Electronic Supplementary Information for Dalton Transactions

Supporting Information

Ferromagnetically Coupled Chiral Cyanide-bridged $\{Ni_6Fe_4\}$ Cages

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Additional Experimental Information

UV/VIS absorption spectra were measured between 200 and 1200 nm with a Shimadzu UV-vis spectrometer UV-3100.

CD spectra for the acetonitrile solutions and KCl pellets were recorded on a JASCO J-810 spectropolarimeter. The measurements of acetonitrile solutions were in the range of 1100-700 nm and 900-220 nm and were performed using the bandwidths of 2 nm and 1 nm, respectively. The measurements on KCl were in the range of 1000-700 nm and 900-245 nm with bandwidths of 10 nm and 4 nm, respectively. 10% diluted KCl pellets were measured in the range of 500-190 nm,with a bandwidth of 4 nm.

Cryospray measurements at -20 °C were carried out at concentrations of the complex in the region of 10^{-5} mol L^{-1} in methanol using a Bruker microTOFQ instrument. Data was collected in positive ion mode and the spectrometer was previously calibrated with the standard tune mix to give a precision of ca. 1.5 ppm in the region of 500-3000 m/z. The standard parameters for a medium mass data acquisition were used, the end plate voltage was set to –500 V and the capillary to +4500 V.

