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Magnetic properties of coordination clusters with $\{Mn_4\}$ and $\{Co_4\}$ antiferromagnetic cores.

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1 Synthesis and characterization

1.1 Materials and synthesis

2-aminophenol (> 98%, TCI) was recrystallised from boiling water, washed with ice-cold water and diethylether and stored under inert atmosphere. 2,6-diacetylpyridine (> 98%, TCI), $Co(OAc)_2{\cdot}4\ H_2O$ (99.999% trace metal basis, Aldrich) and $Zn(OAc)_2{\cdot}2\ H_2O$ (99.999% trace metal basis, Aldrich) were used as received. Solvents were, when indicated, deaerated by three freeze-pump-thaw cycles using argon as inert gas. PE spatulas and PTFE cannulas were employed to avoid magnetic contamination of the samples.

$[Mn_4OAc_4L_2]$ (H_2L=2,6-bis-(1-(2-hydroxyphenyl)iminoethyl)pyridine) ($\{Mn_4\}$)

The complex was synthesized according to the literature.[1]

$[Co_4L_2(OAc)_4]$ (H_2L = 2,6-bis-(1-(2-hydroxyphenyl)iminoethyl) pyridine) ($\{Co_4\}$)

Synthesis of the complex follows the preparation of the manganese analogue,[1] with some modifications. In particular, conducting the reaction under protective atmosphere is necessary to avoid the formation of an unidentified brown precipitate by the reaction of 2-aminophenol, cobalt acetate and dioxygen. 2,6-diacetylpyridine (439 mg, 2.5 mmol, 1 eq.), 2-aminophenol (583 mg, 5.3 mmol, 2.2 eq.) and Co(OAc)2·4 H_2O (1.33 g, 5.3 mmol, 2.2 eq.) were introduced in a Schlenck flask under argon. Deaerated methanol (10 mL) was canulated into the flask and the resulting red solution was refluxed under argon for two hours. After the solution was returned to room temperature, deaerated diethylether (100 mL) was canulated in and allowed to mix with the solution, yielding an orange microcrystalline precipitate. The solid was filtered and washed with diethylether (3×30 mL) to yield $Co_4L_2(OAc)_4{\cdot}4\ CH_3CN$ (1.0-1.2 g, 0.8-0.9 mmol, 60-70 %) as a dark orange powder. The compound was recrystallised by dissolving the solid (130 mg, 0.1 mmol) in acetonitrile (25 mL), sonicating and filtering solution and setting it up for gas phase diffusion of diethylether. Dark red crystals of $Co_4L_2(OAc)_4{\cdot}4\ CH_3CN$ (65-100 mg, 50-75 % recrystallisation yield) were collected by filtration after 3-4 days and used for all further characterization and reactions.

UV (CH_3CN) λ_{max}, nm ($\log\epsilon$): 260sh (4.50), 321 (4.27), 398 (4.14).

CV $E_{1/2}$, V vs. Fc^+/Fc: 0.30, 0.80.

TGA (N_2, 10 K.min^{-1}) -12.3 % (50-150 K, -4 CH_3CN (th. -12.4 %)). -30.5 % (350-400 K), -9.4 % (400-520 K).

Single crystal diffraction quality material can be obtained by gas phase diffusion of n-pentane into a saturated ethanol solution. The compound crystallizes in the P4/n space group with ethanol as a solvate. Due to twinning of

the crystals and disorder of the solvate molecules we were only able to refined to a wR^2 of 36 %. The asymmetric unit unequivocally contains a $Co_4L_2(OAc)_4$ molecule and an ethanol molecule hydrogen bound to one of the acetate oxygens, as well as a second ethanol molecule which refines satisfactorily with a two-parts disorder of the hydroxyl group with approximatively equal occupancies. The SQUEEZE routine was used to account for the residual electronic density localised in the large voids of the unit cell, which corresponds to 8 ethanol molecules per unit cell, yielding a final wR^2 of 36 % ($R_1 = 18$ %) with a formula $Co_4L_2(OAc)_4$·3 EtOH. Crystal structure data is available from Cambridge Structural Database, under CCDC number 1855019.

