Supplementary Material (ESI) for Chemical Communications

Supplementary materials

A Series of Nickel Phosphonate Clusters

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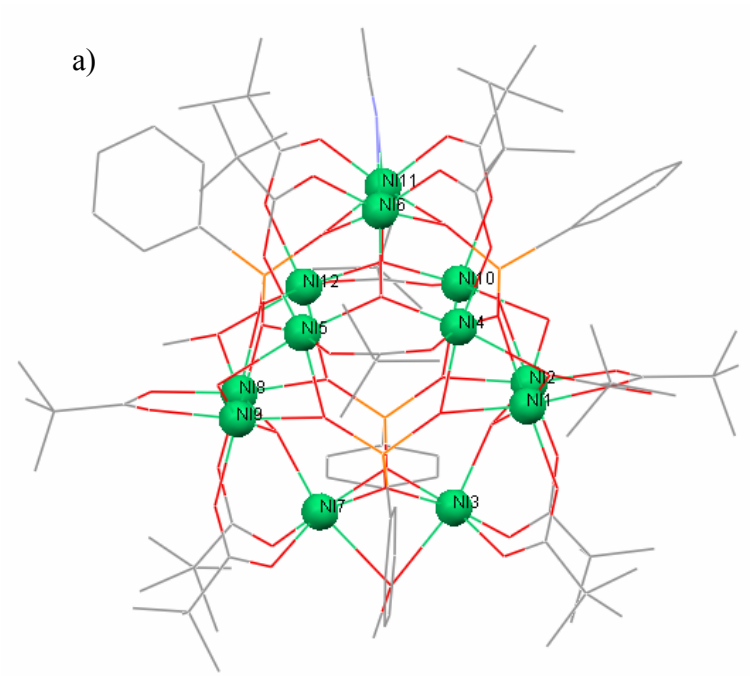
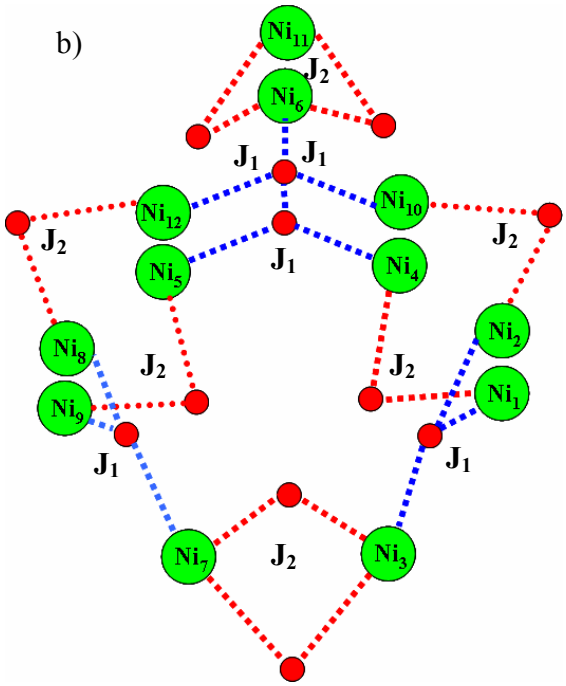




c)

$$H = -J_1\left[\hat{S}_{Ni1}\hat{S}_{Ni4} + \hat{S}_{Ni2}\hat{S}_{Ni10} + \hat{S}_{Ni3}\hat{S}_{Ni7} + \hat{S}_{Ni5}\hat{S}_{Ni9} + \hat{S}_{Ni6}\hat{S}_{Ni11} + \hat{S}_{Ni8}\hat{S}_{Ni12}\right]$$

$$-J_2\left[\hat{S}_{Ni1}\hat{S}_{Ni2} + \hat{S}_{Ni1}\hat{S}_{Ni3} + \hat{S}_{Ni2}\hat{S}_{Ni3} + \hat{S}_{Ni4}\hat{S}_{Ni5} + \hat{S}_{Ni4}\hat{S}_{Ni6} + \hat{S}_{Ni5}\hat{S}_{Ni6} + \hat{S}_{Ni7}\hat{S}_{Ni8} + \hat{S}_{Ni7}\hat{S}_{Ni9} + \hat{S}_{Ni8}\hat{S}_{Ni9} + \hat{S}_{Ni10}\hat{S}_{Ni11} + \hat{S}_{Ni10}\hat{S}_{Ni12} + \hat{S}_{Ni11}\hat{S}_{Ni12}\right]$$

spin Hamiltonian equation 1.

