The examples here also correspond to the same {Mn_6} complex (**Figure 1**) described in the documentation. In example 2, it can be seen from the spin density file (spin_example2) that the spin value on Mn centres Mn1, Mn2, Mn4 and Mn5 is close to 3 which suggests the presence of a high-spin d^3 spin configuration indicating that they are in +IV oxidation state. 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). The difference in oxidation states results in significant asymmetry within the complex and the Hamiltonian for this complex 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.

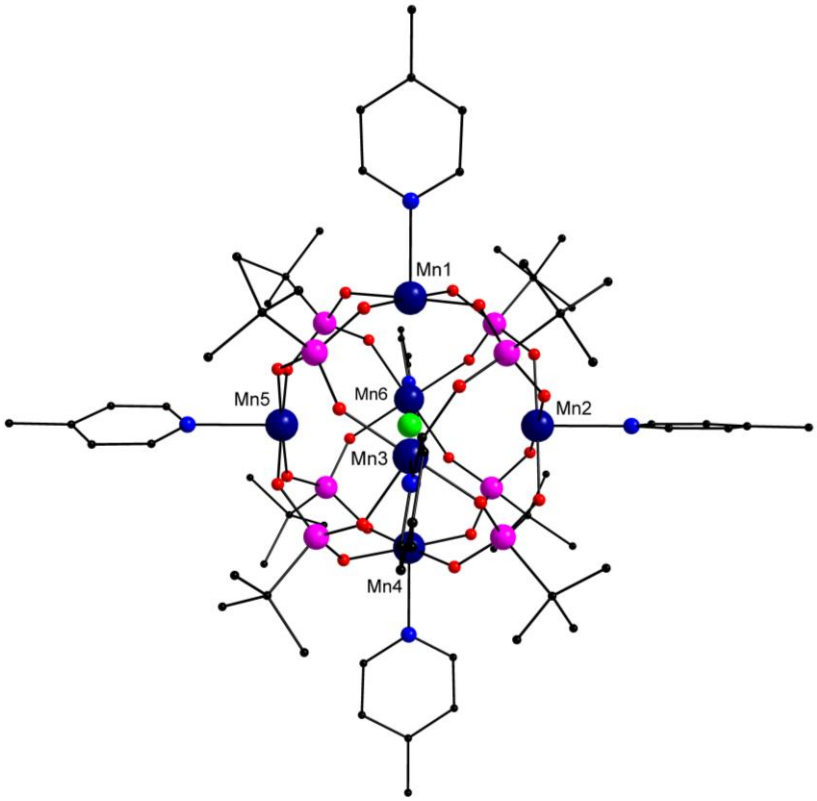

Figure 1: Structure of the {Mn_6} complex. Colour scheme: Mn (dark blue), P (pink), Cl (green), C (black), N (blue) and O (red). Hydrogen atoms have been removed for clarity.

In example 3, the spin density file (spin_example3) shows that the spin value on Mn centres Mn1, Mn2 and Mn4 is close to 3 indicating that they are in +IV oxidation state (corresponding to a d^3 configuration). The spin value on the remaining Mn centres is close to 4 suggesting that they are in +III oxidation state (corresponding to a d^4 configuration). The differences in oxidations state again leads to significant asymmetry and the Hamiltonian for this complex is given as 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.