$Zn_4L_2(OAc)_4$ (H_2L = 2,6-bis-(1-(2-hydroxyphenyl)iminoethyl) pyridine) ({Zn_4})

Synthesis of the complex follows the preparation of the manganese analogue, [1] with some modifications. Specifically, 2,6-diacetylpyridine (186 mg, 1.0 mmol, 1 eq.), 2-aminophenol (250 mg, 2.3 mmol, 2.3 eq.) and $Zn(OAc)_2$·2 H_2O (501 g, 2.3 mmol, 2.3 eq.) were introduced in a Schlenck flask under argon. Deaerated methanol (10 mL) was canulated into the flask and the resulting yellow solution was refluxed under argon for two hours. Note that this step can be conducted in air, but in that case a small amount of strongly red-colored 2-amino-3H-phenoxazin-3-one is formed by the oxidative dimerisation of 2-aminophenol and contaminates the product obtained before recrystallisation. After the solution was returned to room temperature, a microcrystalline yellow solid was precipitated by the addition of diethylether (200 mL). The solid (590-640 mg) was filtered, washed with diethylether (4×25 mL), and redissolved in chloroform (100 mL). Pentane was allowed to diffuse in the solution from the gas phase (to accelerate the process, the solution was divided in three fractions). Yellow single crystal diffraction quality $Zn_4L_2(OAc)_4$·4.5$CHCl_3$ (350-400 mg, 40-45 % yield) was collected by filtration after 3-4 days and used for all further characterization and reactions.

The compound crystallised in the $P2_1/n$ space group, with 4.5 $CHCl_3$ molecules and a $Zn_4L_2(OAc)_4$ complex in the asymmetric unit. One of the chloroform molecules is located close to the inversion center at (0, 0.5, 0) and has an occupancy of 0.5. Another could be refined as an approximately 1:1 disorder between two close positions. Residual electronic density lies mostly in close proximity with the chlorine atoms of the other chloroform molecules, but attempts at refining similar disorder yielded only small occupancy factors and no significant improvement of the R factors, and were abandoned, leaving a final wR^2 factor of 12 % ($R_1 = 4.3\%$). Crystal structure data is available from Cambridge Structural Database, under CCDC number 1855020.

UV (CH_3CN) λ_{max}, nm ($\log \epsilon$): 265sh (4.40), 293 (4.23), 346 (4.17), 407 (4.23).

SQUID: χ_{dia}, $m^3.mol^{-1}$ ($emu.mol^{-1}$): -5.3×10^{-9} (4.2×10^{-4}).

2 Fit of SQUID data

The experimental magnetic susceptibility was fitted exploiting an Heisenberg model Hamiltonian in which the exchange coupling parameters between pairs of ions are left as free parameters. The fit functions are reported in Figure 1 as solid lines, together with the experimental data (points) and the J_n extracted from the fit.

The J_n obtained are in fair agreement with those extracted from the LDA+U calculation. The fitted g-factor is ~ 2 in $\{Mn_4\}$ confirming the validity of the spin-only approximation, while it deviates from 2 in $\{Co_4\}$ reflecting the role of SOC.

Through the model Hamiltonian with parameters obtained from the fit of the experimental data the magnetization was calculated at different temperatures and fields. For large fields or large temperatures the magnetization of $\{Mn_4\}$ is larger than that of $\{Co_4\}$, as observed in the experiments. The saturation value ($gS\mu_B$) of $\{Mn_4\}$ ($20\mu_B$) is indeed larger than for $\{Co_4\}$ ($12\mu_B$ in a spin-only model). At low temperature, fields of 20 T for $\{Co_4\}$ and 25 T for of $\{Mn_4\}$ are needed for the magnetization to reach saturation. These values are significantly large compared to the fields accessible in our experiments (Fig. 3 in the main text).