Fig. S1. a) Molecular X-ray crystal structure of **2** b) model picture which represents different exchange pathways present in **2**; c) Spin-Hamiltonian to describe the two different exchange pathways in **2**.

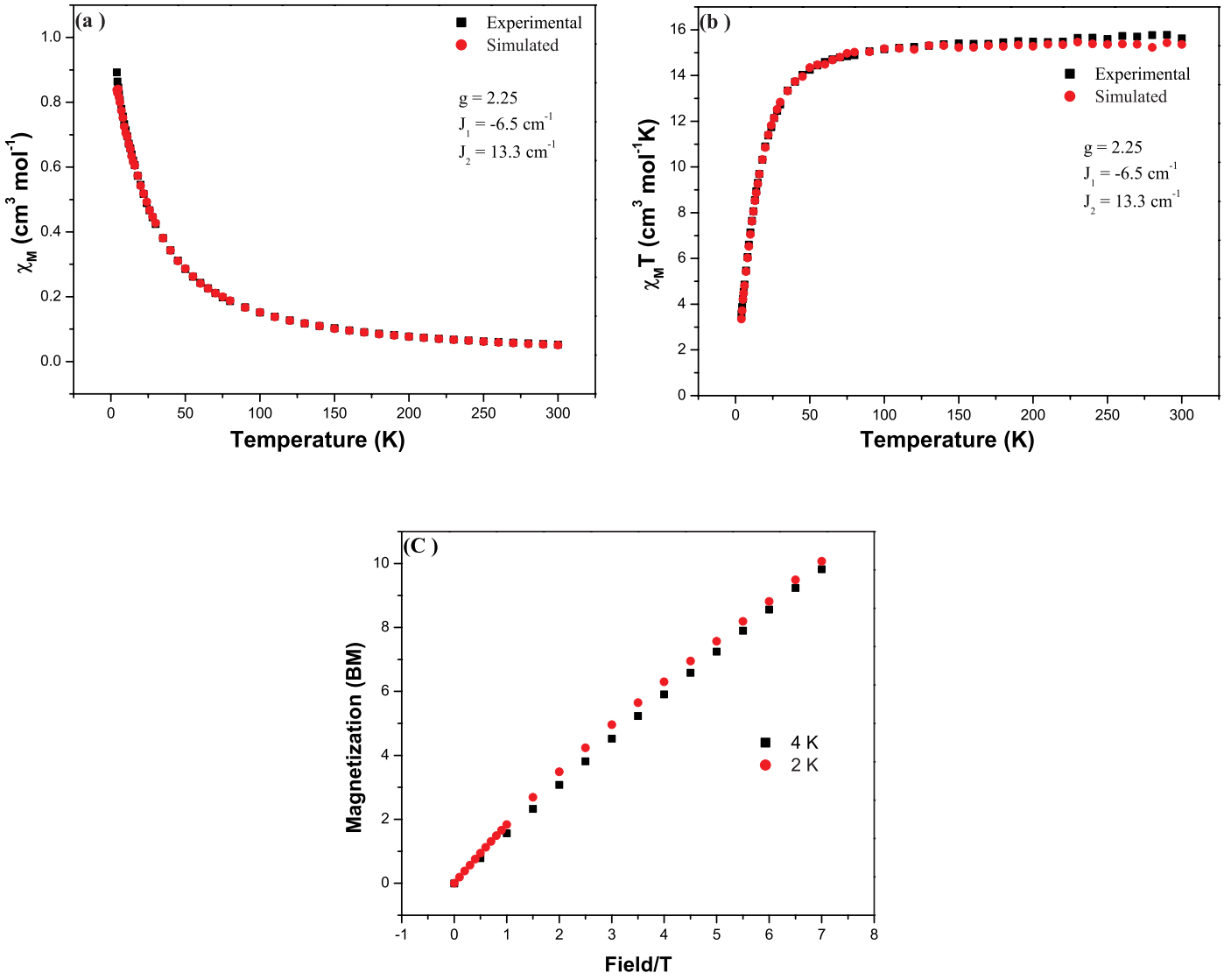
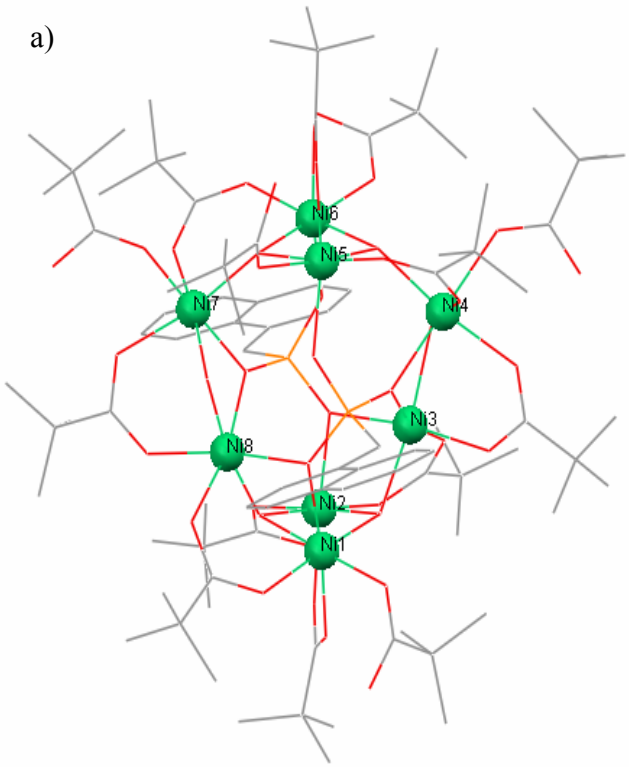
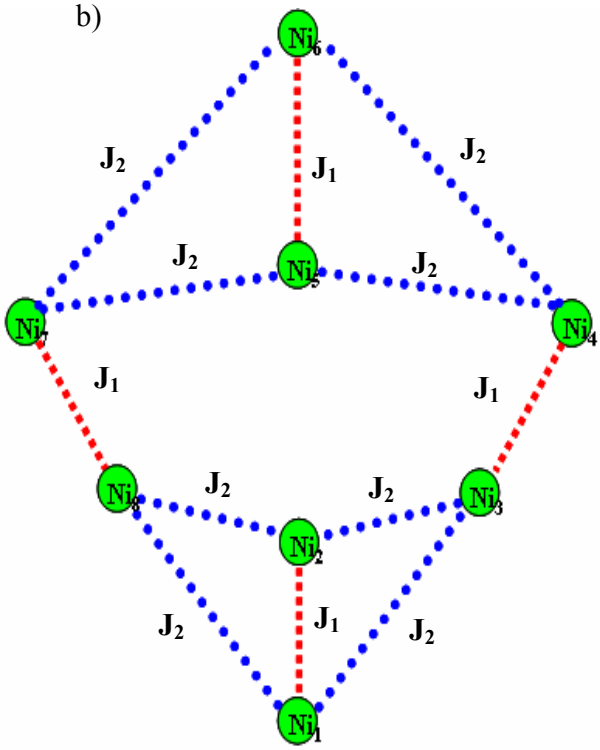


