Supplementary Material (ESI) for Dalton Transactions

Supplementary Materials:

Article Ref : B300539a - Dalton Transactions

(6 figures, 1 table)

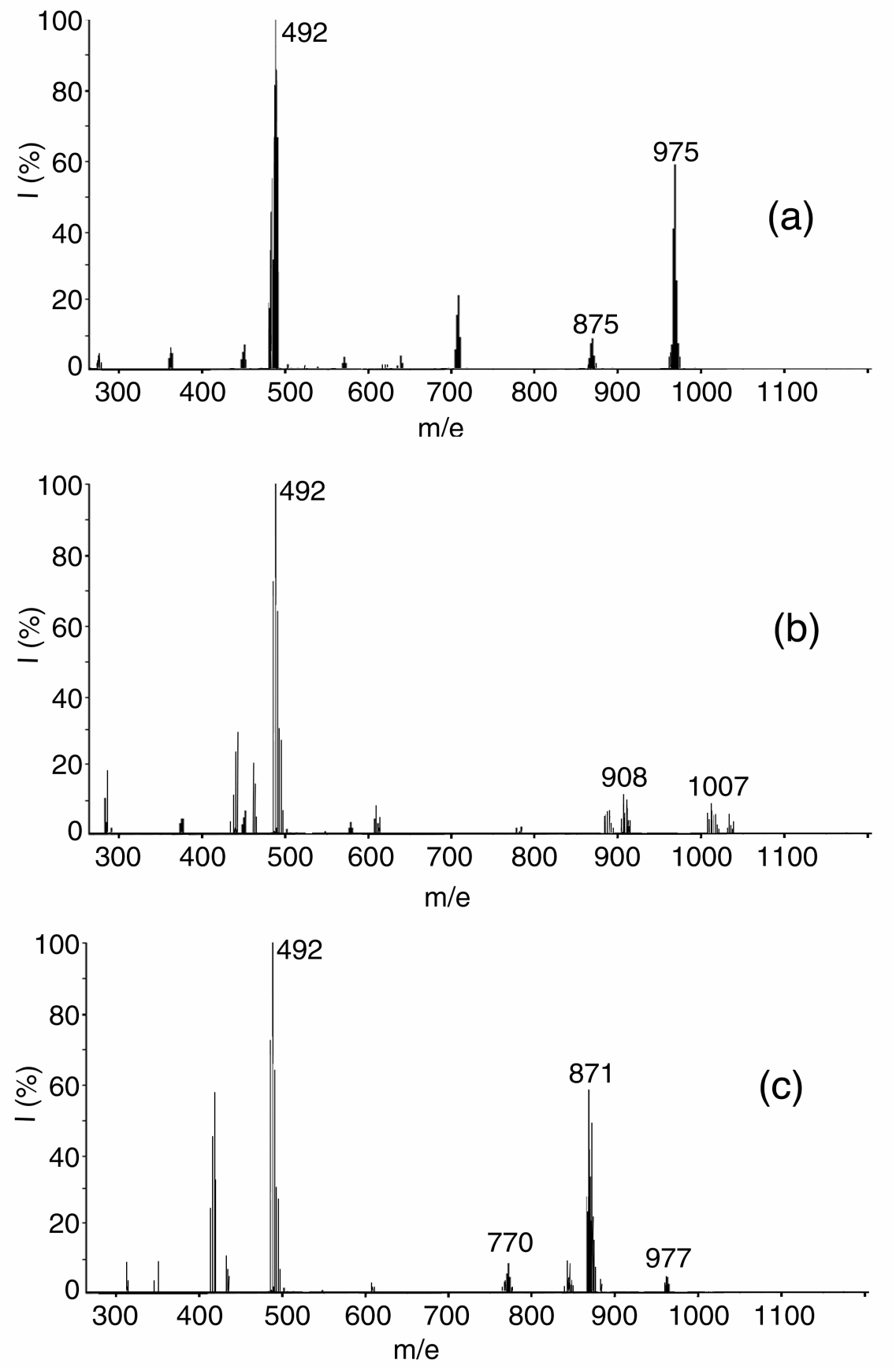

Figure S1 (above): ESI-mass spectra for the $Moda^-$ complexes: (a) $\{Ni(Dien)\}_2(\mu_3\text{-}OH)_2\{Ni_2(Moda)_4\}(ClO_4)_2{\cdot}H_2O$, **1**; (b) $\{Ni(Sdien)\}_2(\mu_3\text{-}OH)_2\{Ni_2(Moda)_4\}(ClO_4)_2{\cdot}H_2O$, **2** and (c) $\{Ni(Odien)\}_2(\mu_3\text{-}OH)_2\{Ni_2(Moda)_4\}(ClO_4)_2{\cdot}0.6H_2O$, **3.**