In the low field−low-temperature limit the model shows an inversion of the magnetization curves leading to larger magnetization of $\{Co_4\}$ with respect to $\{Mn_4\}$. Moreover the two curves display opposite curvature, in agreement with SQUID data at low temperature. In particular, the magnetization of $\{Mn_4\}$ shows positive curvature, as expected for an antiferromagnet, while for $\{Co_4\}$ an almost linear dependence on the field can be observed.

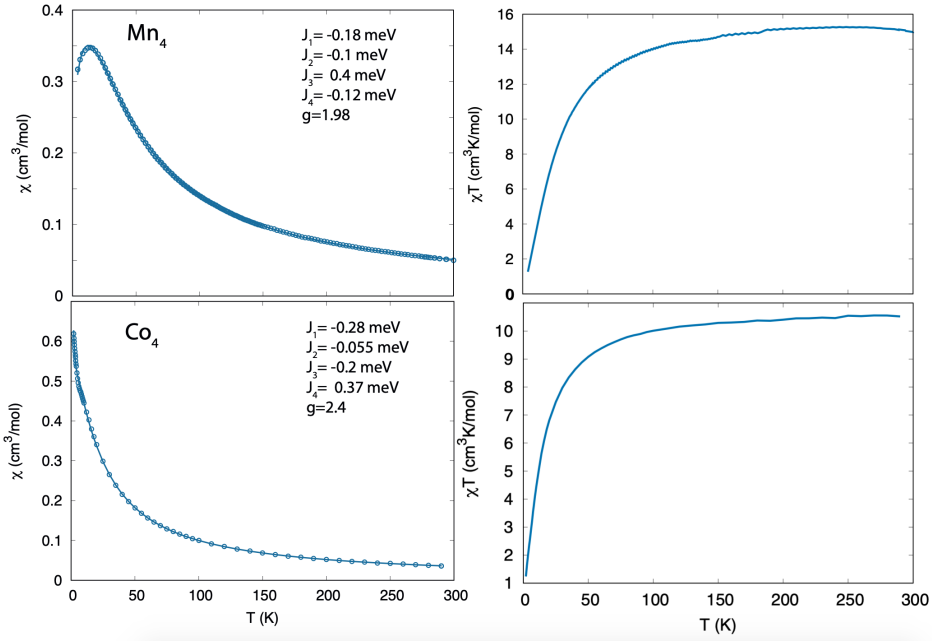

Figure 1: Left panels: Experimental (dots) magnetic susceptibility (χ cm^3/mol) of $\{Mn_4\}$ and $\{Co_4\}$ with the relative fit (line). The J derived from fitting are reported as inset together with the value of g. Right panels: experimental susceptibility times temperature ($\chi \times T$, cm^{3}K/mol) of $\{Mn_4\}$ and $\{Co_4\}$ as a function of the temperature.

The slope of the magnetization is an indication of the coupling between the magnetic centers: the stronger the antiferromagnetic coupling, the smaller the slope. Moreover, the smaller the moment per atom, the stronger the linear dependence of M on the field. Both these aspects explain the fast rise observed for the magnetization of $\{Co_4\}$ in the experimental data, as due to the smaller value of S (or J) (see table 4 and 5 in the main text) and of the AFM coupling, with respect to $\{Mn_4\}$. On the other hand, the saturation value for the magnetization of $\{Co_4\}$ is smaller than for $\{Mn_4\}$, thus the two magnetization curves show a crossing for a certain value of the field which is not reached in the experiments. At high temperature the magnetization curves flatten, resulting in a slower growth as a function of the field with respect to the low temperature limit. The linear dependence on the field $M = Ng^2\mathrm{S}(\mathrm{S}+1)\mu_B^2 B$ in this case is governed by the value of S and it is smaller for $\{Co_4\}$ than for $\{Mn_4\}$, in agreement with what observed in the experiments at high temperature.

