29828	-3972.19889	0.38012	0.03192	0.09691	-3970.88436	-3970.97823
2-triplet	-3971.25960	-3972.15855	0.37832	0.03266	0.09955	-3970.84673	-3970.94325
2-quintet	-3971.20822	-3972.10615	0.37618	0.03323	0.10018	-3970.79692	-3970.89406
2-septet	-3971.17756	-3972.07946	0.37304	0.03410	0.10327	-3970.76853	-3970.86877
2-nonet	-3971.18670	-3972.08410	0.36611	0.03763	0.11327	-3970.78107	-3970.89131
4-singlet	-4281.80303	-4282.87952	0.64371	0.03987	0.11258	-4281.11757	-4281.22712
4-singlet-BS	-4281.95784	-4283.04201	0.64028	0.04219	0.11682	-4281.27443	-4281.38822
4-triplet	-4281.78540	-4282.88119	0.64313	0.04113	0.11476	-4281.10019	-4281.21194
4-quintet	-4281.82616	-4282.90541	0.64268	0.04031	0.11559	-4281.14128	-4281.25384
4-septet	-4281.88891	-4282.97177	0.64175	0.04162	0.11606	-4281.20460	-4281.31764
4-nonet	-4281.93979	-4283.02391	0.64047	0.04129	0.11926	-4281.25614	-4281.37237
4-11et	-4281.92792	-4283.01026	0.63926	0.04140	0.11892	-4281.24538	-4281.36126

[a] Unless stated otherwise, calculations were performed at the wB97XD/6-31G(d) level of theory using SMD to simulate the effects of THF. E is the total DFT energy, ZPE is the zero-point vibrational energy, TC is the thermal correction to the enthalpy, H is the total enthalpy, TS is the temperature times the total entropy, and G is the total Gibbs free energy in solution and includes a correction for change of state from 1 atm to 1 M. [b] Calculated with the wB97XD functional in conjunction with Def2TZVPD for Mn and Def2SVPD for all non-metal atoms based on the wB97XD/6-31G(d) optimal geometry using SMD to model the THF solvent environment. BS indicates the spin broken symmetry state.

Table S5. Charge values of Mn atoms and ligands of a singlet state of **2**, and the broken-symmetry singlet and nonet states of **4**.

Species	Mn	Mn	Ligand	Ligand
2-singlet	-1.6	-1.6	0.8	2.4[a]
4-singlet-BS	1.2	1.2	-1.2	-1.2
4-nonet	1.2	1.2	-1.2	-1.2

[a]Total charge value of all CO ligands.

XYZ coordinates

```
Mn2L(CO)6-singlet.xyz
Mn          8.2491790000         2.8436220000        10.0290420000
O           7.9974670000         2.9626750000        12.9687800000
N           7.7391000000         4.7367900000         9.6328720000
N           8.8235490000         3.0991080000         8.0201360000
O          11.0592800000         3.2342550000        10.7745220000
O           8.5189300000        -0.0469260000        10.6063550000
C           6.8895630000         5.4539070000        10.4047370000
C           8.9913650000         4.4146140000         7.6905340000
C           8.3566700000         5.3502880000         8.6010800000
C           9.6703420000         4.8199150000         6.5358130000
H           9.8155530000         5.8740110000         6.3280780000
C           6.8895630000         6.8704040000        10.4047580000
C           7.6407660000         7.5111080000         9.3906610000
H           7.6438400000         8.5954820000         9.3295260000
C           9.2486420000         2.1629600000         7.1340780000
C           7.8996620000         2.9139080000        11.8081730000
C           8.3148720000         6.7504210000         8.4625890000
H           8.8316370000         7.2335540000         7.6408570000
C          10.1324320000         3.8595190000         5.6596800000
H          10.6548570000         4.1423470000         4.7507200000
C           9.8902660000         2.5187740000         5.9534300000
H          10.1995280000         1.7382350000         5.2657600000
C           9.9580380000         3.0884860000        10.4481660000
C           9.0090130000         0.7141640000         7.4301550000
H           9.7144770000         0.3473320000         8.1831040000
H           9.1513330000         0.1172630000         6.5252940000
H           7.9918440000         0.5501580000         7.7975760000
C           8.3998950000         1.0610560000        10.2901440000
N           6.0400300000         4.7367490000        11.1765840000
N           4.9553720000         3.0990190000        12.7893080000
C           4.7877300000         4.4145610000        13.1189120000
C           5.4224760000         5.3502230000        12.2083970000
C           4.1088040000         4.8200050000        14.2736140000
H           3.9637420000         5.8741300000        14.4813030000
C           6.1383660000         7.5110760000        11.4188750000
H           6.1352820000         8.5954480000        11.4800430000
C           4.5300040000         2.1629700000        13.6753780000
C           5.4642720000         6.7503500000        12.3469260000
H           4.9475200000         7.2334560000        13.1686820000
C           3.6465710000         3.8597270000        15.1497810000
H           3.1242180000         4.1426650000        16.0587480000
C           3.8884720000         2.5189430000        14.8560290000
H           3.5790290000         1.7384730000        15.5436930000