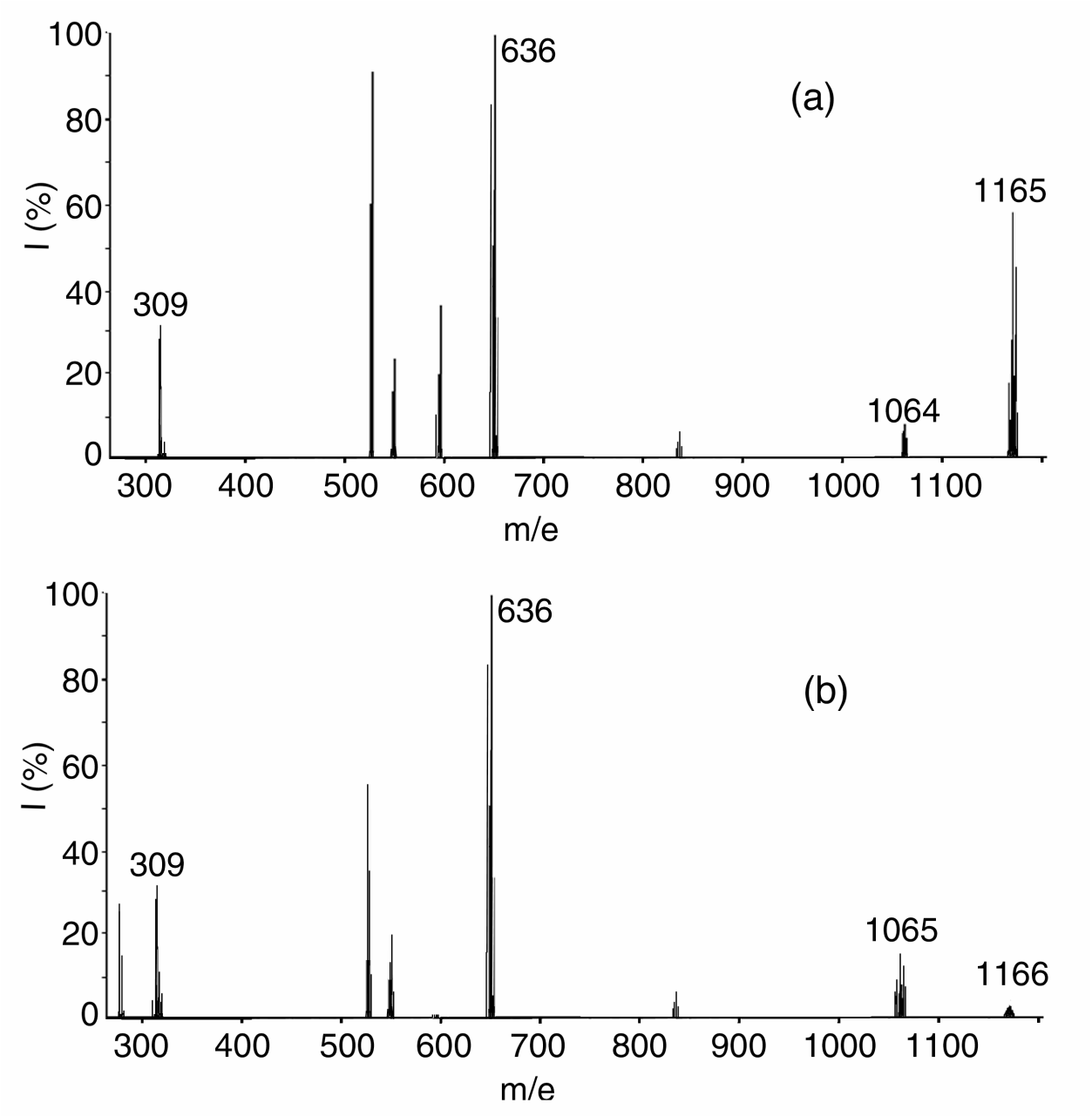

Figure S2 (above): ESI-mass spectra for the $Inaf^-$ complexes: (a) $\{Ni(Dien)\}_2(\mu_3\text{-}OH)_2\{Ni_2(Inaf)_4\}(ClO_4)_2{\cdot}CH_3NO_2$, **4**, (b) $\{Ni(Odien)\}_2(\mu_3\text{-}OH)_2