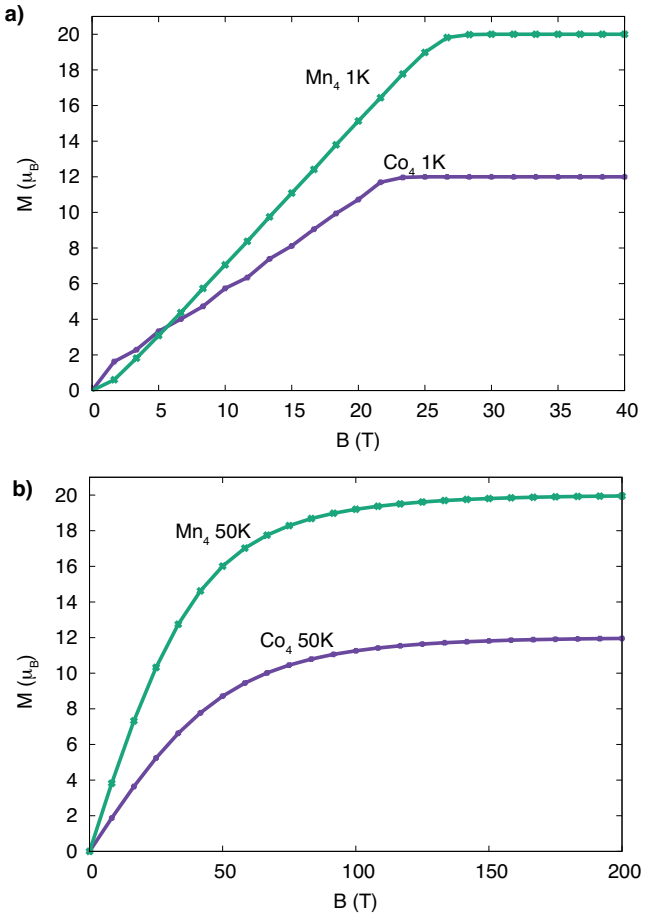

Figure 2: Magnetization versus field dependence for $\{Mn_4\}$ and $\{Co_4\}$ at 1 K (a) and 50 K (b).

3 Exchange parameters from different calculations

The exchange parameters where extracted by fitting a system of equations for the five lowest energy spin configurations of the molecule, as reported in the main text. For a comparison with the available experimental data and previous theoretical calculations on $\{Mn_4\}$ we considered also a set of only three J parameters, despite the oversimplification of this model. Indeed the assumption $J_3 = J_{(1,2)} = J_{(3,4)}$ is not correct, as the M_1/M_2 and M_3/M_3 pairs are not equivalent in terms of chemical coordination and ligands groups. The obtained values are reported in Tables 1 For a system of three exchange parameters, we recover the experimental results of Kampert *et al.* [1].

In Table 2 the J parameters obtained in LDA+SOC calculation are reported. Notably, they are too large compared to those extracted from LDA+U calculation and from the experiments, confirming the need to include the electronic correlation for a reliable estimate of the exchange interaction.

In addition, we also computed the J values with with the Liechtenstein-Katsnelson-Antropov-Gubanov (LKAG) formula[2] implemented in the TB2J package.[3]

Table 1: Computed exchange parameters J (meV and Kelvin) for the $\{Mn_4\}$ molecular complex, using LDA+U and a three-J Heisenberg model. The experimental values from Ref.[1] are reported for comparison.

J	J_1 (1-4,2-3)	J_2 (1-3,2-4)	J_3 (1-2, 3-4)
$\{Mn_4\}$ (meV)	-0.7	-0.4	-0.2
$\{Mn_4\}$ (Kelvin)	-8.1	-4.1	-2.0
Exp[1](Kelvin)	-2.2	-1.1	-0.1

Table 2: Exchange coupling parameters (J_i, meV) of $\{Mn_4\}$ and $\{Co_4\}$ molecular complexes extracted from DFT calculations with SOC included. S is normalized to 1.