C           4.7691870000         0.7140850000        13.3794710000
H           4.0640740000         0.3475880000        12.6260400000
H           4.6259320000         0.1172600000        14.2842360000
H           5.7865530000         0.5495750000        13.0128160000
Mn          5.5301290000         2.8435870000        10.7803540000
O           5.7815360000         2.9628820000         7.8405940000
O           2.7199820000         3.2340060000        10.0349250000
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O	5.2638100000	-0.0469960000	10.2019180000
C	5.8794010000	2.9140170000	9.0011880000
C	3.8211550000	3.0879300000	10.3613660000
C	5.3800670000	1.0609790000	10.5191910000

Mn2L(CO)6-triplet.xyz

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N	7.7102630000	4.7306880000	9.6131780000
N	8.8221270000	3.0904630000	7.9669090000
O	10.9731260000	3.2574090000	10.7669000000
O	8.5729500000	-0.1262570000	10.4290970000
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C	9.0423540000	4.4247890000	7.7233680000
C	8.4147990000	5.3385330000	8.6478030000
C	9.7599510000	4.8600310000	6.5989640000
H	9.9519850000	5.9156320000	6.4464530000
C	6.8895440000	6.8777710000	10.4047230000
C	7.7089320000	7.5161250000	9.4366090000
H	7.7356970000	8.6029010000	9.4006120000
C	9.2213440000	2.1924960000	7.0444230000
C	7.8332450000	2.7654390000	11.7590270000
C	8.4391620000	6.7800990000	8.5474070000
H	9.0437820000	7.2658960000	7.7915680000
C	10.2011490000	3.9273170000	5.6811970000
H	10.7533020000	4.2397820000	4.7997130000
C	9.9034560000	2.5819970000	5.8911330000
H	10.1985230000	1.8274770000	5.1697100000
C	9.8851530000	3.0738790000	10.4347260000
C	8.9183290000	0.7388190000	7.2553040000
H	9.6256100000	0.2915100000	7.9614860000
H	9.0097820000	0.1952500000	6.3112350000
H	7.9039320000	0.5960960000	7.6371190000
C	8.4089770000	0.9858790000	10.1624970000
N	6.0688550000	4.7306890000	11.1962900000
N	4.9569890000	3.0904640000	12.8425500000
C	4.7367460000	4.4247860000	13.0860910000
C	5.3643030000	5.3385320000	12.1616550000
C	4.0191330000	4.8600090000	14.2104920000
H	3.8270810000	5.9156050000	14.3630140000
C	6.0701430000	7.5161240000	11.3728280000
H	6.0433630000	8.6029010000	11.4088120000
C	4.5577820000	2.1924840000	13.7650220000
C	5.3399210000	6.7800990000	12.2620370000
H	4.7352920000	7.2658990000	13.0178670000
C	3.5779310000	3.9272790000	15.1282440000
H	3.0257610000	4.2397300000	16.0097220000
C	3.8756430000	2.5819630000	14.9183040000
H	3.5805750000	1.8274330000	15.6397160000
C	4.8608340000	0.7388180000	13.5541130000
H	4.1535250000	0.2914870000	12.8479710000
H	4.7694610000	0.1952400000	14.4981850000
H	5.8752100000	0.5961310000	13.1722290000
Mn	5.6073450000	2.7700870000	10.8454530000
O	5.7907200000	2.7494240000	7.8962260000
O	2.8059810000	3.2574540000	10.0424960000
O	5.2058880000	-0.1262460000	10.3804400000
C	5.9458740000	2.7654020000	9.0504360000
C	3.8939630000	3.0740120000	10.3746860000
C	5.3699270000	0.9858980000	10.6469690000

Mn2L(CO)6-quintet.xyz

Mn	8.0017970000	2.7669630000	9.8853790000
O	8.0212330000	2.5708100000	12.8587380000

N	7.7156310000	4.7310600000	9.6240240000
N	8.7970650000	3.0973400000	7.9484540000
O	10.7703460000	3.3785900000	10.8918450000
O	8.5314850000	-0.1597800000	10.2522740000
C	6.8895260000	5.4509380000	10.4047230000
C	9.0802720000	4.4449610000	7.7476790000
C	8.4817110000	5.3427400000	8.6636920000
C	9.8578750000	4.8632090000	6.6393500000
H	10.1098870000	5.9116960000	6.5280970000
C	6.8895270000	6.8641620000	10.4047280000
C	7.7678320000	7.5047240000	9.4832010000
H	7.8036900000	8.5908950000	9.4592710000
C	9.1549080000	2.2146500000	6.9867750000
C	7.6179200000	2.6403010000	11.7659390000
C	8.5330010000	6.7730800000	8.6208450000
H	9.1705060000	7.2687280000	7.8981810000
C	10.2619070000	3.9428790000	5.7105850000
H	10.8531680000	4.2479010000	4.8523560000
C	9.8751560000	2.5994810000	5.8655520000
H	10.1396760000	1.8550440000	5.1233350000
C	9.7273210000	3.1284770000	10.5026860000
C	8.7685360000	0.7694410000	7.1276360000
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H	8.8487450000	0.2669150000	6.1605550000
H	7.7391500000	0.6566070000	7.4787380000
C	8.3340660000	0.9445460000	10.0169530000
N	6.0634210000	4.7310530000	11.1854180000
N	4.9819940000	3.0973230000	12.8609840000
C	4.6987930000	4.4449430000	13.0617700000
C	5.2973480000	5.3427260000	12.1457580000
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C	3.5171990000	3.9428590000	15.0988870000
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H	3.6394690000	1.8550280000	15.6861450000
C	5.0105810000	0.7694300000	13.6818380000
H	4.3415890000	0.2462200000	12.9910850000
H	4.9303940000	0.2669230000	14.6489290000
H	6.0399670000	0.6566120000	13.3307290000
Mn	5.7772620000	2.7669310000	10.9240350000
O	5.7578540000	2.5708640000	7.9506670000
O	3.0088270000	3.3787980000	9.9174520000
O	5.2475710000	-0.1598000000	10.5570990000
C	6.1611350000	2.6403240000	9.0434840000
