**Electronic supplementary information (ESI)**

# Structure and magnetism of a mixed-valence octanuclear manganese(II/III) cluster derived from carbamoylcyanonitrosomethanide (ccnm)

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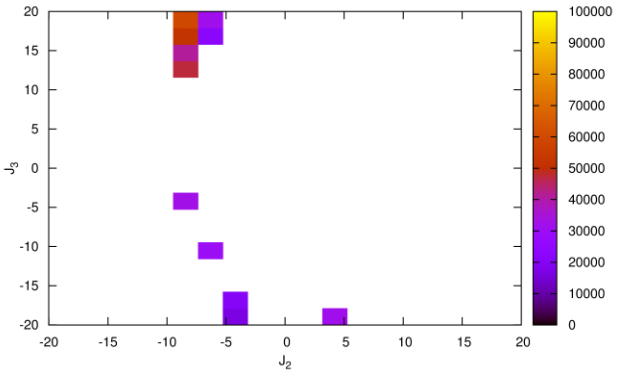


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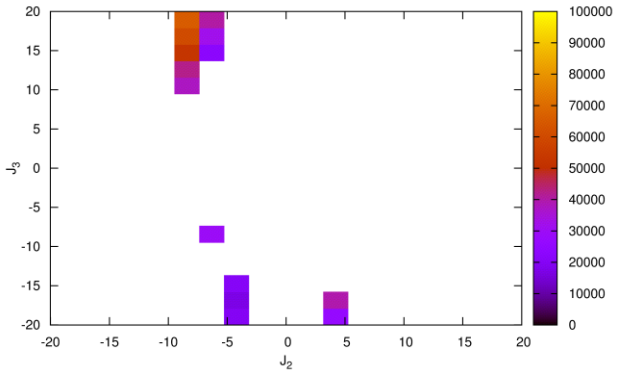


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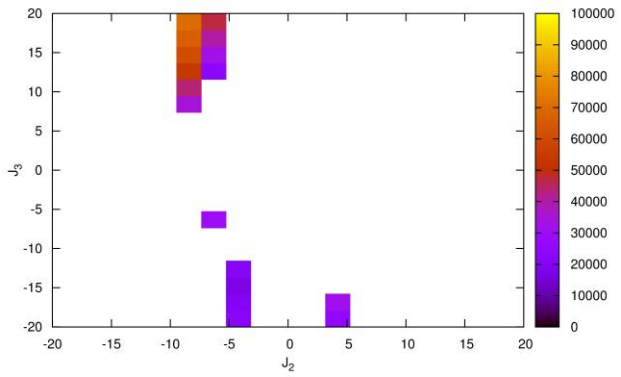


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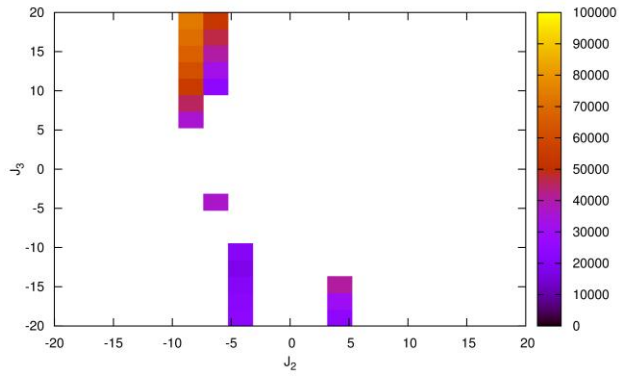


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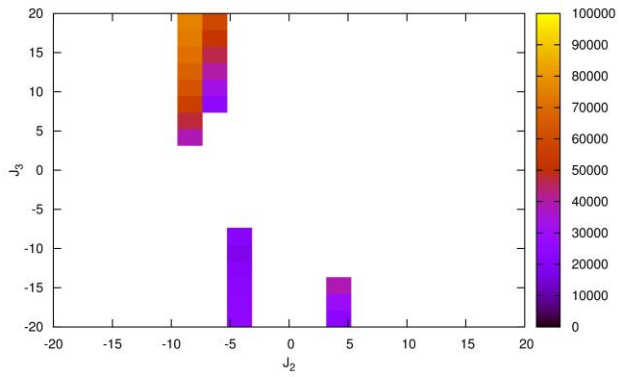