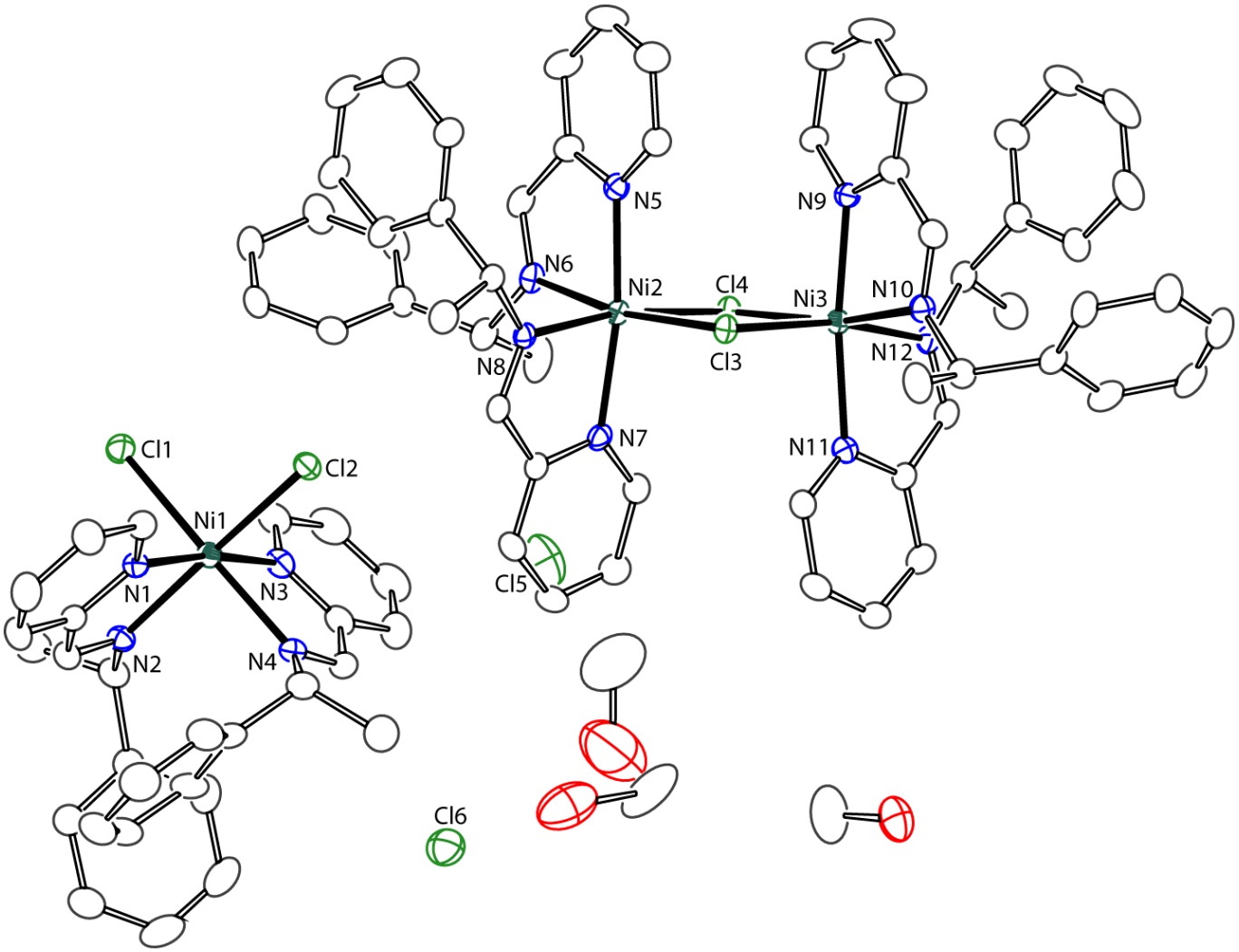

Figure S1. ORTEP drawing of $[Ni_2Cl_2(L^R)_4][NiCl_2(L^R)_2]Cl_2 \cdot 3MeOH$ (**1R**).