C	4.0517870000	3.1285450000	10.3066970000
C	5.4449960000	0.9445250000	10.7924430000

Mn2L(CO)6-septet.xyz

Mn	8.2246740000	2.7036270000	9.7252610000
O	8.0135830000	2.3922010000	12.6997820000
N	7.7035470000	4.6580760000	9.5773900000
N	8.9461600000	3.1084550000	7.8389520000
O	11.1197690000	3.2382260000	10.5830350000
O	8.7323770000	-0.1712530000	10.2554110000
C	6.8883780000	5.3583270000	10.4044870000
C	9.0403370000	4.4777870000	7.6304130000
C	8.4096660000	5.3124440000	8.5872450000
C	9.7030770000	4.9766670000	6.4774590000
H	9.7984640000	6.0452000000	6.3280180000

C	6.8874570000	6.7781730000	10.4043190000
C	7.7040680000	7.4473620000	9.4526990000
H	7.7209510000	8.5342880000	9.4499890000
C	9.4088620000	2.2599170000	6.8862480000
C	7.5150200000	2.4763770000	11.6382460000
C	8.4331110000	6.7413240000	8.5467550000
H	9.0357320000	7.2557210000	7.8086420000
C	10.1904170000	4.1051080000	5.5438610000
H	10.6888350000	4.4770600000	4.6536620000
C	10.0214090000	2.7186410000	5.7350950000
H	10.3739910000	2.0073650000	4.9970910000
C	10.0331480000	3.0534180000	10.3001800000
C	9.2568670000	0.7807210000	7.0970770000
H	9.9451480000	0.4216590000	7.8698070000
H	9.4911600000	0.2432350000	6.1749580000
H	8.2358380000	0.5181470000	7.3907230000
C	8.5616540000	0.9321270000	9.9770480000
N	6.0740920000	4.6572600000	11.2317680000
N	4.8337130000	3.1064320000	12.9705750000
C	4.7377170000	4.4756800000	13.1788620000
C	5.3672170000	5.3109620000	12.2218160000
C	4.0744030000	4.9738980000	14.3317660000
H	3.9774860000	6.0423390000	14.4809050000
C	6.0699830000	7.4465500000	11.3557740000
H	6.0516820000	8.5334540000	11.3581820000
C	4.3724610000	2.2574490000	13.9235840000
C	5.3418980000	6.7398120000	12.2619490000
H	4.7386320000	7.2536030000	12.9999610000
C	3.5884740000	4.1018550000	15.2656500000
H	3.0896380000	4.4732940000	16.1558300000
C	3.7595040000	2.7155830000	15.0747540000
H	3.4081400000	2.0039920000	15.8130330000
C	4.5266160000	0.7784250000	13.7130950000
H	3.8386290000	0.4181280000	12.9406840000
H	4.2934360000	0.2408360000	14.6354350000
H	5.5479350000	0.5173170000	13.4191530000
Mn	5.5549970000	2.7023300000	11.0840770000
O	5.7666570000	2.3907340000	8.1094290000
O	2.6589870000	3.2351970000	10.2278100000
O	5.0492780000	-0.1727490000	10.5537960000
C	6.2648210000	2.4756450000	9.1710970000
C	3.7458850000	3.0509980000	10.5099310000
C	5.2193920000	0.9307180000	10.8322220000

Mn2L(CO)6-nonet.xyz

Mn	8.0307630000	2.6316040000	9.7184870000
O	8.4843750000	2.5159070000	12.8598340000
N	7.3542950000	4.5843520000	9.2855420000
N	9.1243720000	3.0854770000	7.9423610000
O	11.6556680000	4.1671990000	10.2673480000
O	7.0487780000	-0.3471860000	10.0131500000
C	6.6243480000	5.2985760000	10.1629560000
C	8.9881130000	4.4005700000	7.5502940000
C	8.1151150000	5.2228620000	8.3279810000
C	9.7190370000	4.8677090000	6.4257210000
H	9.6222960000	5.8973090000	6.1014270000
C	6.6434670000	6.7145610000	10.1850670000
C	7.3637350000	7.3700890000	9.1420110000
H	7.3579680000	8.4566610000	9.1028340000
C	9.9158910000	2.2423960000	7.2481560000
C	8.4063380000	2.5856650000	11.7138440000
C	8.0624350000	6.6500600000	8.2206020000
H	8.6259940000	7.1600940000	7.4481560000
C	10.5315120000	4.0038640000	5.7369170000
H	11.0863740000	4.3548570000	4.8714120000

C	10.6392200000	2.6582060000	6.1441730000
H	11.2677900000	1.9567160000	5.6072260000
C	11.2634490000	3.1021880000	10.2771500000
C	9.9622630000	0.8184320000	7.7303080000
H	10.1810060000	0.7718580000	8.8036860000
H	10.7284890000	0.2464870000	7.2005990000
H	8.9953460000	0.3284790000	7.5650850000
C	7.2691900000	0.7756890000	9.8595030000
N	5.8845080000	4.5838090000	11.0612690000
N	4.8157090000	3.0162460000	12.8385960000
C	4.8783650000	4.3578980000	13.1857150000
C	5.3706670000	5.2273070000	12.1727400000
C	4.5354770000	4.7744890000	14.4951580000
H	4.5542760000	5.8272800000	14.7522530000
C	5.9814430000	7.3726930000	11.2569060000
H	5.9817580000	8.4596300000	11.2875080000
C	4.5630040000	2.0960520000	13.8002680000
C	5.3938460000	6.6533990000	12.2571470000
H	4.9230490000	7.1554510000	13.0941870000
C	4.2304830000	3.8320540000	15.4416640000
H	3.9846060000	4.1337020000	16.4555620000
C	4.2751900000	2.4644310000	15.1021430000
H	4.0831470000	1.6990270000	15.8455400000
C	4.5972150000	0.6417960000	13.4245160000
H	3.6887010000	0.3505170000	12.8866430000
H	4.6610550000	0.0210140000	14.3218530000
H	5.4578690000	0.4154970000	12.7875020000
Mn	4.8444280000	2.8706870000	10.7922620000
O	4.7772560000	2.7482860000	7.8111830000
O	1.8329470000	4.1908210000	10.8816290000
O	3.6987170000	0.1869000000	10.1210380000
C	4.8767440000	2.8184020000	8.9612000000
C	2.9303920000	3.9008210000	10.8375370000
C	4.1468930000	1.1912540000	10.4711370000

M2L2-singlet.xyz

Mn	-1.4571100000	-0.0164120000	0.0142180000
Mn	1.4570340000	0.0163780000	0.0142410000
N	1.0000920000	-1.8128060000	0.5890030000
N	2.7381290000	-0.2259290000	1.5967880000
N	-2.7118190000	-0.2706330000	-1.5965840000