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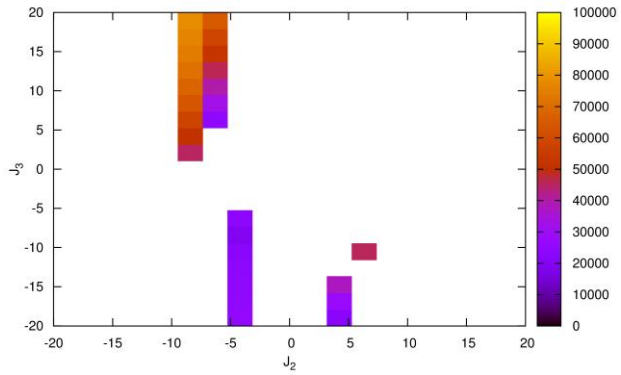


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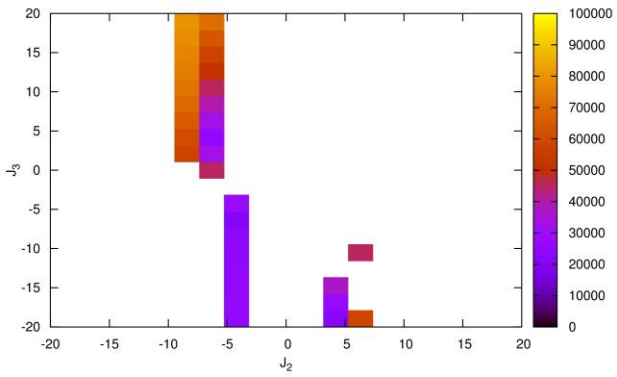


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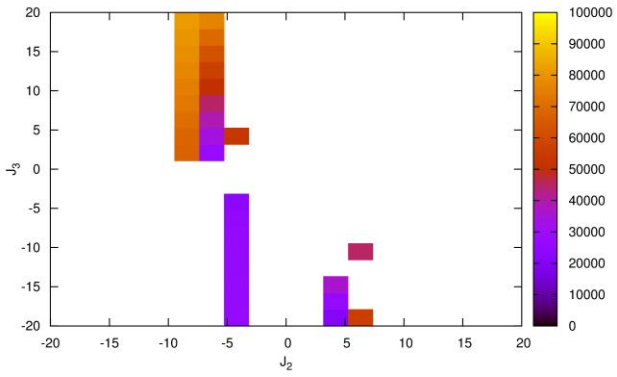


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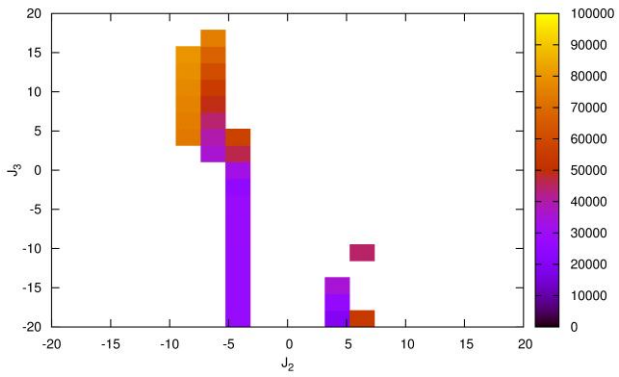


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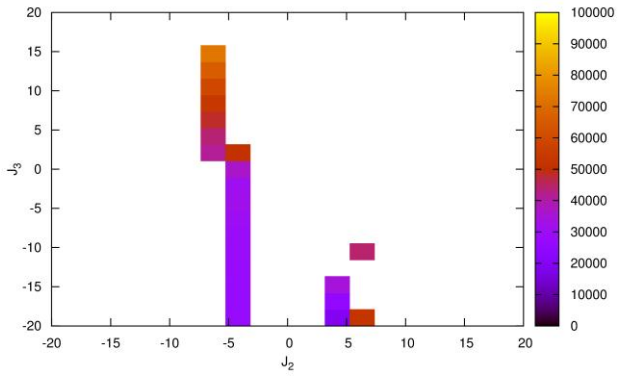