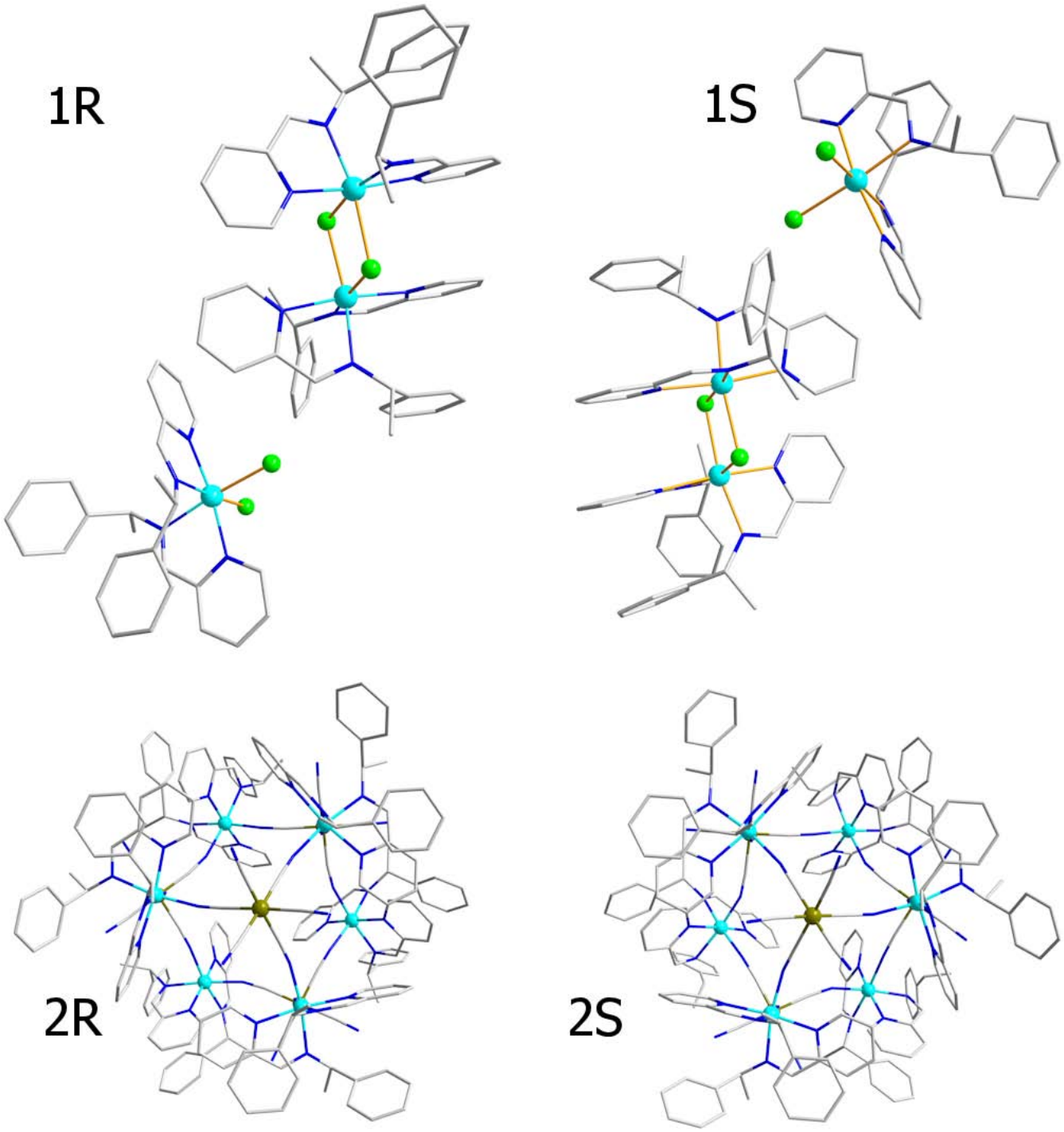

Figure S2. Structural comparison of 1R, 1S, 2R and 2S. All solvent molecules and counterions have been excluded for clarity.

