The examples here also correspond to the same {Mn_6} complex (**Figure 1**) described in the documentation. In example 2, four of the Mn centres, Mn1, Mn2, Mn4 and Mn5, are in +IV oxidation state (d^3 spin configuration) while the others are in +III oxidation state. This decreases the overall symmetry of the complex. Thus, more J-values are required to capture the complete electronic picture leading to the use of the following Hamiltonian:

$$\begin{aligned} H = & -2J_1[\langle s_1.s_4\rangle + \langle s_2.s_5\rangle] - 2J_2[\langle s_3.s_6\rangle] - 2J_3[\langle s_1.s_2\rangle] - 2J_4[\langle s_4.s_5\rangle] \\ & - 2J_5[\langle s_1.s_5\rangle + \langle s_2.s_4\rangle] - 2J_6[\langle s_1.s_3\rangle + \langle s_2.s_3\rangle] - 2J_7[\langle s_1.s_6\rangle] \\ & - 2J_8[\langle s_2.s_6\rangle] - 2J_9[\langle s_3.s_4\rangle + \langle s_3.s_5\rangle] - 2J_{10}[\langle s_4.s_6\rangle + \langle s_5.s_6\rangle] \end{aligned}$$

As the Mn centres Mn1, Mn2, Mn4 and Mn5 are in +IV oxidation state, formally speaking, they should have three electrons in the d-orbitals. This is reflected in the spin density file (spin_example2) where the magnitude of the spin value on Mn centres Mn1, Mn2, Mn4 and Mn5 is close to 3. The magnitude of the spin value on Mn centres Mn3 and Mn6 is close to 4 indicating that they are in +III oxidation state (corresponding to a d^4 configuration). It must be noted that these spin values are determined from Bader analysis of the wavefunction of the optimized structures which were obtained using density functional theory calculations. It is possible to employ a different analysis scheme as well (e.g. Mulliken or Hirshfeld). A total of 16 states have been modelled for this complex as can be seen from the spin density file. The Hamiltonian given above is provided in the file example2. The output files example2_form.txt and example2.txt contain the J-values obtained with the use of formal spin density and the spin density from the file spin_example2 respectively.

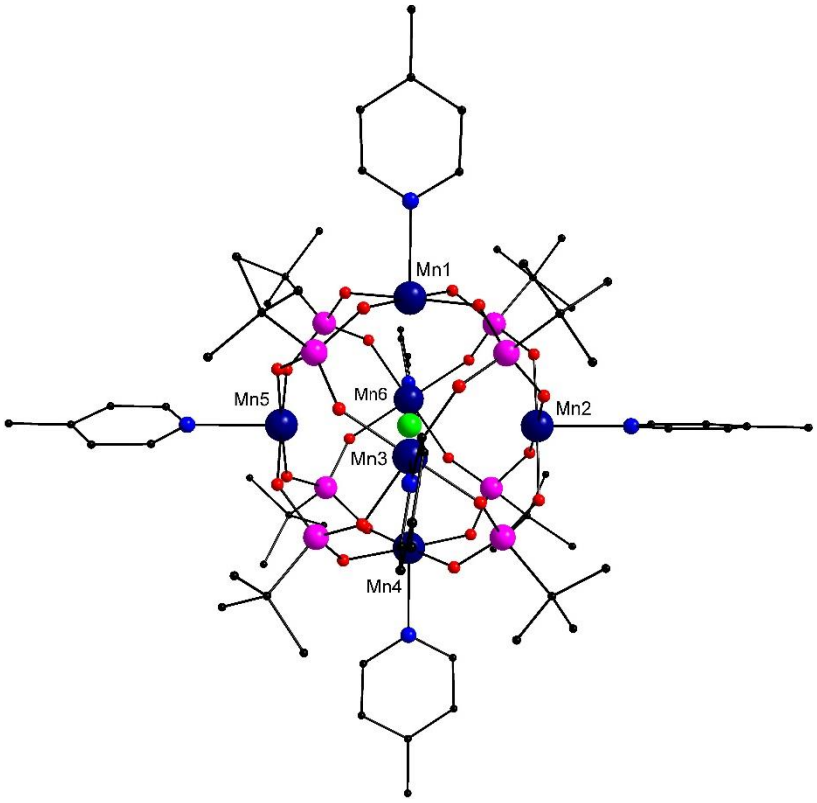

Figure 1: Structure of the {Mn_6} complex. Colour scheme: Mn (dark blue), P (pink), Cl (green), C (black), N (blue) and O (red). Hydrogen atoms have been removed for clarity.

In example 3, the Mn centres Mn1, Mn2 and Mn4 are in +IV oxidation state while the others are in +III oxidation state. The overall symmetry of the complex is significantly reduced and capturing the full electronic picture requires the use of the following Hamiltonian:

$$H = -2\mathrm{J}_1[< s_2.s_5 >] - 2\mathrm{J}_2[< s_1.s_4 >] - 2\mathrm{J}_3[< s_3.s_6 >] - 2\mathrm{J}_4[< s_1.s_2 >] \\ - 2\mathrm{J}_5[< s_1.s_5 >] - 2\mathrm{J}_6[< s_1.s_3 >] - 2\mathrm{J}_7[< s_1.s_6 >] - 2\mathrm{J}_8[< s_2.s_3 >] \\ - 2\mathrm{J}_9[< s_2.s_4 >] - 2\mathrm{J}_{10}[< s_2.s_6 >] - 2\mathrm{J}_{11}[< s_3.s_5 >] - 2\mathrm{J}_{12}[< s_4.s_5 >] \\ - 2\mathrm{J}_{13}[< s_5.s_6 >] - 2\mathrm{J}_{14}[< s_3.s_4 >] - 2\mathrm{J}_{15}[< s_4.s_6 >]$$

The spin density file (spin_example3) shows that the magnitude of the spin value on Mn centres Mn1, Mn2 and Mn4 is close to 3 indicating that they are in +IV oxidation state. The magnitude of the spin value on the remaining Mn centres is close to 4 suggesting that they are in +III oxidation state. The spin values are again obtained from Bader analysis and a total of 21 states have been modelled for this complex as can be seen from the spin density file. The above given Hamiltonian is provided in the file example3. The output files example3_form.txt and example3.txt contain the J-values obtained with the use of formal spin density and the spin density from the file spin_example3 respectively.