N	-2.7379960000	0.2256740000	1.5969220000
N	2.7118760000	0.2708620000	-1.5965850000
N	0.9596030000	1.8367080000	-0.5688710000
N	-1.0000370000	1.8126880000	0.5892180000
N	-0.9594020000	-1.8365790000	-0.5692970000
C	0.0368040000	-2.5450540000	-0.0056470000
C	-1.8596690000	-2.4713170000	-1.4195540000
C	1.9292710000	-2.4398480000	1.4085470000
C	-1.9292370000	2.4396220000	1.4088430000
C	1.8597750000	2.4715450000	-1.4191360000
C	-0.0714240000	3.9708640000	-0.0313250000
C	2.8362630000	-1.5207280000	2.0375360000
C	2.7925780000	1.5751800000	-2.0267550000
C	-2.8362080000	1.5204510000	2.0377400000
C	-2.7924770000	-1.5748850000	-2.0270230000
C	-0.0367610000	2.5450540000	-0.0053270000
C	3.5271770000	0.7267110000	2.1506320000
C	-1.8227180000	-3.8615930000	-1.5520920000
H	-2.5369980000	-4.3653490000	-2.1958300000
C	3.5403690000	-0.6589710000	-2.1408620000
C	0.0713100000	-3.9708760000	-0.0316430000
C	-3.5270900000	-0.7270200000	2.1506000000
C	1.0689560000	-4.5968870000	0.7527270000
H	1.1145890000	-5.6815250000	0.7912600000

C	-4.4454190000	-0.4237670000	3.1416450000
H	-5.0635220000	-1.2103140000	3.5601200000
C	1.9618270000	-3.8298620000	1.4907880000
H	2.7047250000	-4.3217670000	2.1107280000
C	-3.7648600000	1.8748150000	3.0356120000
H	-3.8278780000	2.9018980000	3.3771620000
C	-0.8979480000	-4.6123600000	-0.8442770000
H	-0.8898210000	-5.6954090000	-0.9279990000
C	-3.7428100000	-1.9533020000	-3.0029030000
H	-3.7975850000	-2.9847430000	-3.3326550000
C	4.4693840000	-0.3310860000	-3.1089790000
H	5.1114120000	-1.1016960000	-3.5214510000
C	0.8977890000	4.6124720000	-0.8439050000
H	0.8895450000	5.6955200000	-0.9276200000
C	-1.0691730000	4.5967700000	0.7530250000
H	-1.1149050000	5.6814030000	0.7915750000
C	-1.9619370000	3.8296470000	1.4910850000
H	-2.7048800000	4.3214450000	2.1110590000
C	1.8226740000	3.8618110000	-1.5516900000
H	2.5368690000	4.3656440000	-2.1954610000
C	-4.5675750000	0.9011020000	3.5824660000
H	-5.2844350000	1.1547710000	4.3578630000
C	-3.3862340000	-2.1281010000	1.6324600000
H	-3.6648950000	-2.1811360000	0.5747650000
H	-4.0320130000	-2.8110450000	2.1901080000
H	-2.3539250000	-2.4805520000	1.7159950000
C	3.4205740000	-2.0653090000	-1.6321090000
H	3.7049940000	-2.1215370000	-0.5758120000
H	4.0723460000	-2.7372260000	-2.1962780000
H	2.3921440000	-2.4304370000	-1.7128540000
C	3.7429560000	1.9537490000	-3.0025240000
H	3.7977790000	2.9852370000	-3.3321150000
C	-3.5403270000	0.6592790000	-2.1407690000
C	3.3864180000	2.1278130000	1.6325400000
H	3.6646880000	2.1808160000	0.5747510000
H	4.0325250000	2.8106330000	2.1899610000
H	2.3541960000	2.4804480000	1.7164790000
C	4.4453280000	0.4233820000	3.1418170000
H	5.0633870000	1.2098900000	3.5604310000
C	4.5674110000	-0.9015160000	3.5825520000
H	5.2841360000	-1.1552480000	4.3580540000
C	4.5741280000	1.0035340000	-3.5391160000
H	5.3031510000	1.2774720000	-4.2961550000
C	3.7647880000	-1.8751860000	3.0354840000
H	3.8278100000	-2.9023020000	3.3769320000
C	-4.5739460000	-1.0030140000	-3.5394020000
H	-5.3029200000	-1.2768210000	-4.2965340000
C	-4.4692340000	0.3315450000	-3.1090220000
H	-5.1112190000	1.1022250000	-3.5214310000
C	-3.4207680000	2.0654970000	-1.6316290000
H	-3.7055920000	2.1214030000	-0.5754170000
H	-4.0723830000	2.7375190000	-2.1958540000
H	-2.3923440000	2.4307360000	-1.7118660000

M2L2-singlet-BS.xyz

Mn	1.4577980000	-0.0675700000	-0.0422220000
Mn	-1.4577110000	0.0678310000	-0.0425850000
N	-0.9332230000	1.9566610000	0.6258010000
N	-2.9048880000	0.4749740000	1.5757730000
N	2.8696960000	0.3510220000	-1.6487330000
N	2.9047720000	-0.4750420000	1.5768150000
N	-2.8696220000	-0.3509840000	-1.6486750000
N	-1.0326890000	-1.9085300000	-0.5504580000
N	0.9334520000	-1.9566100000	0.6259220000
N	1.0330240000	1.9087210000	-0.5502220000

C	0.0818160000	2.6461440000	0.0640020000
C	1.9995500000	2.5430540000	-1.3314870000
C	-1.8667080000	2.6133370000	1.4239870000
C	1.8668090000	-2.6133890000	1.4242170000
C	-1.9995080000	-2.5429580000	-1.3313370000
C	-0.1436960000	-4.0727280000	0.1166990000
C	-2.8922900000	1.7789250000	1.9887090000
C	-2.9383630000	-1.6758490000	-1.9838660000
C	2.8923640000	-1.7791310000	1.9892190000
C	2.9381910000	1.6758510000	-1.9842050000
C	-0.0816240000	-2.6459950000	0.0640150000
C	-3.8379680000	-0.3785590000	2.0542250000
C	2.0603760000	3.9397060000	-1.3656660000
H	2.8287650000	4.4373870000	-1.9481410000
C	-3.7364000000	0.5351360000	-2.1892710000
C	0.1436760000	4.0728780000	0.1164680000
C	3.8378840000	0.3783850000	2.0554000000
C	-0.8301050000	4.7317600000	0.9052390000
H	-0.7997330000	5.8143540000	0.9925550000
C	4.7986960000	-0.0247080000	2.9661180000
H	5.5310950000	0.6849690000	3.3350550000
C	-1.8023540000	4.0019230000	1.5675660000
H	-2.5330320000	4.5220830000	2.1781750000
C	3.8612560000	-2.2381530000	2.9133770000
H	3.8508820000	-3.2682960000	3.2497930000
C	1.1702950000	4.7010250000	-0.6291710000
H	1.2390990000	5.7853700000	-0.6314980000