\{Ni_2(Inaf)_4\}(ClO_4)_2{\cdot}2NaClO_4{\cdot}2H_2O$, **5**.

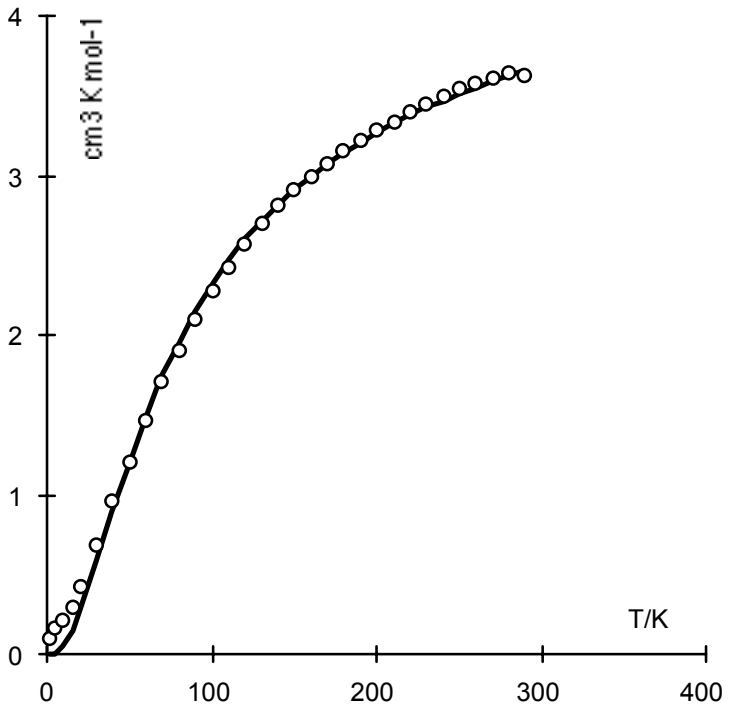

Figure S3 (above)**:** χT *vs* T plot for compound **1b**. Solid line represents fit to eq. 3-5, with parameters from Table 4.

