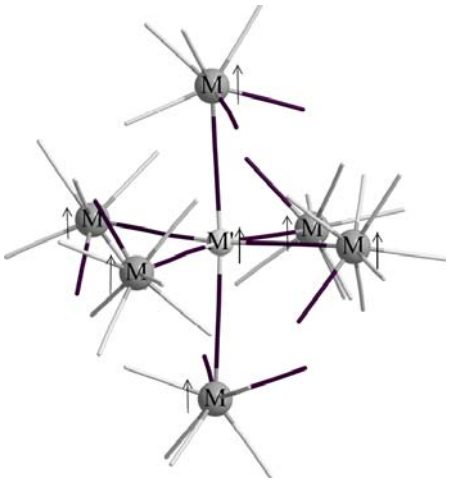
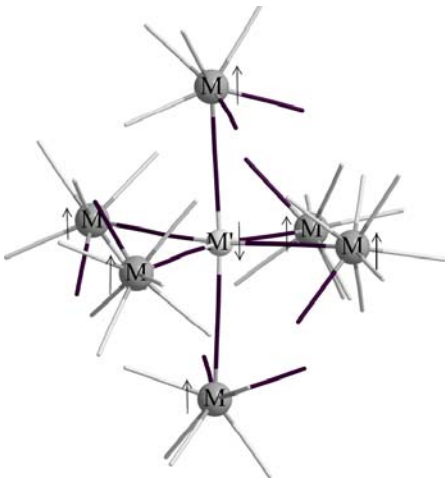
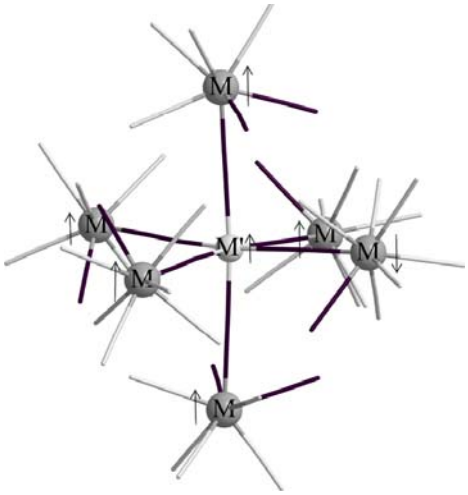
Three spin states for models $\mathbf{A}^6$, $\mathbf{B}^6$, $\mathbf{C}^6$ and $\mathbf{D}^6$ are as follows:



1

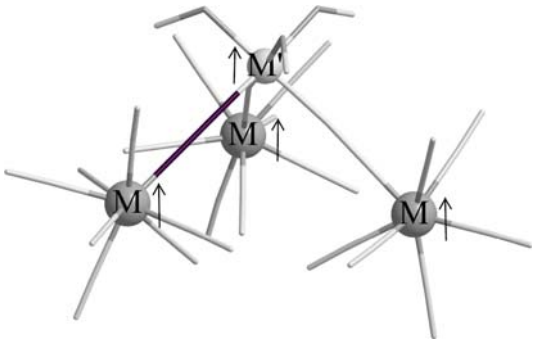


2

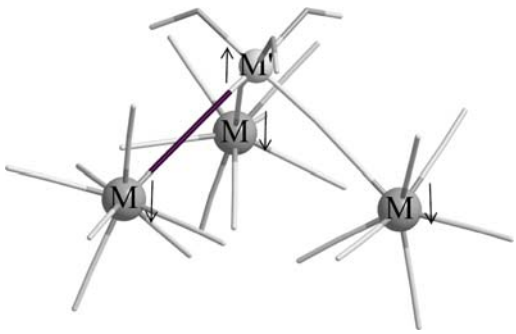


3

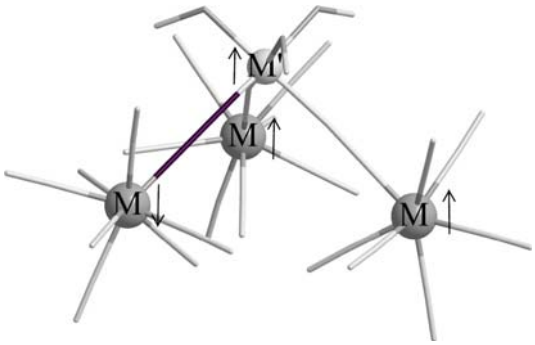
Five spin states for models $\mathbf{A}^3$, $\mathbf{B}^3$, $\mathbf{C}^3$ and $\mathbf{D}^3$ are as follows:



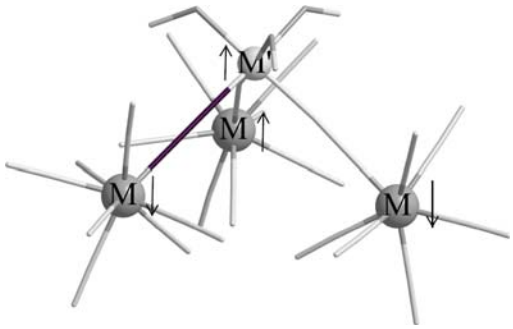
1



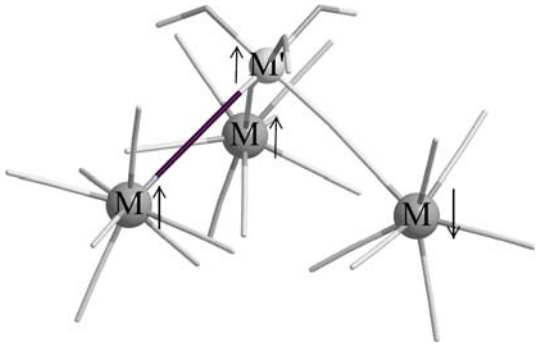
2



3



4



5

The equations to extract *J* values using different spin state energies for each of models $\mathbf{A}^6$, $\mathbf{B}^6$, $\mathbf{C}^6$, $\mathbf{D}^6$, $\mathbf{A}^3$, $\mathbf{B}^3$, $\mathbf{C}^3$ and $\mathbf{D}^3$.

For models $\mathbf{A}^6$ and $\mathbf{B}^6$, the equations are thus: $J_{ap} = (E_2 - E_1)/36$ (1)

$$J_{ap} = (E_2 - E_3)/30 \quad (2)$$

For models $\mathbf{C}^6$ and $\mathbf{D}^6$, the equations are thus: $J_{ap} = (E_2 - E_1)/18$ (3)

$$J_{ap} = (E_2 - E_3)/15 \quad (4)$$

For models $\mathbf{A}^3$ and $\mathbf{B}^3$, the equations are thus: $J_{ap} = (E_3 - E_1)/6$ (5)

$$J_{ap} = (E_4 - E_5)/6 \quad (6)$$

$$J_{ap} = (E_2 - E_4)/6 \quad (7)$$

$$J_{eq} = (E_2 - E_3)/12 \quad (8)$$

$$J_{eq} = (E_4 - E_3)/6 \quad (9)$$

$$J_{eq} = (E_5 - E_1)/6 \quad (10)$$

For models $\mathbf{C}^3$ and $\mathbf{D}^3$, the equations are thus: $J_{ap} = (E_3 - E_1)/3$ (11)

$$J_{ap} = (E_4 - E_5)/3 \quad (12)$$

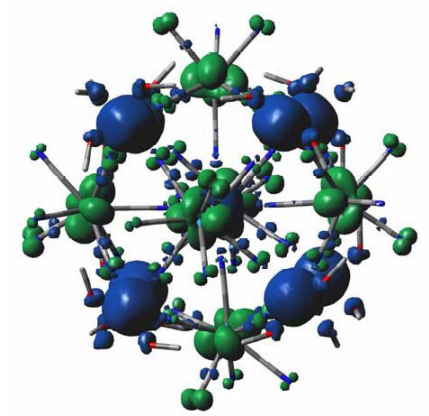
$$J_{ap} = (E_2 - E_4)/3 \quad (13)$$

$$J_{eq} = (E_2 - E_3)/6 \quad (14)$$

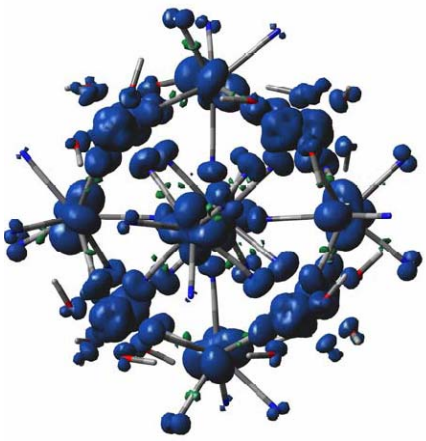
$$J_{eq} = (E_4 - E_3)/3 \quad (15)$$

$$J_{eq} = (E_5 - E_1)/3 \quad (16)$$

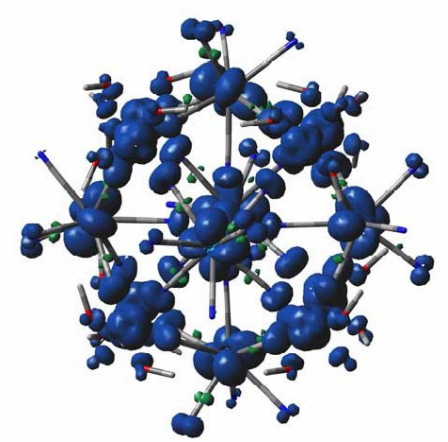
Representation of the spin density maps of complexes **B** (*S*=39/2 ground spin state), **C** (*S*=12 ground spin state) and **D** (*S*=12 ground spin state) in their ground spin states, respectively (blue and green regions indicate positive and negative spin populations, respectively; the isodensity surface represented corresponds to a value of 0.005 e^- /$bohr^3$).



B



C



D