C	3.9119360000	2.1165320000	-2.9142040000
H	3.9583800000	3.1599560000	-3.2036960000
C	-4.7053420000	0.1483340000	-3.0962250000
H	-5.3855870000	0.8819030000	-3.5147180000
C	-1.1704430000	-4.7008940000	-0.6287370000
H	-1.2393940000	-5.7852300000	-0.6308220000
C	0.8300110000	-4.7316940000	0.9054730000
H	0.7994720000	-5.8142770000	0.9928600000
C	1.8023600000	-4.0019680000	1.5677460000
H	2.5329440000	-4.5222060000	2.1783960000
C	-2.0605500000	-3.9396060000	-1.3651990000
H	-2.8291480000	-4.4372880000	-1.9473910000
C	4.8036650000	-1.3623390000	3.3947490000
H	5.5469760000	-1.7024940000	4.1102170000
C	3.7998580000	1.7860240000	1.5305700000
H	4.1008070000	1.8107770000	0.4775000000
H	4.4786780000	2.4329820000	2.0923800000
H	2.7899720000	2.2030990000	1.5918480000
C	-3.6025640000	1.9606710000	-1.7340770000
H	-3.8235920000	2.0464800000	-0.6639680000
H	-4.2896170000	2.6148420000	-2.2771400000
H	-2.5826410000	2.3286860000	-1.8892250000
C	-3.9125350000	-2.1165560000	-2.9134260000
H	-3.9591960000	-3.1600100000	-3.2027670000
C	3.7364320000	-0.5350590000	-2.1895020000
C	-3.7999980000	-1.7860200000	1.5289440000
H	-4.1009530000	-1.8104210000	0.4758650000
H	-4.4788400000	-2.4331380000	2.0905460000
H	-2.7901440000	-2.2031690000	1.5901560000
C	-4.7985530000	0.0242360000	2.9653100000
H	-5.5308740000	-0.6855560000	3.3341800000
C	-4.8034070000	1.3617350000	3.3943770000
H	-5.5465400000	1.7016600000	4.1101400000
C	-4.7842550000	-1.2079890000	-3.4605420000
H	-5.5306440000	-1.5358660000	-4.1785200000
C	-3.8610580000	2.2376810000	2.9131240000
H	-3.8505300000	3.2677090000	3.2498960000
C	4.7834960000	1.2079750000	-3.4615810000
H	5.5295310000	1.5358140000	-4.1799430000

C	4.7049050000	-0.1482720000	-3.0969780000
H	5.3850760000	-0.8818190000	-3.5156310000
C	3.6032380000	-1.9605590000	-1.7339940000
H	3.8246100000	-2.0460910000	-0.6639480000
H	4.2903770000	-2.6145640000	-2.2771480000
H	2.5834080000	-2.3289710000	-1.8887940000

M2L2-triplet.xyz

Mn	-1.4198750000	0.0254180000	-0.0163440000
Mn	1.4731620000	-0.0184770000	-0.0134180000
N	0.9596870000	-1.7902610000	0.6952890000
N	2.6901500000	-0.1495420000	1.6343260000
N	-2.7734820000	-0.3656460000	-1.5567340000
N	-2.7295630000	0.4152590000	1.5430740000
N	2.7361560000	0.1148910000	-1.6259970000
N	1.0069480000	1.7683880000	-0.7143700000
N	-0.9628890000	1.8931170000	0.4340470000
N	-1.0157640000	-1.8695840000	-0.4479590000
C	-0.0215780000	-2.5469880000	0.1593890000
C	-1.9126820000	-2.5505640000	-1.2582230000
C	1.8734830000	-2.3689000000	1.5692380000
C	-1.8309700000	2.5851340000	1.2681620000
C	1.9343120000	2.3367600000	-1.5811030000
C	0.1060710000	3.9720690000	-0.2182830000
C	2.7885580000	-1.4278690000	2.1343210000
C	2.8342300000	1.3792350000	-2.1511940000
C	-2.7717830000	1.7331690000	1.9295520000
C	-2.8468300000	-1.6866290000	-1.9201530000
C	0.0483240000	2.5482330000	-0.1682380000
C	3.4990920000	0.8222830000	2.1338000000
C	-1.8844760000	-3.9451840000	-1.3109350000
H	-2.5950090000	-4.4833040000	-1.9301160000
C	3.5212080000	-0.8744330000	-2.1217180000
C	-0.0048880000	-3.9708010000	0.2295550000
C	-3.5764760000	-0.4708650000	2.1264670000
C	0.9781670000	-4.5553030000	1.0680620000
H	1.0021860000	-5.6348640000	1.1869490000
C	-4.4876590000	-0.0826290000	3.0922420000
H	-5.1483370000	-0.8199300000	3.5348470000
C	1.8752070000	-3.7543060000	1.7551840000
H	2.6011400000	-4.2123750000	2.4195230000
C	-3.6905050000	2.1716500000	2.9073200000
H	-3.7061920000	3.2134770000	3.2068380000
C	-0.9717510000	-4.6558660000	-0.5461160000
H	-0.9727900000	-5.7421740000	-0.5584180000
C	-3.7936860000	-2.1193530000	-2.8725210000
H	-3.8377270000	-3.1641390000	-3.1582400000
C	4.4320440000	-0.6401850000	-3.1361040000
H	5.0460180000	-1.4536540000	-3.5064580000
C	1.1021420000	4.5405010000	-1.0500250000
H	1.1587180000	5.6203930000	-1.1528540000
C	-0.8373330000	4.6726490000	0.5743160000
H	-0.8062720000	5.7581660000	0.6031150000
C	-1.7631290000	3.9776820000	1.3373800000
H	-2.4519910000	4.5267940000	1.9714610000
C	1.9761910000	3.7211990000	-1.7487880000
H	2.7186540000	4.1657650000	-2.4040580000
C	-4.5449140000	1.2641550000	3.4833060000
H	-5.2538990000	1.5835740000	4.2415120000
C	-3.5045550000	-1.9000520000	1.6743700000
H	-3.7940170000	-1.9908160000	0.6224990000
H	-4.1779630000	-2.5247130000	2.2668360000
H	-2.4896800000	-2.2969130000	1.7691970000
C	3.3816220000	-2.2370860000	-1.5083860000
H	3.6632220000	-2.2173030000	-0.4501580000

H	4.0250930000	-2.9576850000	-2.0193990000
H	2.3488730000	-2.5944450000	-1.5642640000
C	3.7594370000	1.6639240000	-3.1772870000
H	3.8235880000	2.6662170000	-3.5862450000
C	-3.6179730000	0.5292910000	-2.1263040000
C	3.3596270000	2.1966190000	1.5481180000
H	3.6314430000	2.1960300000	0.4868120000
H	4.0093900000	2.9060950000	2.0668350000
H	2.3278990000	2.5548130000	1.6197670000
C	4.4252210000	0.5613400000	3.1243800000
H	5.0520200000	1.3629550000	3.4994590000
C	4.5499690000	-0.7476510000	3.6244230000