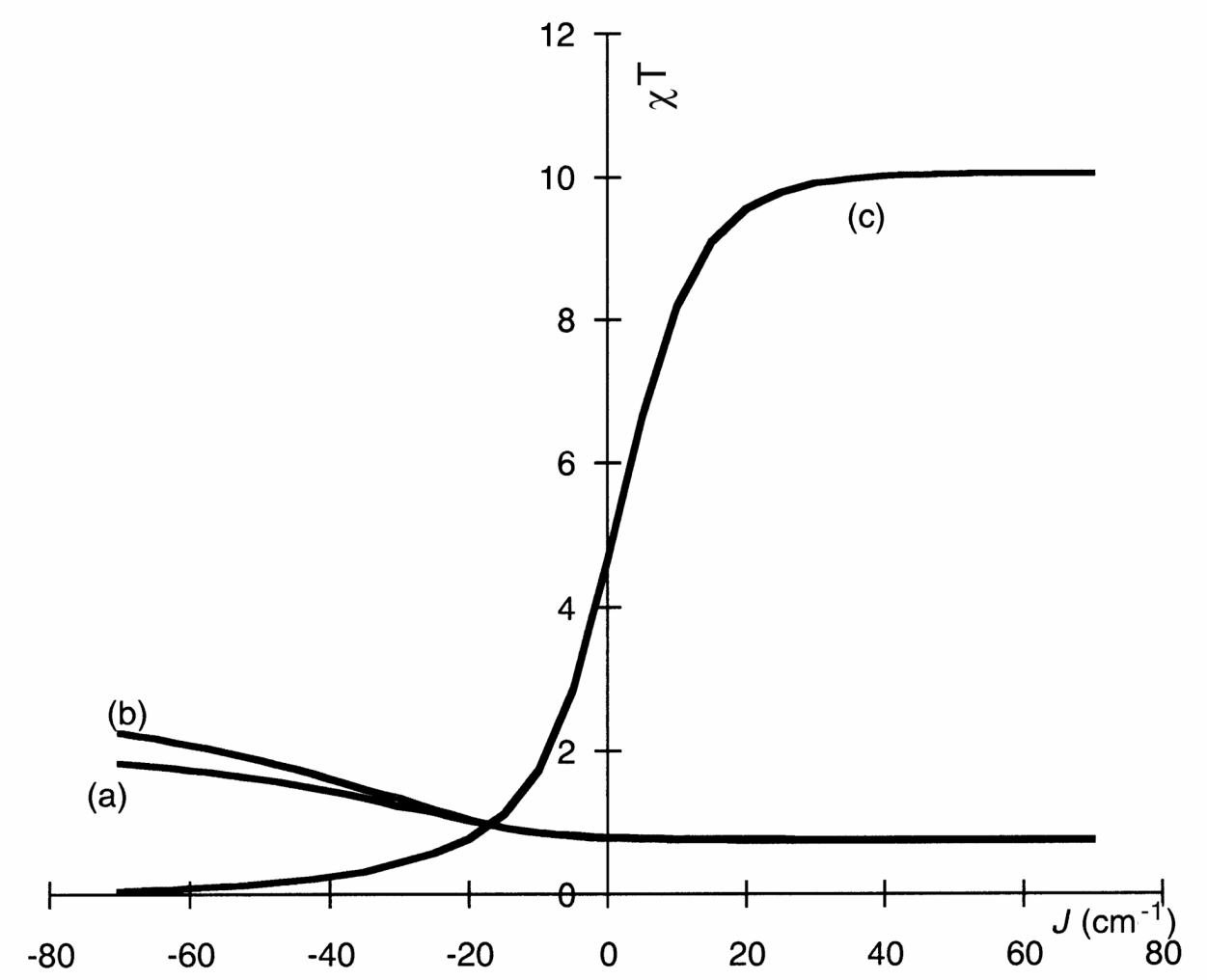

Fig S4 (above)**:** Illustration of the response of the magnetic properties of tetranickel rhombū s to the *J*-values, as plots of the dependence of χT at 50 K, for (a) J_b varied with J_a=-20, J_c=0 cm^{-1}; (b) J_c varied with J_a=-20, J_b=+10 cm^{-1}; (c) J_a varied with J_b=+10, J_c=0 cm^{-1} (all with g=2.0, ρ, *tip*=0).