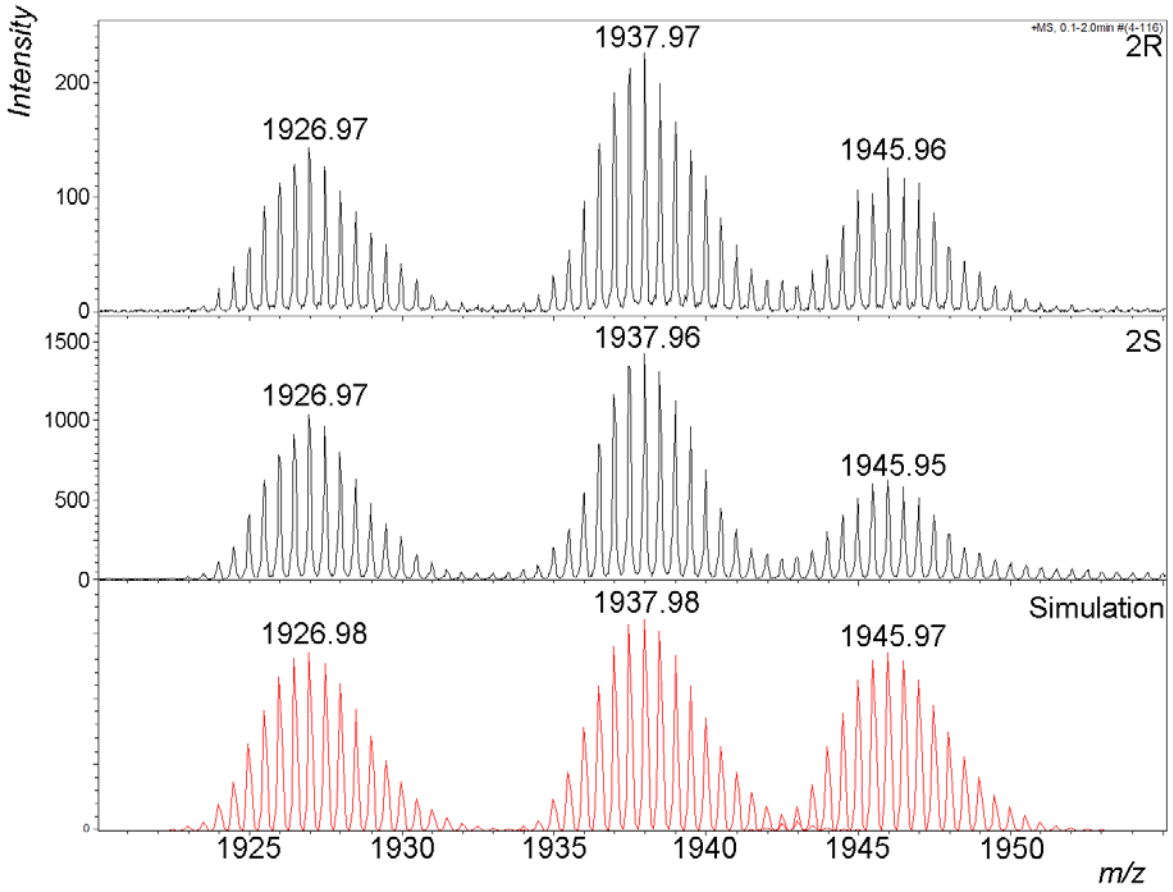

Figure S3. CSI-MS spectra of **2R** and **2S** observed (black) and simulated (red): 1926.98 = $[(Et_4N)H[Ni(L^{R/S})_2]_6[Fe(CN)_6]_4]^{2+}$; 1937.98 = $[(Et_4N)Na[Ni(L^{R/S})_2]_6[Fe(CN)_6]_4]^{2+}$; 1945.97 = $[(Et_4N)K[Ni(L^{R/S})_2]_6[Fe(CN)_6]_4]^{2+}$.

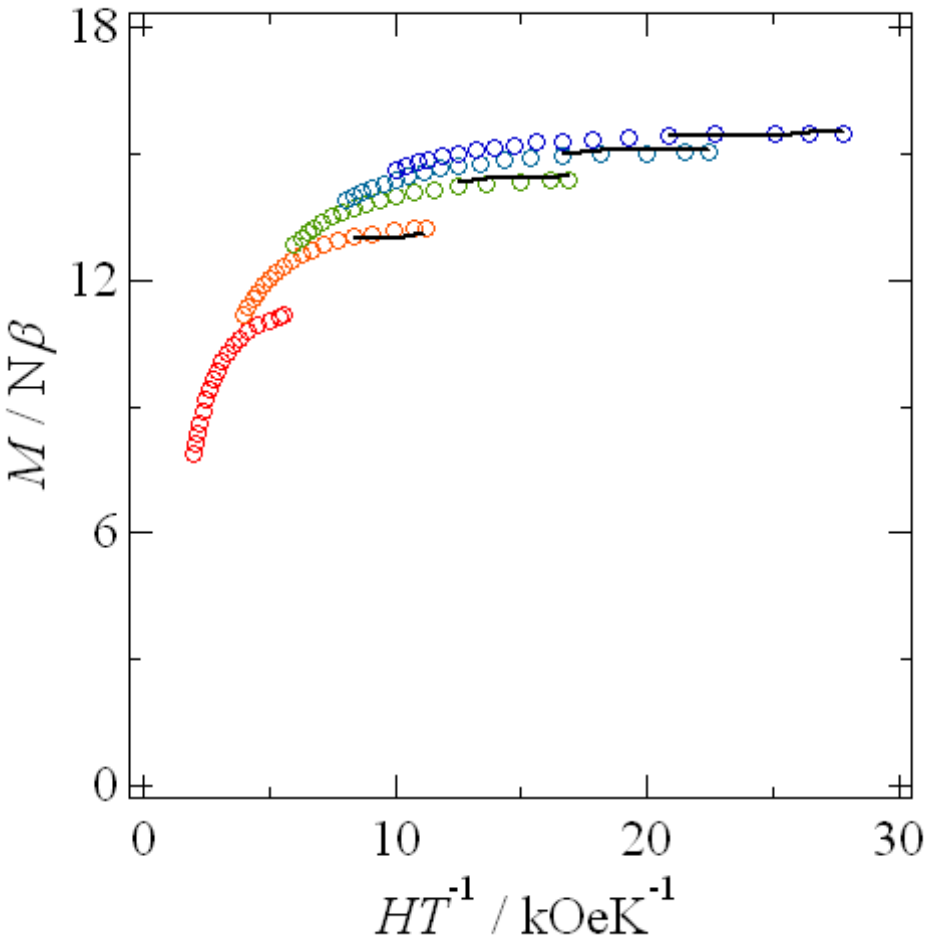

Figure S4. Plot of reduced magnetization ($M / N\beta$) versus H / T for **2R** in the temperature range 1.8 – 4.0 K and in applied fields of 1 – 5 T. Solid lines are the fit; see the text for the fitting parameters