SOC (meV)	J_1	J_2	J_3	J_4
$\{Mn_4\}$	-5.0	-4.2	9.3	31.8
$\{Co_4\}$	-7.35	-1.42	2.58	5.52

TB2J evaluates the J for each couple of atoms. So there are six J parameters (Table 3). The non-equivalent J for pairs M_1/M_3 and M_2/M_4 is related to the not perfect symmetry of the electronic structure associated with these pairs of atoms, probably due to some orbital polarization in the Mn/Co.

When the Heisenberg equation is solved for four exchange parameters, The TB2J results for the LDA+U case give the same trend obtained using SIESTA total energies: the ferromagnetic coupling between atoms M1 and M2 is not reproduced ($J_3 < 0$) and the exchange coupling parameters are larger for $\{Co_4\}$ than for $\{Mn_4\}$

With SOC included, the exchange parameters obtained with TB2J are in fair agreement with those reported in the main text supporting the robustness of the results. The comparison between the two molecules confirms indeed the larger strength of the magnetic coupling in $\{Mn_4\}$ with respect to $\{Co_4\}$ but the absolute value of the J is too large.

All the methods agree in the qualitative description of the magnetic coupling within the two molecules and in these terms, i.e. only qualitatively, these parameters should be taken into account.

Table 3: J of the $\{Mn_4\}$ and $\{Co_4\}$ molecular complexes obtained with TB2J in LDA+U and with SOC included. The values are reported in meV.

LDA+U	J_1 (1-4,2-3)	J_2 (1-3,2-4)	J_3 (1-2)	J_4 (3-4)
$\{Mn_4\}$	-1.21/-1.23	-1.77/-1.84	-0.8	0.1
$\{Co_4\}$	-3.47/-3.29	-1.70/-1.82	0.03	-2.25
SOC	J_1 (1-4,2-3)	J_2 (1-3,2-4)	J_3 (1-2)	J_4 (3-4)
$\{Mn_4\}$	-34.5/1.3	-55.7/-29.2	12.94	3.29
$\{Co_4\}$	-3.24/-5.09	-11.84/-10.68	1.18	18.35

