Supplementary Information for

Weak antiferromagnetic coupling for novel linear hexanuclear nickel(II) string complexes (Ni_6^{12+}) and partial metal-metal bonds in their one-electron reduction products (Ni_6^{11+})

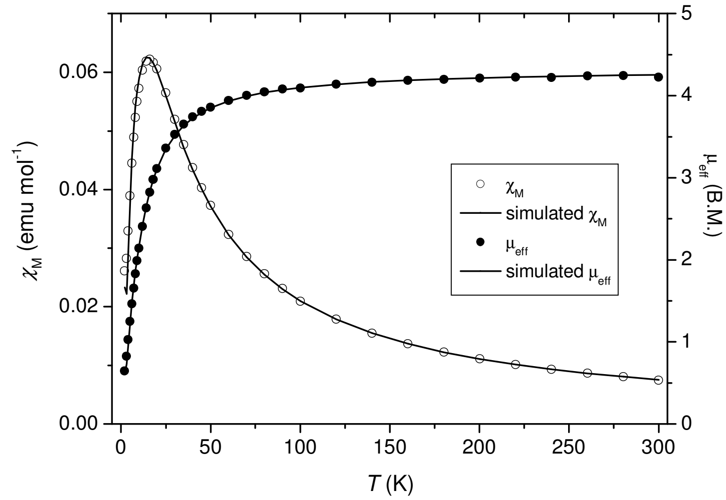


Fig. S1 The magnetic behavior for compound **3**: molar magnetic susceptibility χ_M (○), temperature-dependent effective magnetic moments μ_{eff} (●), and simulations (solid line, —).

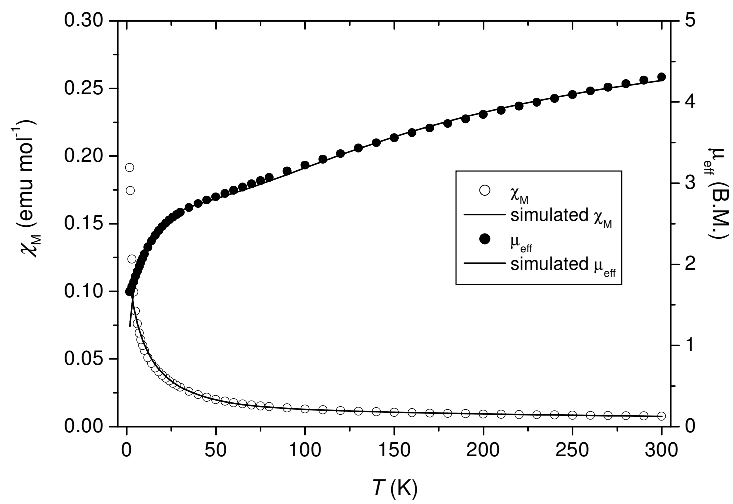
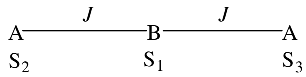


Fig. S2 The magnetic behavior for compound **4**: molar magnetic susceptibility χ_M (○), temperature-dependent effective magnetic moments μ_{eff} (●), and simulations (solid line, —).

Scheme S1 The linear trinuclear (A—B—A) model.



$$\mathbf{H}=-2J(\mathbf{S}_1\mathbf{S}_2+\mathbf{S}_1\mathbf{S}_3)-2J'\mathbf{S}_2\mathbf{S}_3$$

$$E(S_T,S_{23}) = -J[S_T(S_T+1)-\sum_{i=1}^{3}S_i(S_i+1)]-(J'-J)[S_{23}(S_{23}+1)-S_2(S_2+1)-S_3(S_3+1)]$$

$J' = 0$

$$E(S_T,S_{23}) = -JS_T(S_T+1)+JS_{23}(S_{23}+1)+J\sum_{i=1}^{3}S_i(S_i+1)-J[S_2(S_2+1)+S_3(S_3+1)]$$

$\mathbf{S}_{23} = \mathbf{S}_2 + \mathbf{S}_3$, $\mathbf{S}_T = \mathbf{S}_{23} + \mathbf{S}_1$