H	5.2785640000	-0.9685200000	4.3990310000
C	4.5544120000	0.6546890000	-3.6641090000
H	5.2666150000	0.8544680000	-4.4594150000
C	3.7392090000	-1.7390360000	3.1333120000
H	3.8090810000	-2.7513680000	3.5158350000
C	-4.6421490000	-1.2018130000	-3.4433920000
H	-5.3721550000	-1.5180880000	-4.1826990000
C	-4.5553630000	0.1479270000	-3.0698090000
H	-5.2141640000	0.8909320000	-3.5055420000
C	-3.5125120000	1.9571040000	-1.6764280000
H	-3.7853320000	2.0506700000	-0.6199080000
H	-4.1808990000	2.5962430000	-2.2589330000
H	-2.4908340000	2.3332040000	-1.7841850000

M2L2-quintet.xyz

Mn	-1.4272190000	-0.0001230000	0.0000580000
Mn	1.4234340000	0.0001450000	0.0000840000
N	0.9724150000	-1.8460770000	0.5491210000
N	2.7303850000	-0.2907320000	1.5764760000
N	-2.7026020000	-0.2385800000	-1.7091040000
N	-2.7026670000	0.2382700000	1.7091300000
N	2.7303810000	0.2910050000	-1.5763780000
N	0.9721080000	1.8461940000	-0.5492200000
N	-1.0313900000	1.8456230000	0.5591320000
N	-1.0311780000	-1.8457890000	-0.5590680000
C	-0.0216010000	-2.5623020000	-0.0204760000
C	-1.9423780000	-2.4647980000	-1.4103540000
C	1.9015600000	-2.4935620000	1.3560880000
C	-1.9427650000	2.4645700000	1.4102640000
C	1.9011710000	2.4937480000	-1.3562040000
C	-0.0140730000	3.9877310000	0.0472210000
C	2.8279710000	-1.5988960000	1.9809870000
C	2.8277800000	1.5991780000	-1.9809540000
C	-2.8420450000	1.5551950000	2.0607950000
C	-2.8417900000	-1.5555010000	-2.0608340000
C	-0.0220140000	2.5622840000	0.0203580000
C	3.5388710000	0.6414500000	2.1415920000
C	-1.9267570000	-3.8545390000	-1.5411570000
H	-2.6439430000	-4.3485680000	-2.1888190000
C	3.5391080000	-0.6410390000	-2.1413930000
C	-0.0133510000	-3.9877470000	-0.0475550000
C	-3.4919540000	-0.6981890000	2.2864080000
C	0.9859080000	-4.6345460000	0.7208760000
H	1.0057620000	-5.7198830000	0.7628520000
C	-4.4484310000	-0.3646750000	3.2289040000
H	-5.0618040000	-1.1394270000	3.6756960000
C	1.9044980000	-3.8872270000	1.4400430000
H	2.6451490000	-4.3944020000	2.0502180000
C	-3.8169390000	1.9426550000	3.0072860000
H	-3.9264820000	2.9859880000	3.2803670000
C	-1.0070140000	-4.6168290000	-0.8383660000
H	-1.0149750000	-5.7000580000	-0.9194130000
C	-3.8166410000	-1.9430600000	-3.0073220000

H	-3.9260520000	-2.9863970000	-3.2804400000
C	4.4730230000	-0.3071320000	-3.1048330000
H	5.1035540000	-1.0783140000	-3.5334740000
C	0.9850390000	4.6346260000	-0.7213150000
H	1.0046560000	5.7199620000	-0.7634600000
C	-1.0078680000	4.6167160000	0.8379460000
H	-1.0160730000	5.6999570000	0.9188160000
C	-1.9274510000	3.8543450000	1.5408420000
H	-2.6447740000	4.3483310000	2.1883830000
C	1.9038150000	3.8874110000	-1.4403470000
H	2.6443680000	4.3946790000	-2.0505620000
C	-4.6121610000	0.9832290000	3.5856980000
H	-5.3614910000	1.2656960000	4.3194880000
C	-3.2927390000	-2.1205380000	1.8484630000
H	-3.5457610000	-2.2407500000	0.7889380000
H	-3.9235390000	-2.7984250000	2.4291980000
H	-2.2488950000	-2.4261350000	1.9712050000
C	3.4010040000	-2.0558240000	-1.6612820000
H	3.6941020000	-2.1382450000	-0.6094560000
H	4.0376090000	-2.7248500000	-2.2457680000
H	2.3670180000	-2.4044390000	-1.7402410000
C	3.7810080000	1.9856790000	-2.9483290000
H	3.8491420000	3.0220600000	-3.2591960000
C	-3.4920400000	0.6977970000	-2.2863020000
C	3.4005000000	2.0562280000	1.6615250000
H	3.6933690000	2.1387340000	0.6096400000
H	4.0371270000	2.7253240000	2.2459070000
H	2.3664830000	2.4047030000	1.7407190000
C	4.4728000000	0.3076640000	3.1050640000
H	5.1031850000	1.0789300000	3.5337680000
C	4.5981060000	-1.0325470000	3.5054190000
H	5.3304320000	-1.3113760000	4.2574640000
C	4.5981270000	1.0330810000	-3.5052420000
H	5.3304530000	1.3120030000	-4.2572520000
C	3.7811900000	-1.9852740000	2.9484150000
H	3.8494810000	-3.0216560000	3.2592500000
C	-4.6120150000	-0.9837150000	-3.5856680000
H	-5.3613220000	-1.2662600000	-4.3194530000
C	-4.4484820000	0.3641900000	-3.2288070000
H	-5.0619780000	1.1388720000	-3.6755520000
C	-3.2931040000	2.1201430000	-1.8482140000
H	-3.5465760000	2.2402550000	-0.7887830000
H	-3.9237380000	2.7980050000	-2.4291560000
H	-2.2492430000	2.4258490000	-1.9705020000

M2L2-septet.xyz

Mn	-1.4706980000	0.0291730000	-0.0732450000
Mn	1.4350360000	0.0192020000	0.0419400000
N	0.9076100000	-2.0267920000	0.1832420000
N	2.8580350000	-0.8030830000	1.4733350000
N	-2.6949380000	0.1479910000	-1.7364030000
N	-2.7125610000	-0.1888670000	1.7576240000
N	2.8608910000	0.8571530000	-1.4338550000
N	0.9063670000	2.0512120000	-0.1203800000
N	-1.0672020000	1.6857890000	0.9708210000
N	-1.0515680000	-1.6969140000	-0.9697930000
C	-0.1018020000	-2.5741180000	-0.5325500000
C	-2.0123270000	-2.1191410000	-1.8617460000
C	1.8452140000	-2.8433870000	0.7753920000
C	-2.0485360000	2.0925270000	1.8740620000
C	1.7961950000	2.8886570000	-0.7896680000
C	-0.2987430000	3.9814460000	0.7429850000
C	2.8692270000	-2.1803530000	1.5162740000
C	2.8369400000	2.2210280000	-1.5226320000
C	-2.8729150000	1.0183020000	2.3751180000