4 Spin dynamics calculation

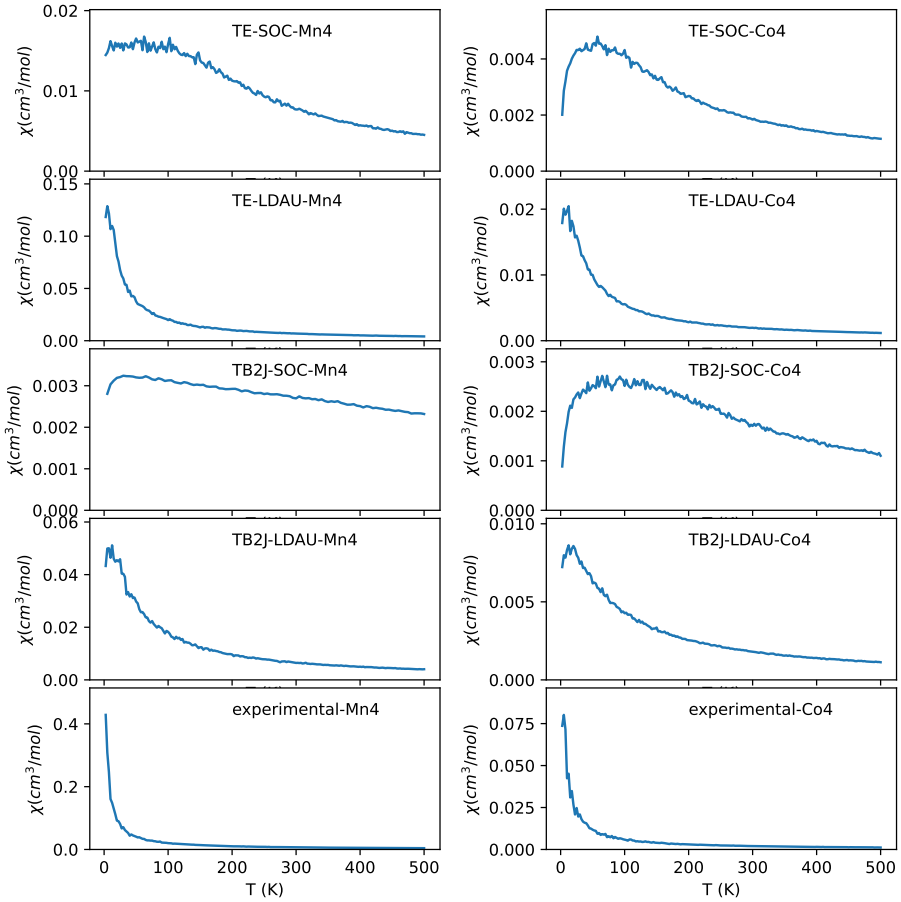

Figure 3: The susceptibilities computed with spin dynamics using various set of parameters. TE-SOC: fit from DFT (with SOC) energies. TE-LDAU: fit from DFT (with +U correction). TB2J-SOC: computed with TB2J from DFT with SOC. TB2J-LDAU: computed from TB2J with DFT+U. Experimental: fit from experimental data. The left and the right panels are from Mn4 and Co4, respectively.

Using the Heisenberg model constructed from DFT results, we perform Ginzberg-Landau-Lifshitz (GLL) atomic spin dynamics[4,5] (ASD) to compute the magnetic susceptibility with the MULTIBINIT code[6]. The isothermal magnetic susceptibility is calculated with the fluctuation-dissipation theorem[7]:

$$\chi = \frac{1}{k_B T}(\langle m^2 \rangle - \langle m \rangle^2), \tag{1}$$

where $\langle\rangle$ means the average over the ensembles, m is the magnetization of the system.

Four sets of parameters from DFT results with either SOC or Hubbard U correction, computed by total energy (TE) method or TB2J, were used as input. Another set of exchange parameters by fitting to experimental data is also taken as comparison. The results are shown in Fig. 3.

The "λ"-shape of the susceptibility curves are similar to extended structures, where the susceptibility diverges at the critical temperature, which is ill-defined in molecules. Nevertheless the temperature of the peak (definded as T_P), the decay of the susceptibility above the T_P, and the value of the susceptibilities, all shows that the exchange parameters from the DFT results with the "+U" correction agrees better with experiments, in which the exchange values are smaller in general.

5 Relaxed structures

The atomic coordinates (in Å) obtained through structural relaxation performed in DFT-LDA and SOC included are reported below for $\{Co_4\}$ and $\{Mn_4\}$.

$\{Co_4\}$:

Co 11.784660 24.970504 9.657395
Co 10.497270 22.083542 10.349018
Co 13.826910 22.493219 9.595356
Co 11.640250 22.424358 7.355454
O 12.276659 23.190641 10.768667
O 13.053111 23.738692 8.233238
O 12.150853 21.350956 8.965670
O 10.536075 23.509294 8.730816
N 11.150917 25.250576 11.697139
N 10.234291 26.256309 9.631992
N 11.898964 25.955696 7.819901
C 12.573409 23.459183 12.047217
C 13.501743 22.727320 12.800231
H 14.089320 21.934242 12.292846
C 13.683728 23.040467 14.147378
H 14.424537 22.471937 14.743995
C 12.967844 24.084895 14.745447
H 13.125847 24.329670 15.812985
C 12.094520 24.862400 13.986050
H 11.619728 25.748710 14.442161
C 11.894341 24.565336 12.624100
C 10.126773 26.025442 11.948916
C 9.578037 26.345785 13.287772
H 10.175627 27.151091 13.781884
H 8.530036 26.715922 13.221056
H 9.604646 25.444738 13.951800
C 9.538585 26.565027 10.740648
C 8.341386 27.295098 10.668957
H 7.820799 27.608225 11.593808
C 7.833021 27.630308 9.415343
H 6.862677 28.154484 9.327204
C 8.583412 27.341326 8.274367
H 8.239272 27.639455 7.265994
C 9.816490 26.700082 8.429924
C 10.790725 26.483101 7.373647
C 10.499096 26.837914 5.965518
H 11.118355 26.205940 5.283527
H 9.420716 26.654751 5.742013
H 10.706556 27.914849 5.751836
C 13.024326 25.741449 7.058258
C 13.537168 26.594422 6.071137
H 13.031246 27.555676 5.858676
C 14.722039 26.250453 5.422129
H 15.143996 26.930256 4.657679
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H 16.319763 24.794952 5.214912
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C 13.063406 17.859247 8.376878
H 13.502886 17.200660 7.602911
C 12.747203 17.325275 9.633942
H 12.915108 16.251224 9.840454
C 12.205322 18.140545 10.625957
H 11.907104 17.720989 11.605658
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C 11.650265 20.474168 12.485497
C 12.636444 19.653283 13.225367
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C 7.023869 24.354608 9.088815
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H 5.679835 25.092977 7.561875
C 7.661627 24.652798 6.770087
H 7.379020 24.906744 5.729114
C 8.956450 24.210011 7.041607
H 9.719280 24.084856 6.245056
C 9.303374 23.877674 8.358257
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O 14.950837 23.896252 10.435570
C 14.509448 25.023697 10.844952
C 15.140291 25.589838 12.078773
H 16.108362 25.094580 12.300594
H 15.260569 26.691401 11.992143
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O 9.264080 21.016327 9.158996
O 9.981759 21.377015 7.029957
C 9.077203 21.170511 7.908653
C 7.656352 21.159999 7.435931
H 7.600703 21.151344 6.327734
H 7.105154 20.298050 7.871949
H 7.167930 22.096305 7.813696
O 14.512862 20.887840 10.767680
O 15.138232 21.186628 8.688865
C 15.122061 20.452460 9.730707

C 15.736798 19.099933 9.768206
H 16.570752 19.090335 10.507721
H 14.961592 18.371446 10.113626
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C 13.128020 23.549145 3.938469
H 14.056502 22.988709 3.703249
H 12.409620 23.476724 3.089349
H 13.369196 24.629938 4.096111

{Mn_4}
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Mn 10.424819 22.105112 10.320622
Mn 13.969259 22.519930 9.574551
Mn 11.607671 22.312376 7.271543
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C 8.310229 23.711196 11.775950
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H 7.137163 24.854052 13.184148
H 7.048056 25.426713 11.463985
C 8.294030 23.971264 9.377957
C 6.985741 24.402518 9.078548
H 6.208726 24.395808 9.864623
C 6.645107 24.768102 7.776819
H 5.611433 25.100776 7.560535
C 7.584354 24.666278 6.741623
H 7.286273 24.909318 5.702311
C 8.882809 24.228377 7.004842
H 9.636329 24.102363 6.198341
C 9.255876 23.909629 8.319972
O 13.629165 25.693699 10.335326
O 15.054352 23.949492 10.419150
C 14.579768 25.047346 10.878908
C 15.148944 25.577028 12.154026
H 16.102522 25.070021 12.411438
H 15.283882 26.679496 12.085672
H 14.405273 25.377946 12.971604
O 9.240174 20.965235 9.109180
O 9.939535 21.279195 6.990173

C 9.017738 21.132906 7.868470
C 7.596402 21.202296 7.413526
H 7.528188 21.226430 6.305692
H 7.019675 20.346110 7.830899
H 7.143116 22.142987 7.825555
O 14.587882 20.910049 10.688605
O 15.351206 21.082424 8.631351
C 15.226349 20.400428 9.687313
C 15.757963 19.019043 9.815996
H 16.581455 19.010146 10.568026
H 14.940826 18.348605 10.182828
H 16.133811 18.655074 8.836485
O 12.967978 21.908972 5.586999
O 11.521639 23.566847 5.647444
C 12.523106 22.978168 5.081699
C 13.126088 23.607245 3.878303
H 14.073814 23.096458 3.606186
H 12.402614 23.547213 3.031790
H 13.323867 24.686749 4.095232

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