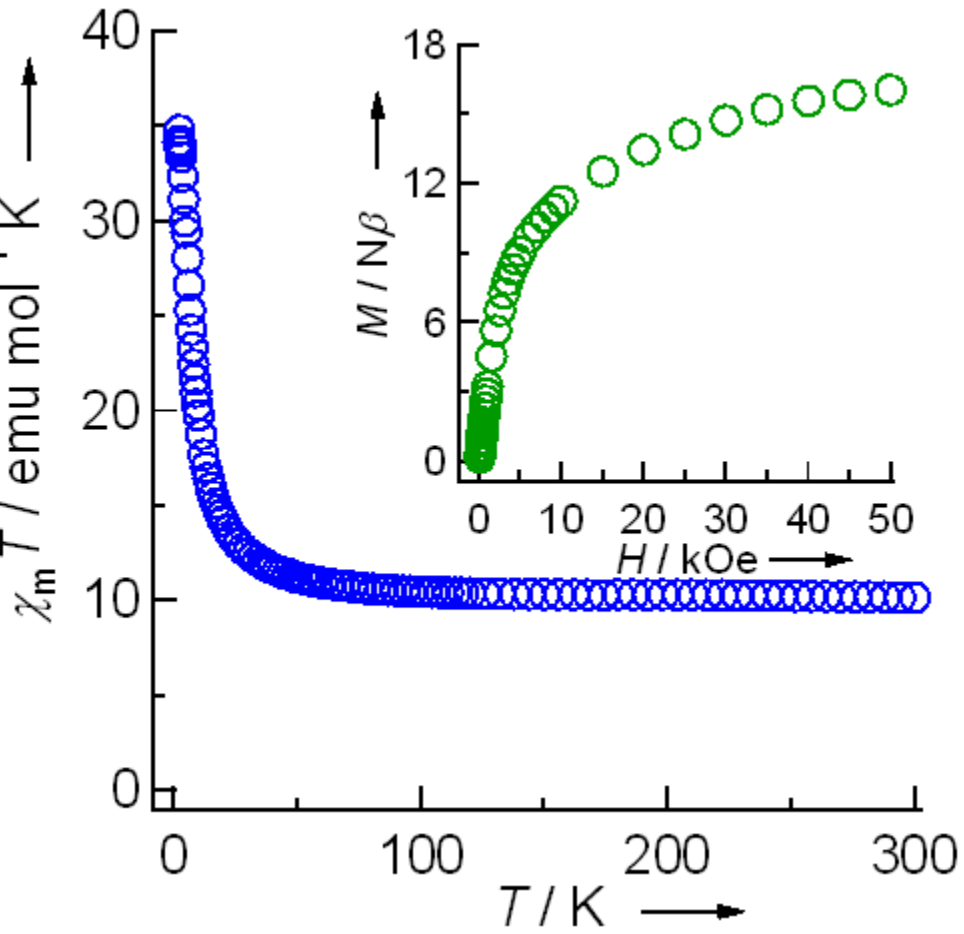

Figure S5. Plot of $\chi_m T$ vs. T of **2S** at applied field of 500 Oe. Inset: Field dependence of the magnetization at 1.8 K.