Fig. S2. a) Plot of molar magnetic susceptibility as a function of temperature of **2** b) plot of $\chi_M T$ vs T of **2**; the red circles represents best fit obtained using the above spin-Hamiltonian c) Field dependence of magnetization at constant temperatures for **2.**

a)



b)



c)

$$H = -J_1\left[\hat{S}_{Ni1}\hat{S}_{Ni2} + \hat{S}_{Ni3}\hat{S}_{Ni4} + \hat{S}_{Ni5}\hat{S}_{Ni6} + \hat{S}_{Ni7}\hat{S}_{Ni8}\right] - J_2\left[\hat{S}_{Ni1}\hat{S}_{Ni3} + \hat{S}_{Ni1}\hat{S}_{Ni8} + \hat{S}_{Ni2}\hat{S}_{Ni3} + \hat{S}_{Ni2}\hat{S}_{Ni8} + \hat{S}_{Ni4}\hat{S}_{Ni5} + \hat{S}_{Ni4}\hat{S}_{Ni6} + \hat{S}_{Ni5}\hat{S}_{Ni7} + \hat{S}_{Ni6}\hat{S}_{Ni7}\right]$$

Fig. S3. a) Molecular X-ray crystal structure of **3** b) model picture which represents different exchange pathways present in **3**; c) Spin-Hamiltonian to describe the two different exchange pathways in **3**.