C	-2.8886780000	-1.0939930000	-2.3137190000
C	-0.1445650000	2.5735810000	0.5271110000
C	3.7980100000	-0.1000550000	2.1422030000
C	-2.0951230000	-3.4993980000	-2.2256480000
H	-2.8720720000	-3.8349710000	-2.9030220000
C	3.7994630000	0.1487970000	-2.0992540000
C	-0.1788630000	-3.9517130000	-0.8128180000
C	-3.4366670000	-1.2534390000	2.1640720000
C	0.8075390000	-4.7931820000	-0.2129590000
H	0.7682610000	-5.8645320000	-0.3937810000
C	-4.3526240000	-1.1602340000	3.2002890000
H	-4.9179120000	-2.0342700000	3.5047160000
C	1.7785130000	-4.2600740000	0.5802190000
H	2.5209700000	-4.9052440000	1.0358460000
C	-3.7910380000	1.1634940000	3.4354180000
H	-3.8969930000	2.1183890000	3.9377030000
C	-1.2202040000	-4.3930750000	-1.6829330000
H	-1.2919190000	-5.4508910000	-1.9238150000
C	-3.8969400000	-1.2744400000	-3.2941330000
H	-4.0503390000	-2.2509520000	-3.7399770000
C	4.7626960000	0.7618370000	-2.8806740000
H	5.5004880000	0.1651260000	-3.4058200000
C	0.6363250000	4.8228840000	0.0885060000
H	0.5400790000	5.9010770000	0.1813680000
C	-1.3599150000	4.3882650000	1.5784570000
H	-1.5026000000	5.4457160000	1.7824650000
C	-2.1945600000	3.4395520000	2.1716360000
H	-2.9753420000	3.7681760000	2.8505110000
C	1.6469180000	4.2735070000	-0.6834120000
H	2.3380410000	4.9356670000	-1.1949980000
C	-4.5286120000	0.0739240000	3.8396690000
H	-5.2354710000	0.1681070000	4.6591010000
C	-3.2126950000	-2.5472460000	1.4350500000
H	-3.4979850000	-2.4532000000	0.3814810000
H	-3.8034280000	-3.3527770000	1.8786560000
H	-2.1568320000	-2.8348930000	1.4658140000
C	3.7541060000	-1.3434430000	-1.9322130000
H	4.0373180000	-1.6254290000	-0.9119070000
H	4.4402570000	-1.8389400000	-2.6241400000
H	2.7444150000	-1.7275300000	-2.1118750000
C	3.8087970000	2.8929570000	-2.3028170000
H	3.7972630000	3.9741410000	-2.3787740000
C	-3.4529280000	1.1983430000	-2.1393340000
C	3.7247370000	1.3960360000	2.0155780000
H	3.9737870000	1.7083560000	0.9948860000
H	4.4230550000	1.8854240000	2.6997330000
H	2.7147170000	1.7591840000	2.2330660000
C	4.7898020000	-0.7159160000	2.8833210000
H	5.5269950000	-0.1194040000	3.4096520000
C	4.8216160000	-2.1256940000	2.9329030000
H	5.5917040000	-2.6324960000	3.5076630000
C	4.7602690000	2.1631110000	-2.9734970000
H	5.5063780000	2.6697670000	-3.5792130000
C	3.8763480000	-2.8537590000	2.2576810000
H	3.8914350000	-3.9369650000	2.2998240000
C	-4.6584020000	-0.2045330000	-3.6838770000
H	-5.4291240000	-0.3274630000	-4.4392500000
C	-4.4303950000	1.0631050000	-3.1054810000
H	-5.0139810000	1.9262160000	-3.4063500000
C	-3.1843280000	2.5218680000	-1.4820200000
H	-3.4072870000	2.4813000000	-0.4099080000
H	-3.7982970000	3.3081250000	-1.9286330000
H	-2.1315810000	2.8042370000	-1.5879030000

M2L2-nonet.xyz

Mn	-1.4600110000	0.0553360000	-0.1030010000
Mn	1.5000100000	0.0774580000	0.0836210000
N	0.9418290000	-1.9042950000	0.6797330000
N	2.8690280000	-0.3622020000	1.6632250000
N	-2.9087990000	-0.4381830000	-1.6048850000
N	-2.8261840000	0.4526970000	1.6322560000
N	2.8269510000	0.3771420000	-1.6633710000
N	0.9722450000	1.9452410000	-0.6554710000
N	-0.9403540000	1.9724590000	0.5803260000
N	-0.9532150000	-1.9319070000	-0.6181940000
C	0.0024220000	-2.6431230000	0.0342300000
C	-1.8974870000	-2.5859040000	-1.3780790000
C	1.8951770000	-2.5319120000	1.4494680000
C	-1.8716040000	2.6216150000	1.3892970000
C	1.8980580000	2.5625280000	-1.4946670000
C	0.0213280000	4.1084640000	-0.0756290000
C	2.8903050000	-1.6912660000	2.0335840000
C	2.8446680000	1.6709070000	-2.1083670000
C	-2.8291650000	1.7590840000	2.0324030000
C	-2.9120510000	-1.7693760000	-1.9632490000
C	0.0156650000	2.6743680000	-0.0499430000
C	3.7961200000	0.4926120000	2.1544370000
C	-1.8680750000	-4.0139920000	-1.4786740000
H	-2.6008590000	-4.5304980000	-2.0876910000
C	3.6810690000	-0.5311380000	-2.1847810000
C	0.0163540000	-4.0539870000	0.0401660000
C	-3.6893540000	-0.4274240000	2.1803670000
C	0.9972660000	-4.6966780000	0.8503740000
H	1.0141800000	-5.7829710000	0.8960510000
C	-4.5991110000	-0.0506680000	3.1551150000
H	-5.2771260000	-0.7822450000	3.5807370000
C	1.8968420000	-3.9601860000	1.5604500000
H	2.6404580000	-4.4569930000	2.1726130000
C	-3.7408030000	2.1923260000	3.0228010000
H	-3.7336060000	3.2226500000	3.3594650000
C	-0.9506920000	-4.7248110000	-0.7655860000
H	-0.9421580000	-5.8114200000	-0.8046950000
C	-3.9139070000	-2.2550200000	-2.8460500000
H	-3.9208880000	-3.2972360000	-3.1436090000
C	4.5884010000	-0.1978060000	-3.1747590000
H	5.2577020000	-0.9503590000	-3.5770740000
C	0.9907730000	4.7241110000	-0.9003990000
H	1.0142190000	5.8077700000	-0.9770190000
C	-0.9472880000	4.7560200000	0.7261580000
H	-0.9662100000	5.8417030000	0.7669420000
C	-1.8614410000	4.0121510000	1.4656050000
H	-2.5893710000	4.5316940000	2.0807250000
C	1.8951860000	3.9510160000	-1.6204090000
H	2.6215510000	4.4430370000	-2.2595270000
C	-4.6167950000	1.2878090000	3.5756670000
H	-5.3141340000	1.6078520000	4.3447780000