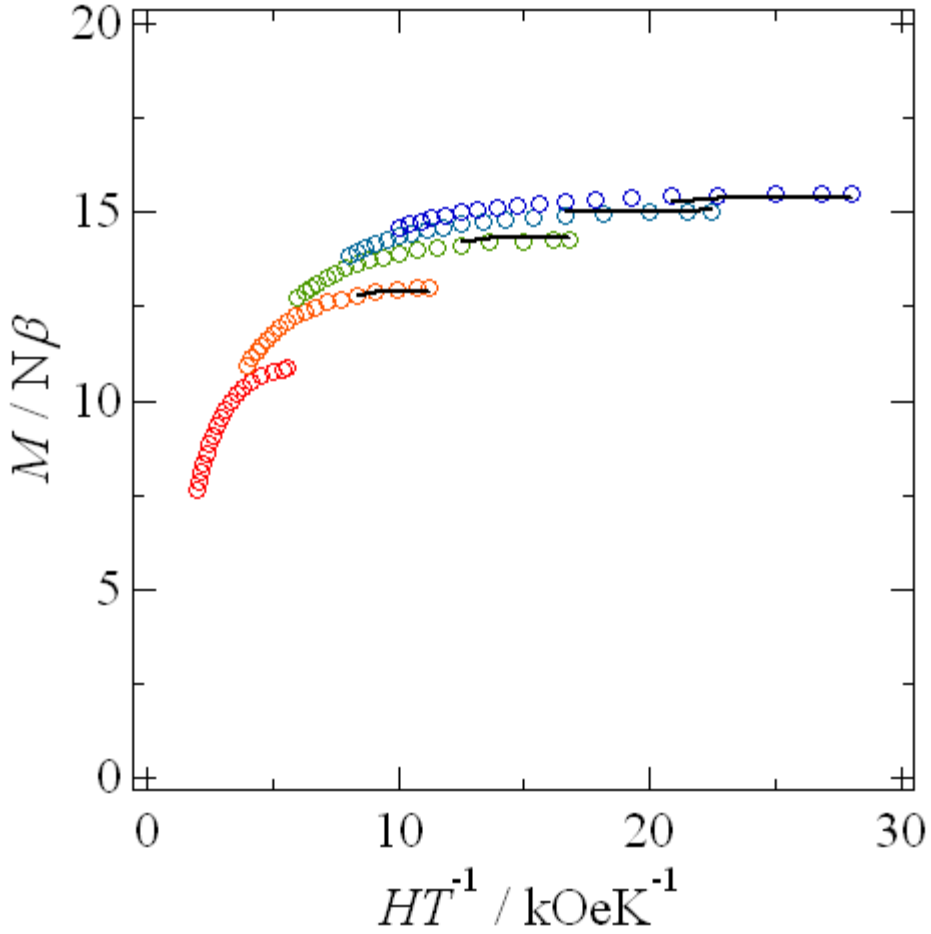

Figure S6. Plot of reduced magnetization (M / $N\beta$) versus H / T for **2S** in the temperature range 1.8 – 4.0 K and in applied fields of 1 – 5 T. Solid lines are the fit; see the text for the fitting parameters

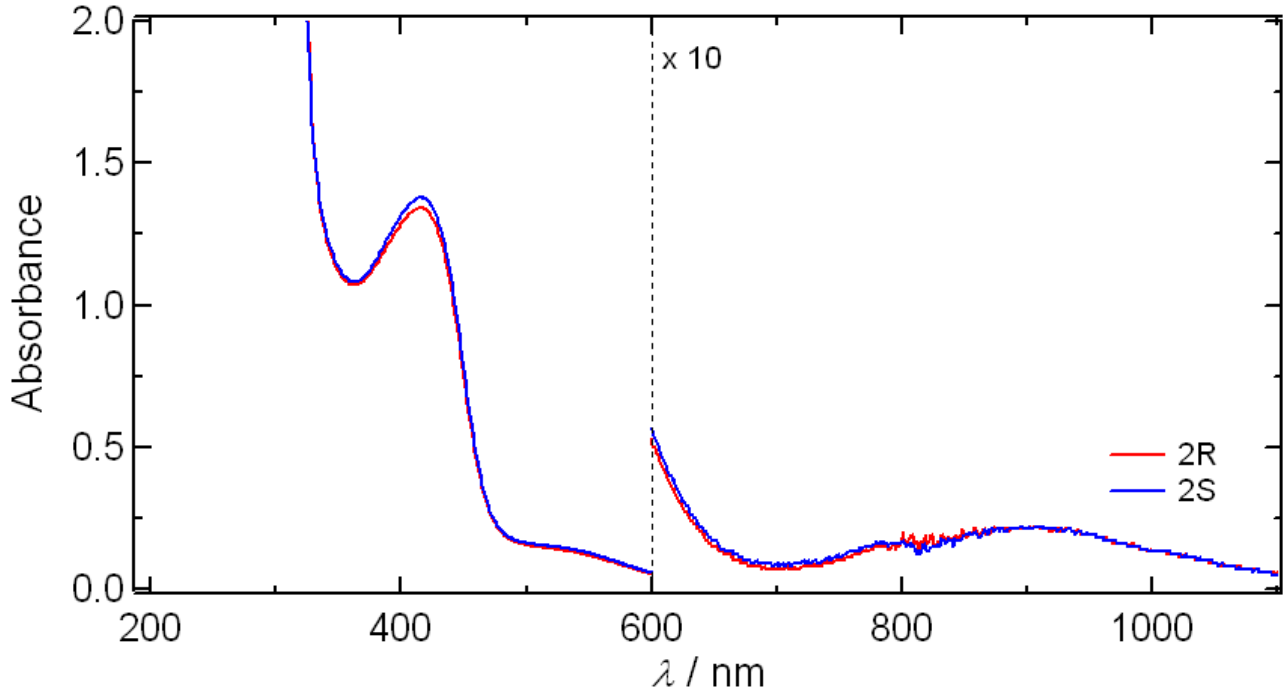

Figure S7. UV-vis spectra of **2R** and **2S**.