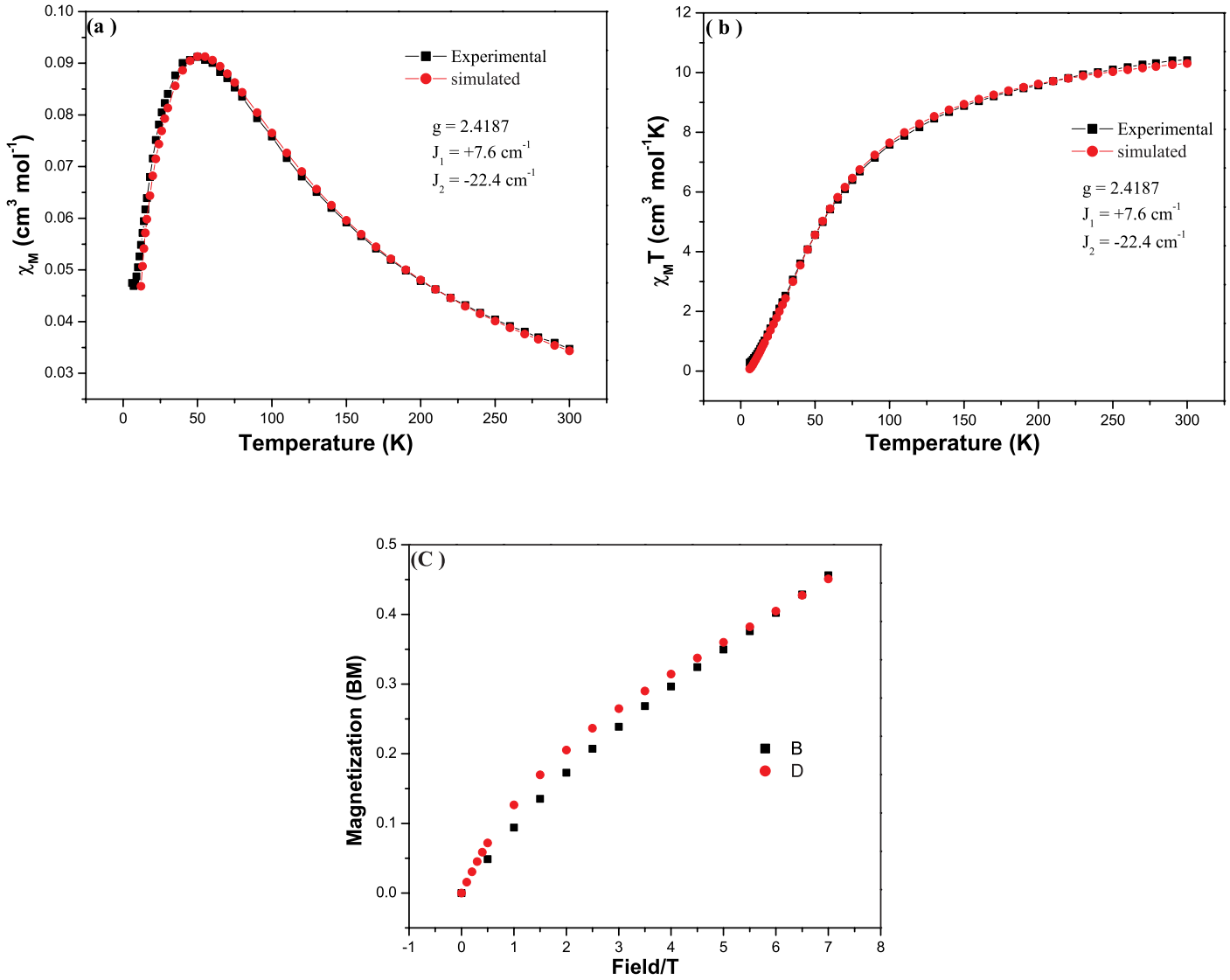
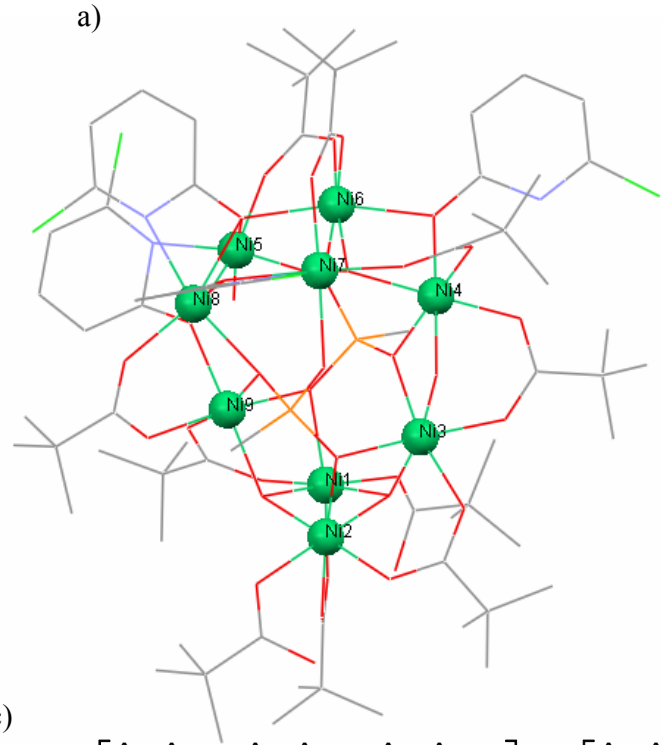
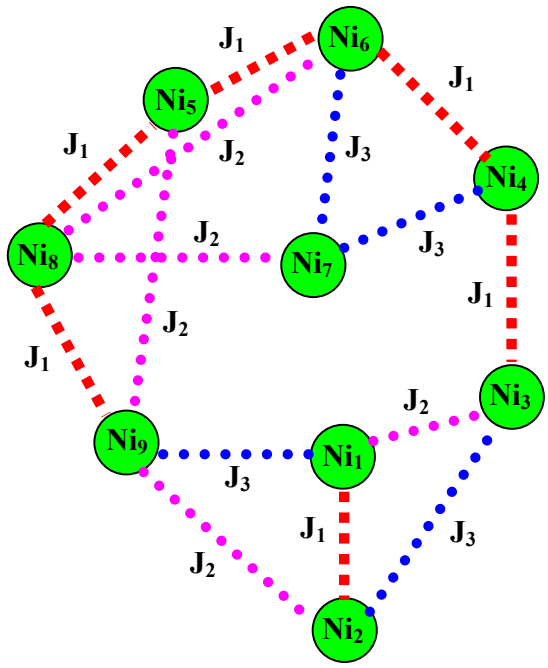