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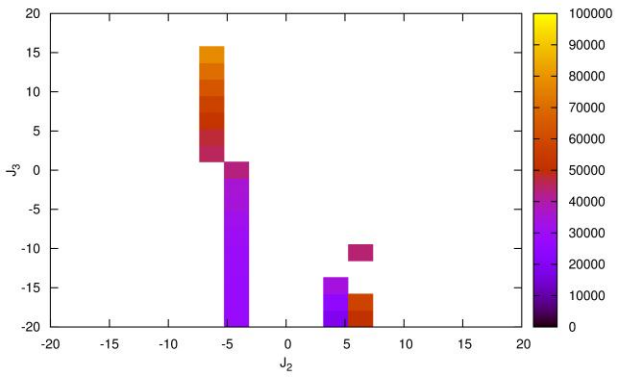


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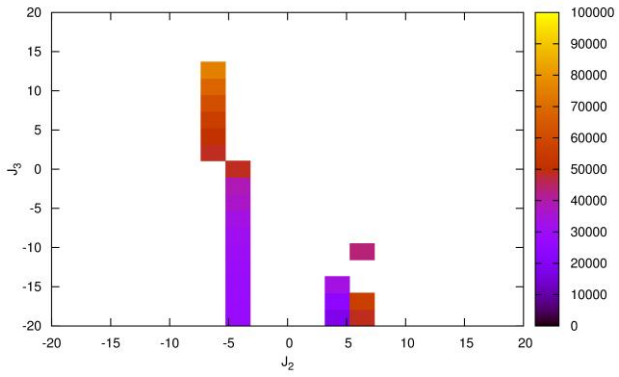


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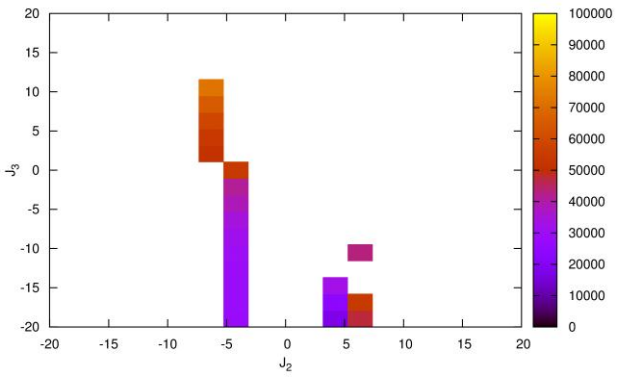


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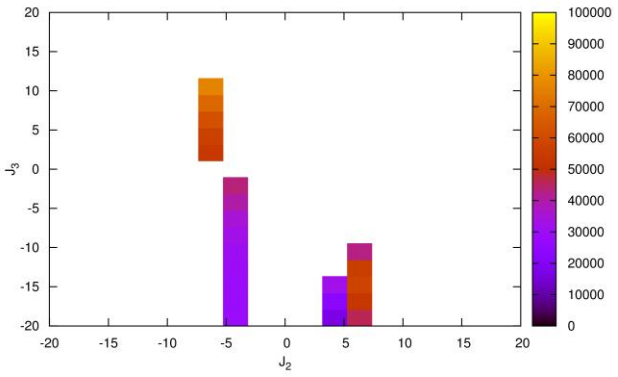


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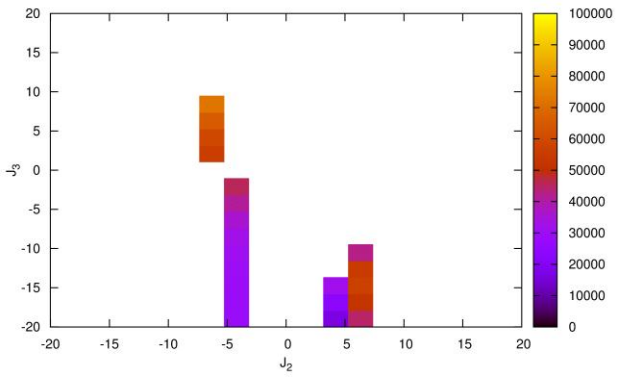