C	-3.6253720000	-1.8389450000	1.6685680000
H	-3.9243910000	-1.8803910000	0.6152660000
H	-4.2893170000	-2.4951530000	2.2372410000
H	-2.6065980000	-2.2344130000	1.7373630000
C	3.6040920000	-1.9210570000	-1.6195970000
H	3.8849470000	-1.9224140000	-0.5603320000
H	4.2750470000	-2.6008490000	-2.1511600000
H	2.5852280000	-2.3167450000	-1.6903410000
C	3.7586900000	2.0593950000	-3.1162670000
H	3.7633220000	3.0790510000	-3.4843660000
C	-3.8609090000	0.3949330000	-2.0834150000
C	3.7067430000	1.9135560000	1.6716650000
H	3.8738770000	1.9667110000	0.5892760000
H	4.4527690000	2.5453370000	2.1608330000
H	2.7154200000	2.3345180000	1.8725950000

C	4.7805690000	0.0836120000	3.0320130000
H	5.5084360000	0.7954680000	3.4055580000
C	4.8202460000	-1.2737290000	3.4223940000
H	5.5852330000	-1.6192770000	4.1119300000
C	4.6205370000	1.1270870000	-3.6414540000
H	5.3193710000	1.4120060000	-4.4228720000
C	3.8910040000	-2.1522040000	2.9311160000
H	3.9141510000	-3.1926000000	3.2341860000
C	-4.8664020000	-1.3966850000	-3.3297450000
H	-5.6325880000	-1.7599490000	-4.0088100000
C	-4.8502970000	-0.0382020000	-2.9446450000
H	-5.5985250000	0.6569910000	-3.3094080000
C	-3.8018940000	1.8178530000	-1.6016470000
H	-4.0015370000	1.8683700000	-0.5250960000
H	-4.5414310000	2.4396530000	-2.1130280000
H	-2.8108570000	2.2521910000	-1.7724540000

M2L2-11-et.xyz

Mn	-1.4779740000	0.0727270000	-0.1340070000
Mn	1.4950460000	-0.0971820000	0.0186200000
N	0.9857290000	1.9092260000	-0.6588380000
N	2.8451630000	0.3263040000	-1.7120070000
N	-2.8923130000	0.5340720000	1.5956890000
N	-2.8344560000	-0.3358560000	-1.6774540000
N	2.8560440000	-0.4332010000	1.6237350000
N	0.9278640000	-1.9668860000	0.6701690000
N	-1.0072410000	-1.9138590000	-0.5489740000
N	-0.8826980000	1.9769050000	0.6501210000
C	0.0948050000	2.6550700000	0.0208030000
C	-1.7723610000	2.6417760000	1.4450090000
C	1.9425610000	2.5219780000	-1.4217600000
C	-1.9923390000	-2.5509240000	-1.3390290000
C	1.8677260000	-2.6091520000	1.4934060000
C	-0.1444330000	-4.0802500000	0.1607320000
C	2.8683090000	1.6131130000	-2.1205030000
C	2.8674780000	-1.7709550000	2.0341180000
C	-2.9216240000	-1.7016720000	-1.9716940000
C	-2.7953010000	1.7905810000	2.0806090000
C	-0.0775290000	-2.6504360000	0.0944230000
C	3.6753770000	-0.5798240000	-2.2551930000
C	-1.7202510000	4.0229860000	1.5798170000
H	-2.4410860000	4.5464510000	2.1972980000
C	3.7837220000	0.4254640000	2.1259970000
C	0.1782630000	4.0836800000	0.0694680000
C	-3.7268830000	0.5312990000	-2.2290670000
C	1.1888290000	4.6933990000	-0.7035150000
H	1.2847740000	5.7747590000	-0.7031520000
C	-4.7224010000	0.1342430000	-3.0859330000
H	-5.4109020000	0.8607740000	-3.5043280000
C	2.0523550000	3.9063960000	-1.4609100000
H	2.8275190000	4.3795810000	-2.0526580000
C	-3.9544710000	-2.1456960000	-2.8600320000
H	-4.0315430000	-3.1997870000	-3.1063560000
C	-0.7587230000	4.7513760000	0.8819350000
H	-0.7266080000	5.8340560000	0.9568300000
C	-3.6233480000	2.2345800000	3.1140140000
H	-3.5214680000	3.2344420000	3.5185540000
C	4.7509060000	0.0415340000	3.0232800000
H	5.4677550000	0.7634950000	3.3999790000
C	0.8074230000	-4.7280730000	0.9879830000
H	0.7612260000	-5.8100260000	1.0932540000
C	-1.1521080000	-4.7120680000	-0.6162680000
H	-1.2121340000	-5.7982560000	-0.6209920000
C	-2.0331330000	-3.9633980000	-1.3684110000
H	-2.7876240000	-4.4692460000	-1.9627260000

C	1.7768540000	-4.0074910000	1.6595510000
H	2.4890110000	-4.5283260000	2.2918890000
C	-4.8290660000	-1.2535380000	-3.4051490000
H	-5.6061360000	-1.5956980000	-4.0838680000
C	-3.5663980000	1.9702470000	-1.8184890000
H	-3.7120710000	2.0838540000	-0.7372040000
H	-4.2894600000	2.6143270000	-2.3268040000
H	-2.5596080000	2.3357410000	-2.0554900000
C	3.7040100000	1.8405300000	1.6197280000
H	3.9255160000	1.8812440000	0.5465380000
H	4.4180050000	2.4887380000	2.1354510000
H	2.6991630000	2.2543320000	1.7635770000
C	3.8755650000	-2.2064840000	2.9503940000
H	3.8962900000	-3.2442510000	3.2679580000
C	-3.8128940000	-0.3121020000	2.0873980000
C	3.5996630000	-1.9764600000	-1.7101480000
H	3.8292500000	-1.9838980000	-0.6386430000
H	4.3060750000	-2.6367920000	-2.2189260000
H	2.5923980000	-2.3881070000	-1.8335020000
C	4.5655870000	-0.2220960000	-3.2637570000
H	5.2255550000	-0.9681510000	-3.6924970000
C	4.5885950000	1.0975070000	-3.7050290000
H	5.2684480000	1.3972200000	-4.4966250000
C	4.7936960000	-1.3228220000	3.4364200000
H	5.5531900000	-1.6542460000	4.1398090000
C	3.7372150000	2.0295840000	-3.1330190000
H	3.7388220000	3.0572710000	-3.4763260000
C	-4.5676000000	1.3617870000	3.6320120000
H	-5.2183110000	1.6816930000	4.4400820000
C	-4.6707880000	0.0755370000	3.1146930000
H	-5.4025010000	-0.6261550000	3.4998890000
C	-3.8878890000	-1.6754710000	1.4657950000
H	-4.2307060000	-1.6011440000	0.4280910000
H	-4.5796770000	-2.3199630000	2.0134670000
H	-2.9030180000	-2.1520100000	1.4469510000

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