Fig. S4. a) Plot of molar magnetic susceptibility as a function of temperature of **3** b) plot of $\chi_M T$ vs T of **3**; the red circles represents best fit obtained using the above spin-Hamiltonian c) Field dependence of magnetization at constant temperatures for **3**.

a)



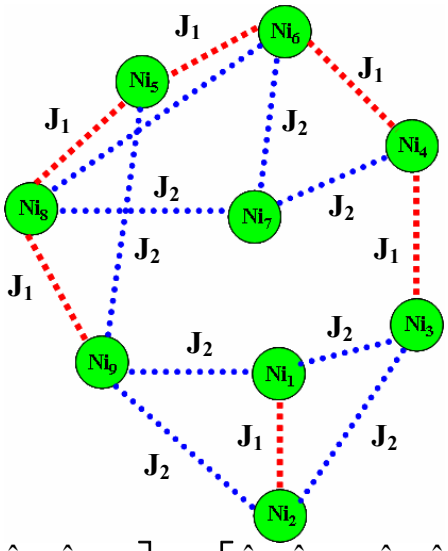
b)



c)

$$H = -J_1\left[\begin{matrix}\hat{S}_{Ni1}\hat{S}_{Ni2}+\hat{S}_{Ni3}\hat{S}_{Ni4}+\hat{S}_{Ni4}\hat{S}_{Ni6}\\+\hat{S}_{Ni5}\hat{S}_{Ni6}+\hat{S}_{Ni5}\hat{S}_{Ni8}+\hat{S}_{Ni8}\hat{S}_{Ni9}\end{matrix}\right]-J_2\left[\begin{matrix}\hat{S}_{Ni1}\hat{S}_{Ni3}+\hat{S}_{Ni2}\hat{S}_{Ni9}+\hat{S}_{Ni5}\hat{S}_{Ni9}\\+\hat{S}_{Ni6}\hat{S}_{Ni8}+\hat{S}_{Ni7}\hat{S}_{Ni8}\end{matrix}\right]-J_3\left[\begin{matrix}\hat{S}_{Ni1}\hat{S}_{Ni9}+\hat{S}_{Ni2}\hat{S}_{Ni3}\\+\hat{S}_{Ni4}\hat{S}_{Ni7}+\hat{S}_{Ni6}\hat{S}_{Ni7}\end{matrix}\right]$$

spin Hamiltonian equation 3



d)

$$H = -J_1\left[\begin{matrix}\hat{S}_{Ni1}\hat{S}_{Ni2}+\hat{S}_{Ni3}\hat{S}_{Ni4}+\hat{S}_{Ni4}\hat{S}_{Ni6}\\+\hat{S}_{Ni5}\hat{S}_{Ni6}+\hat{S}_{Ni5}\hat{S}_{Ni8}+\hat{S}_{Ni8}\hat{S}_{Ni9}\end{matrix}\right]-J_2\left[\begin{matrix}\hat{S}_{Ni1}\hat{S}_{Ni3}+\hat{S}_{Ni1}\hat{S}_{Ni9}+\hat{S}_{Ni2}\hat{S}_{Ni3}+\hat{S}_{Ni2}\hat{S}_{Ni9}+\hat{S}_{Ni4}\hat{S}_{Ni7}\\+\hat{S}_{Ni5}\hat{S}_{Ni9}+\hat{S}_{Ni6}\hat{S}_{Ni7}+\hat{S}_{Ni6}\hat{S}_{Ni8}+\hat{S}_{Ni7}\hat{S}_{Ni8}\end{matrix}\right]$$

spin Hamiltonian equation 4.

Fig. S5. a) Molecular X-ray crystal structure of **4;** b) model picture which represents different exchange pathways present in **4**; c) Spin-Hamiltonian to describes the three different exchange pathways in **4**; d) Simplified spin Hamiltonian, to describes the different exchange pathways in for 4.