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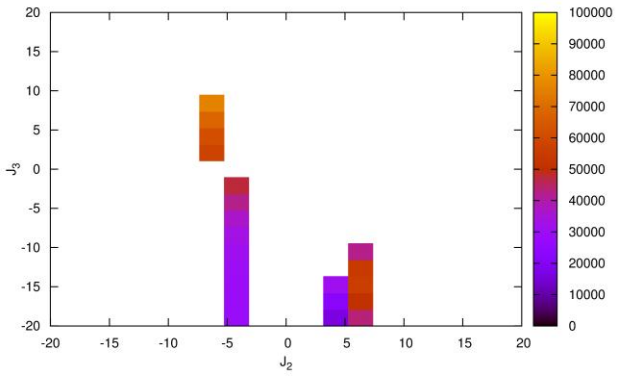


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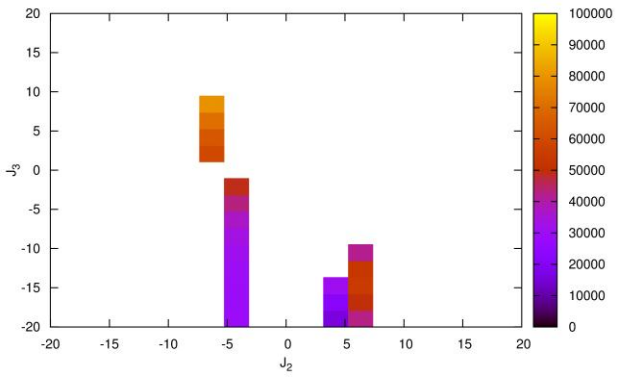


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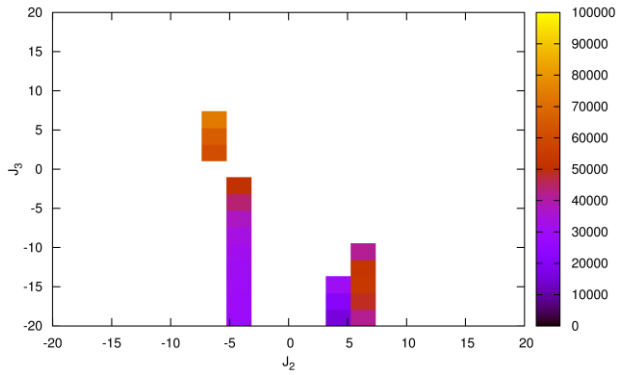


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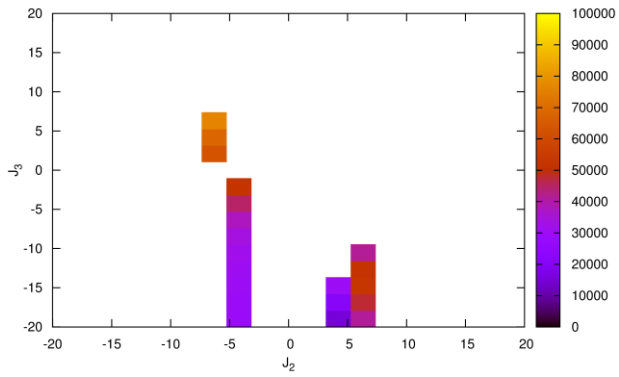


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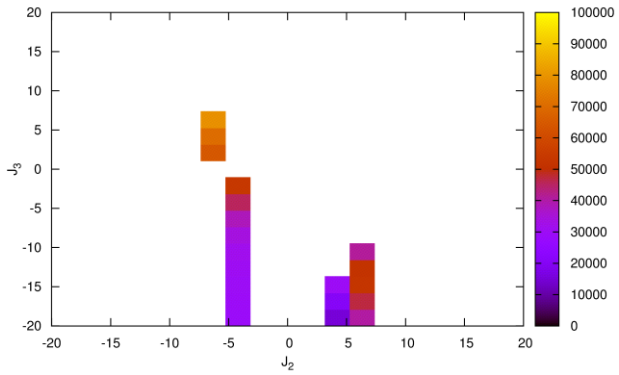