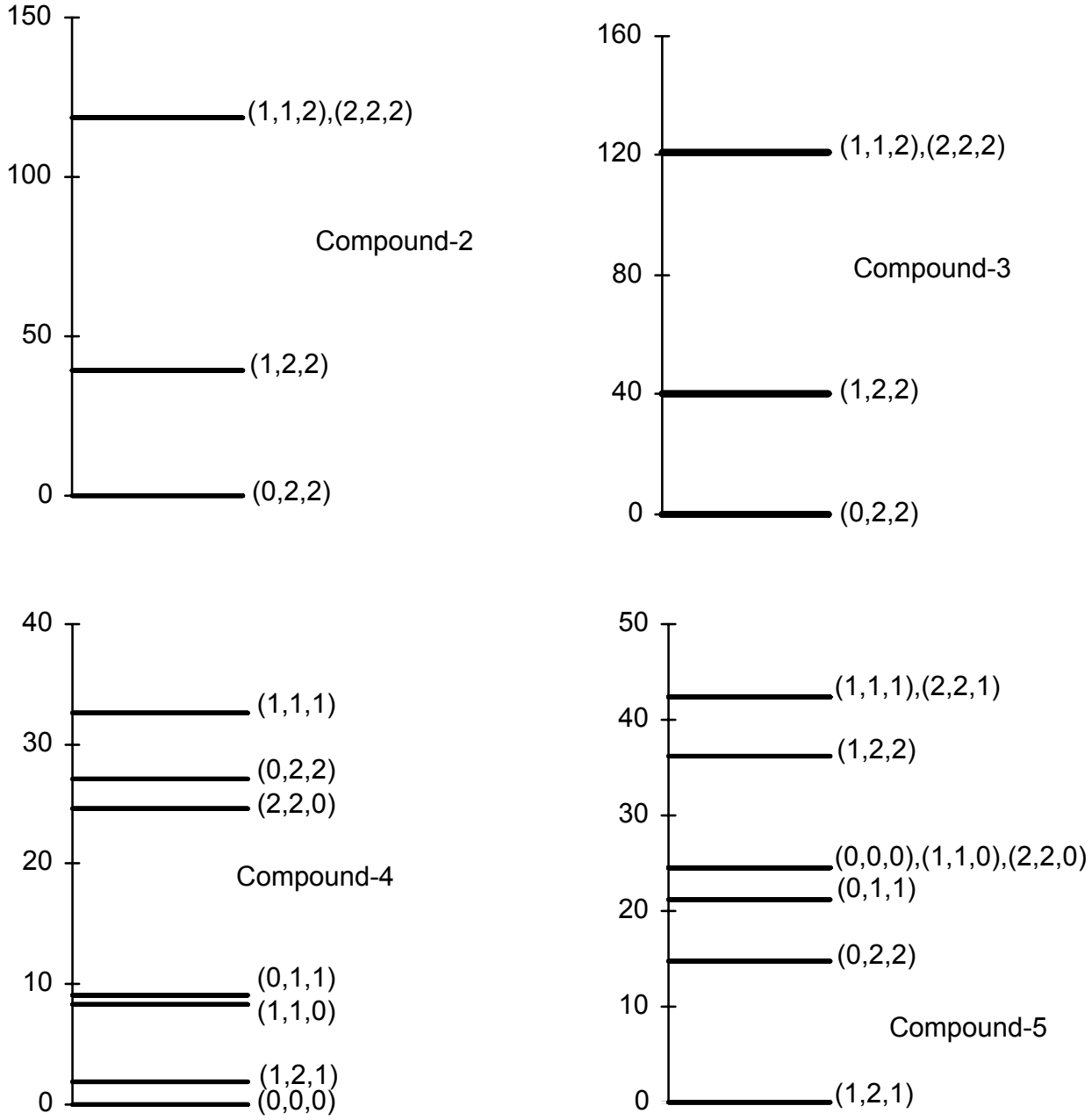

Figure S5 (above): Low-lying spin levels in the complexes **2**, **3**, **4** & **5**.