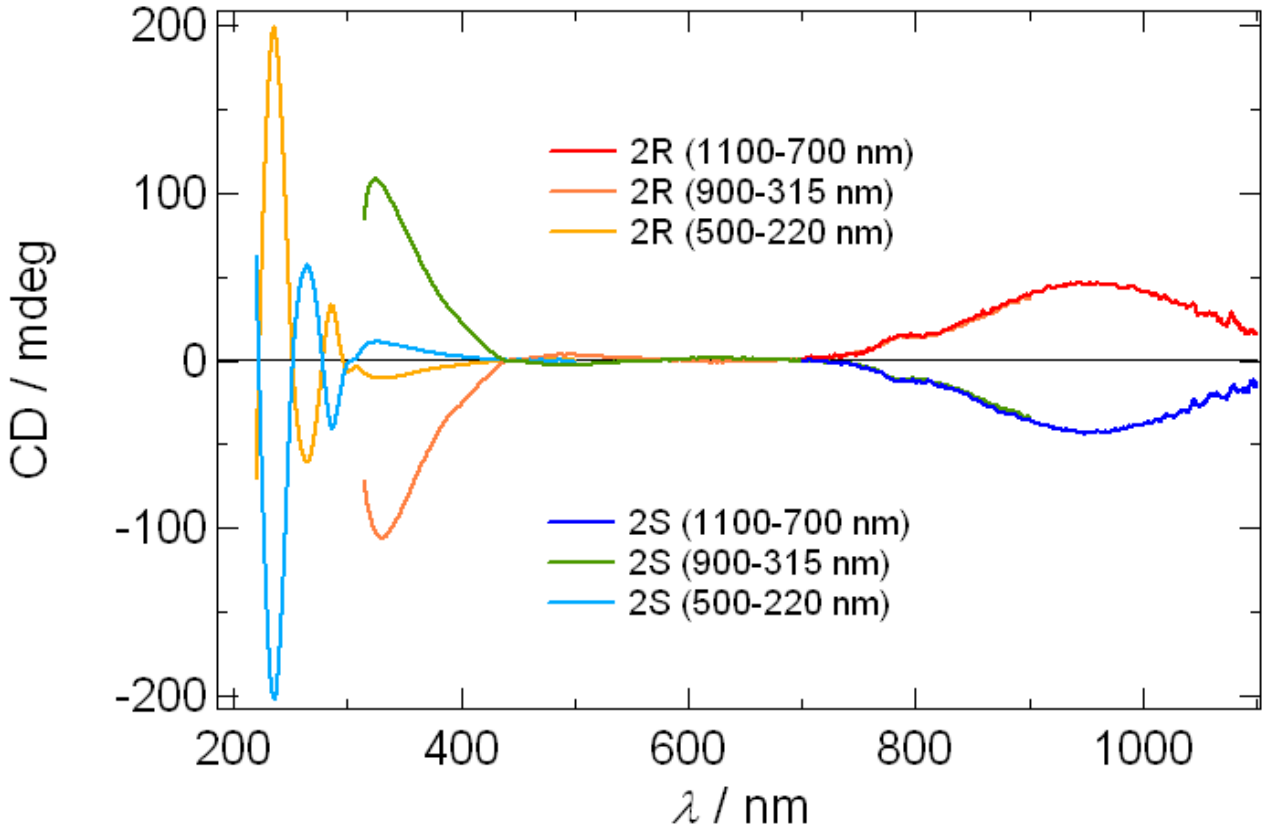

Figure S8. CD spectra of **2R** and **2S** in acetonitrile solution.