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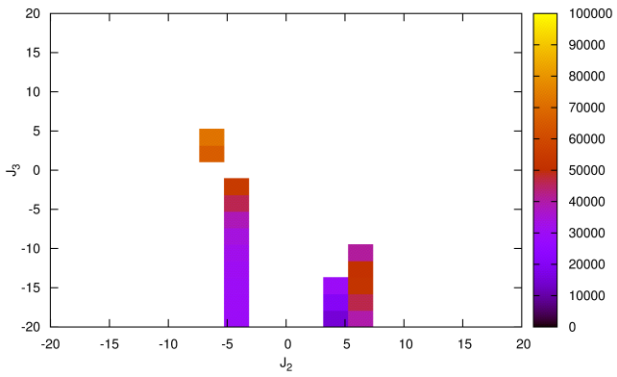


u)

**Figure S1** Plots of residual error *vs.* $J_2$ and $J_3$ for different values of $J_1$, $J_1$ = -20 (a), -18 (b), -16 (c), -14 (d), -12 (e), -10 (f), -8 (g), -6 (h), -4 (i), -2 (j), 0 (k), +2 (l), +4 (m), +6 (n), +8 (o), +10 (p), +12 (q), +14 (r), +16 (s), +18 (t) and +20 (u) $cm^{-1}$.

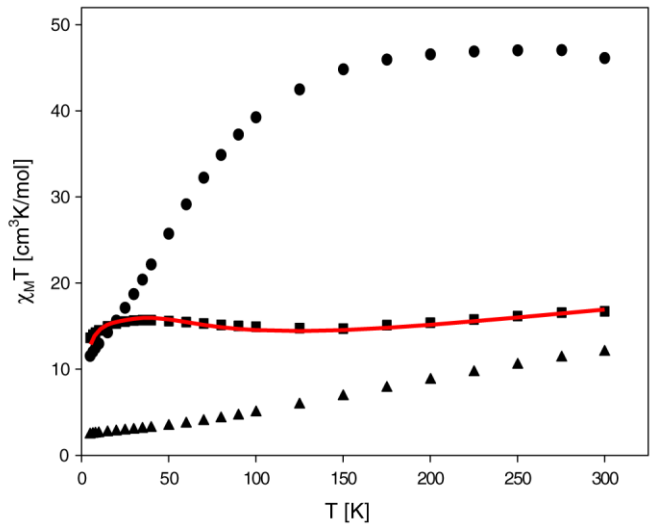


**Figure S2** Plots of magnetic data taken from A. Masello, M. Murugesu, K. A. Abboud, G. Christou, *Polyhedron*, 2007, **26**, 2276, with the black squares for a $Mn_8$ cluster analogous to **1**·3MeCN·$H_2O$, *viz.* $[Mn_8O_4(fdc)_6(DMF)_2(H_2O)_2]$.4DMF.4$H_2O$. The red line is that calculated using the model and the three *J* values given in the text.

**Table S1.** Bond valence sum calculations for **1**. The oxidation state for each metal is the whole number closest to the value in bold.

| Atoms | Mn(II) | Mn(III) | Mn(IV) |
|---|---|---|---|
| Mn1 | 3.30 | **3.05** | 2.99 |
| Mn2 | 3.28 | **3.05** | 2.99 |
| Mn3 | 3.30 | **3.05** | 2.99 |
| Mn4 | 3.28 | **3.05** | 2.99 |
| Mn5 | **2.24** | 2.10 | 2.04 |
| Mn6 | **2.05** | 1.93 | 1.87 |
| Mn7 | **2.04** | 1.92 | 1.86 |
| Mn8 | **2.14** | 2.01 | 1.95 |