$S_1 = 1/2$, $S_2 = S_3 = 1$

So $S_{23} = 0 \rightarrow S_T = 1/2$

$S_{23} = 1 \rightarrow S_T = 1/2, 3/2$

$S_{23} = 2 \rightarrow S_T = 1/2, 3/2, 5/2$

$E(1/2,0) = -3J/4 \rightarrow -6J$

$E(1/2,1) = -3J/4 + 2J \rightarrow -4J$

$E(3/2,1) = -15J/4 + 2J \rightarrow -7J$

$E(1/2,2) = -3J/4 + 6J \rightarrow 0$

$E(3/2,2) = -15J/4 + 6J \rightarrow -3J$

$E(5/2,2) = -35J/4 + 6J \rightarrow -8J$

$$\chi=\frac{Ng^2\beta^2}{4kT}\times\frac{1+10e^{3J/kT}+e^{4J/kT}+e^{6J/kT}+10e^{7J/kT}+35e^{8J/kT}}{1+2e^{3J/kT}+e^{4J/kT}+e^{6J/kT}+2e^{7J/kT}+3e^{8J/kT}}$$

When the impurities are taken into account, the equation of χ_M is corrected by Weiss constant as following:

$$\chi=\frac{Ng^2\beta^2}{4k(T-\theta)}\times\frac{1+10e^{3J/kT}+e^{4J/kT}+e^{6J/kT}+10e^{7J/kT}+35e^{8J/kT}}{1+2e^{3J/kT}+e^{4J/kT}+e^{6J/kT}+2e^{7J/kT}+3e^{8J/kT}}\times(1-\rho)+\frac{Ng^2\beta^2\sum S_i(S_i+1)}{3k(T-\theta)}\times\rho$$
$$=\frac{Ng^2\beta^2}{4k(T-\theta)}\times\frac{1+10e^{3J/kT}+e^{4J/kT}+e^{6J/kT}+10e^{7J/kT}+35e^{8J/kT}}{1+2e^{3J/kT}+e^{4J/kT}+e^{6J/kT}+2e^{7J/kT}+3e^{8J/kT}}\times(1-\rho)+\frac{4Ng^2\beta^2}{k(T-\theta)}\times\rho$$

where $\sum S_i(S_i+1) = 6 \times 1 \times (1+1) = 12$

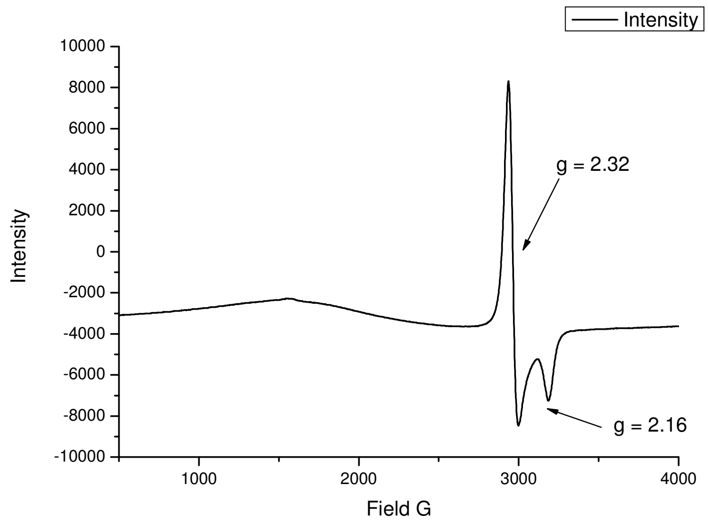


Fig. S3 The EPR spectrum of compound **2** in CH_2Cl_2 at 77 K.

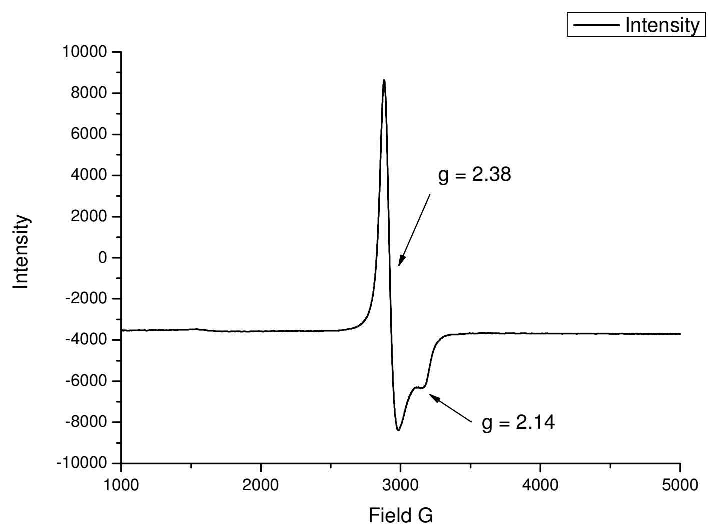


Fig. S4 The EPR spectrum of compound **4** in CH_2Cl_2 at 77 K.