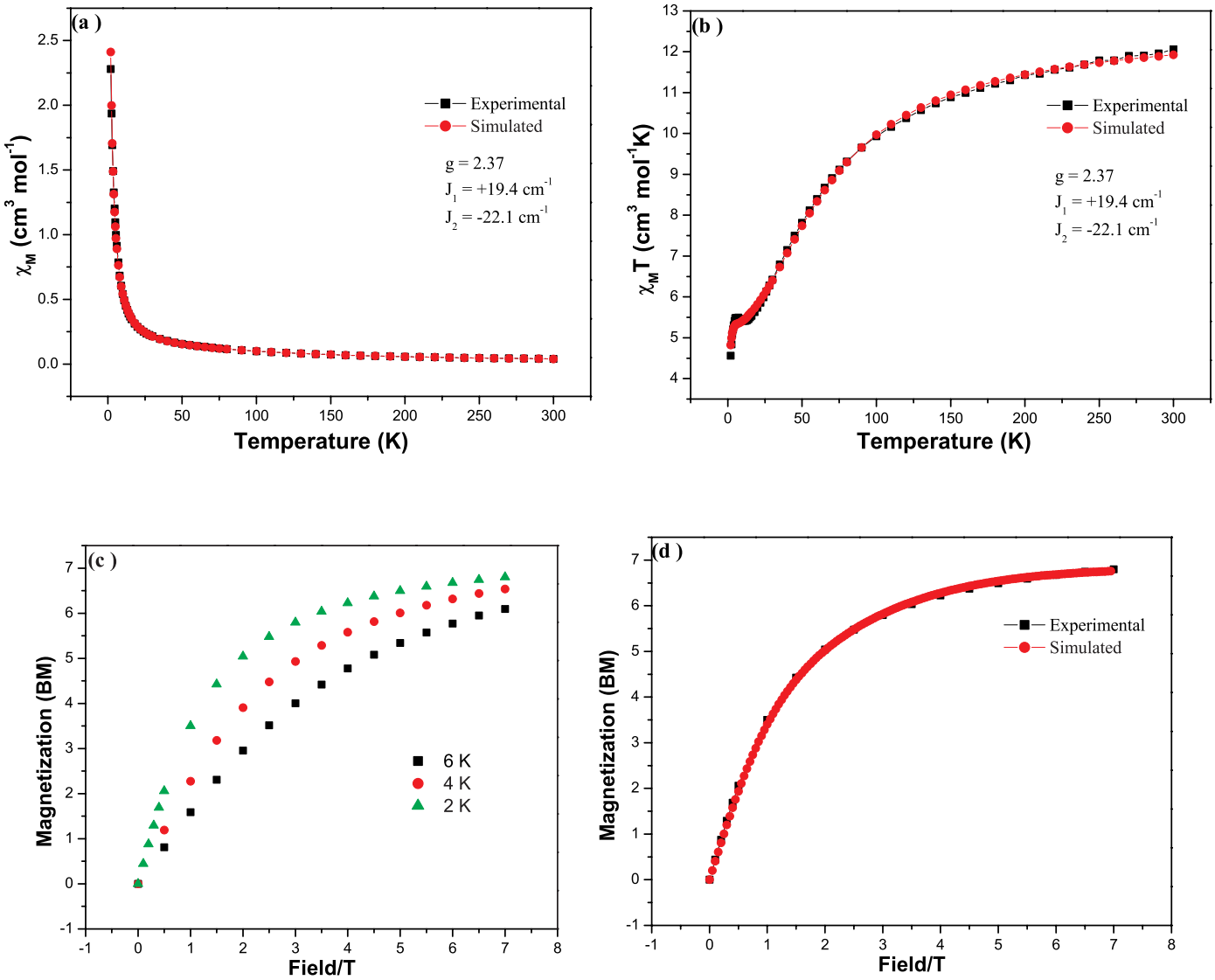


Fig. S6. a) Plot of molar magnetic susceptibility as a function of temperature of **4** b) plot of $\chi_M T$ vs T of **4**; the red circles represents best fit obtained using the above spin-Hamiltonian; c) Field dependence of magnetization at constant temperature for **4**; d) Field dependence of magnetization at 1.8 K for **4** with simulation.