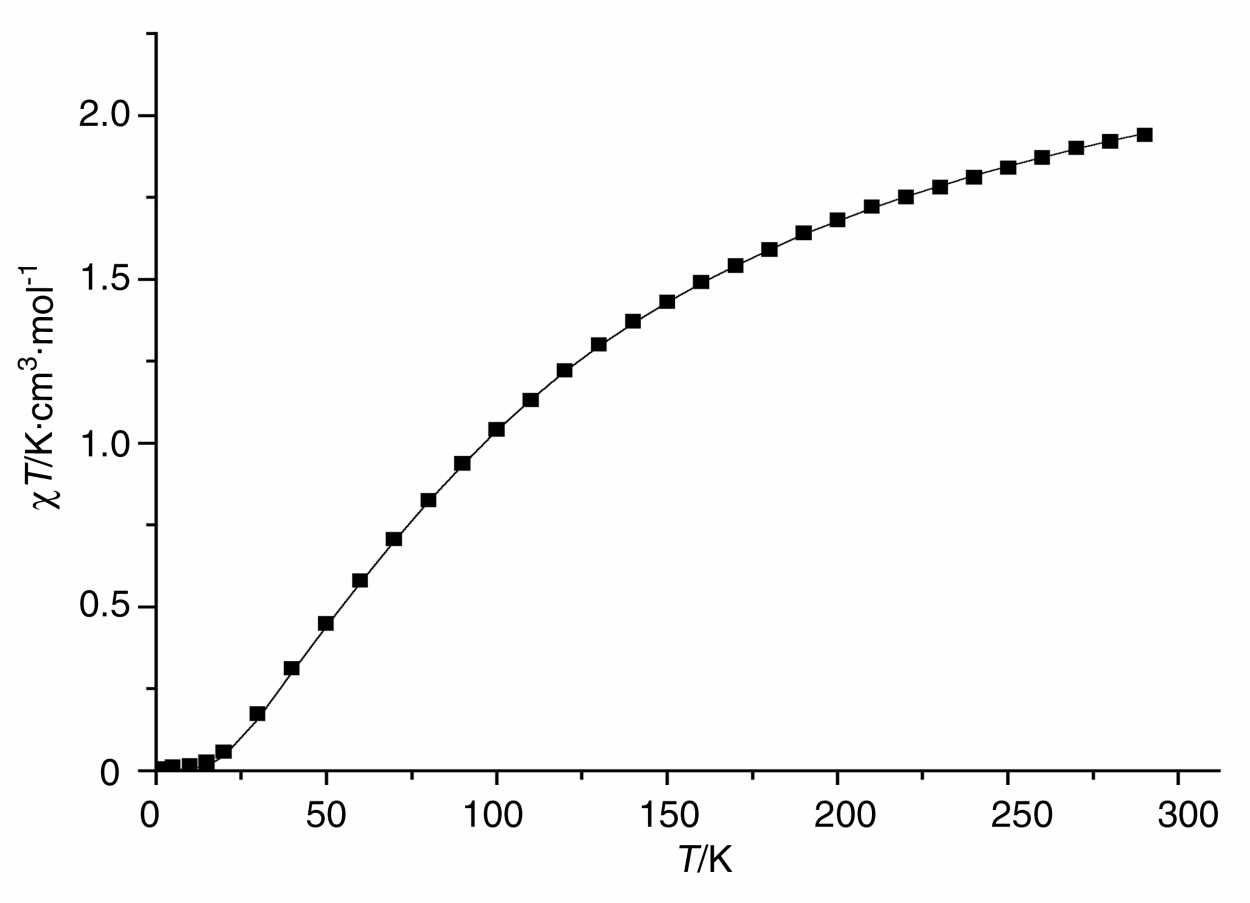

Figure S6 (above): χT *vs* T plot for the dinuclear compound **6**. The solid line represents the theoretical fit to eq. 6, with the parameters from Table 4.

Table S1. Spectroscopic properties of the nickel(II) complexes 1 – 5.

Ligand set	λ_{max}/nm (ε/cm^{-1} dm^3 mol^{-1}) in CH_3CN	λ_{max}/nm (ε/cm^{-1} dm^3 mol^{-1}) in CH_3NO_2
1 Dien/Moda$^-$	310 ($3.5\infty10^4$), 560 (sh, 250)	555 (220)
2 Sdien/Moda$^-$	295 ($2.8\infty10^4$), 571 (150)	571 (150)
3 Odien/Moda$^-$	303 ($2.1\infty10^4$), 575 (120)	559 (sh, 120)
4 Dien/Inaf$^-$	571 (200)	571 (190)
5 Odien/Inaf$^-$	588 (120)	571 (130)