Spin Crossover in Iron(III) Schiff-base 1-D Chain Complexes

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Contents:

S1: Single Crystal X-ray Diffraction

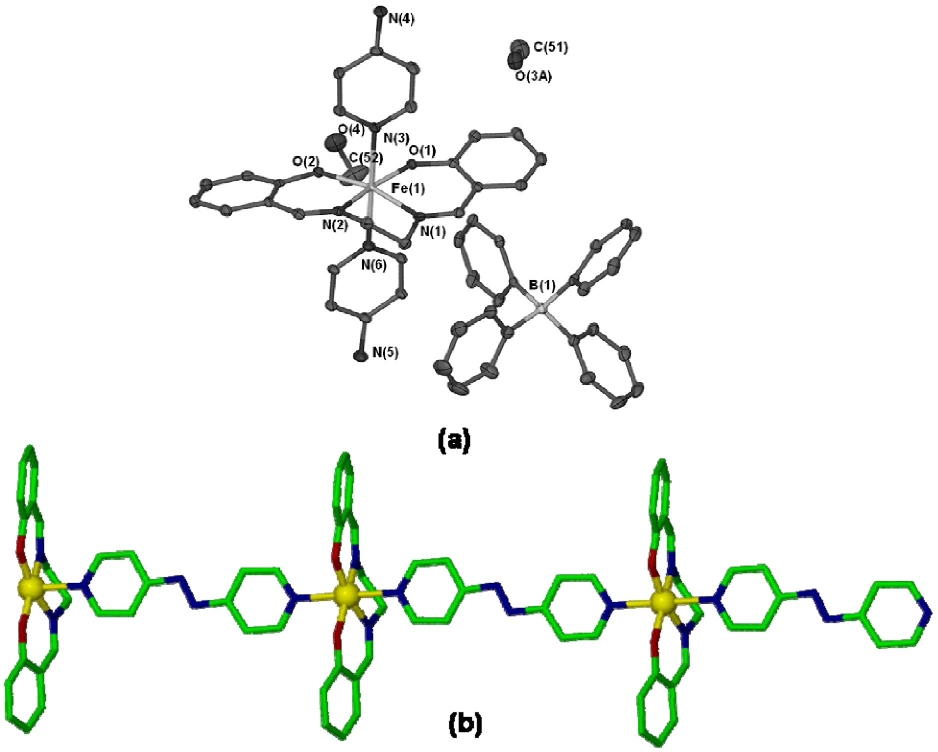

Figure S1: (a) Asymmetric unit and (b) the 1-D chain structure of **1a.** Hydrogen atoms and carbon labels omitted for clarity.

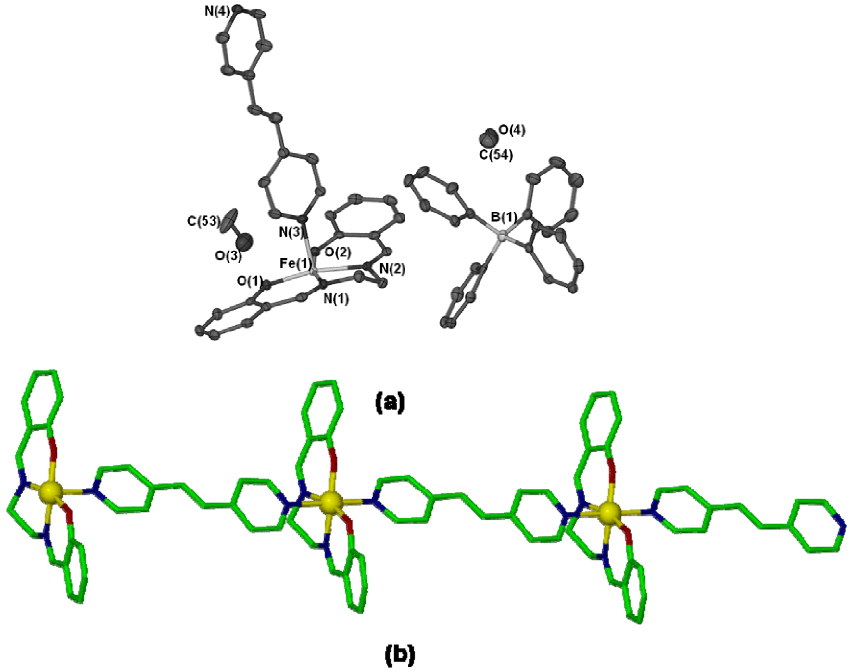

Figure S2: (a) Asymmetric unit and (b) the 1-D chain structure of **1b.** Hydrogen atoms and carbon labels omitted for clarity.

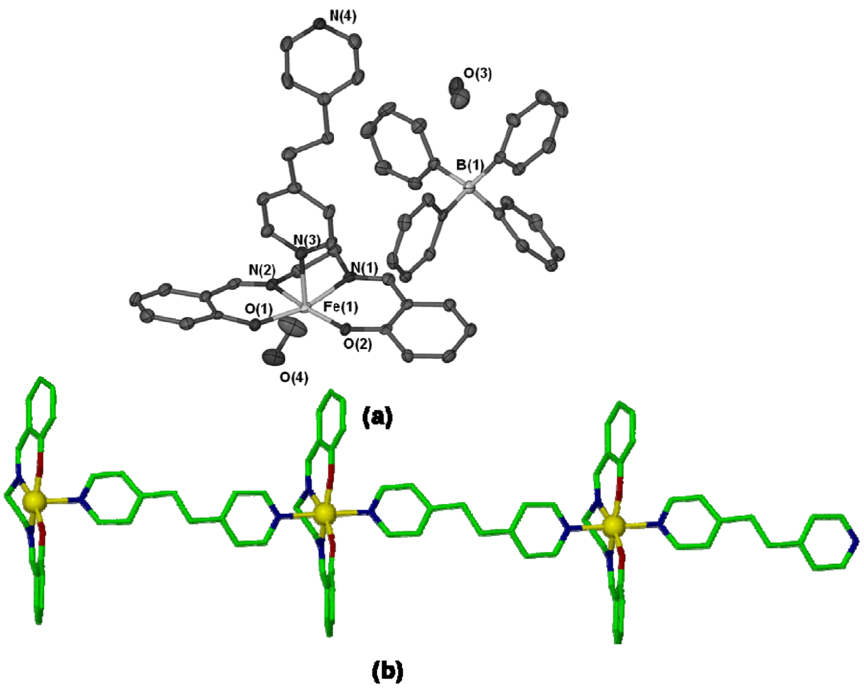

Figure S3: (a) Asymmetric unit and (b) the 1-D chain structure of **1c.** Hydrogen atoms and carbon labels omitted for clarity.

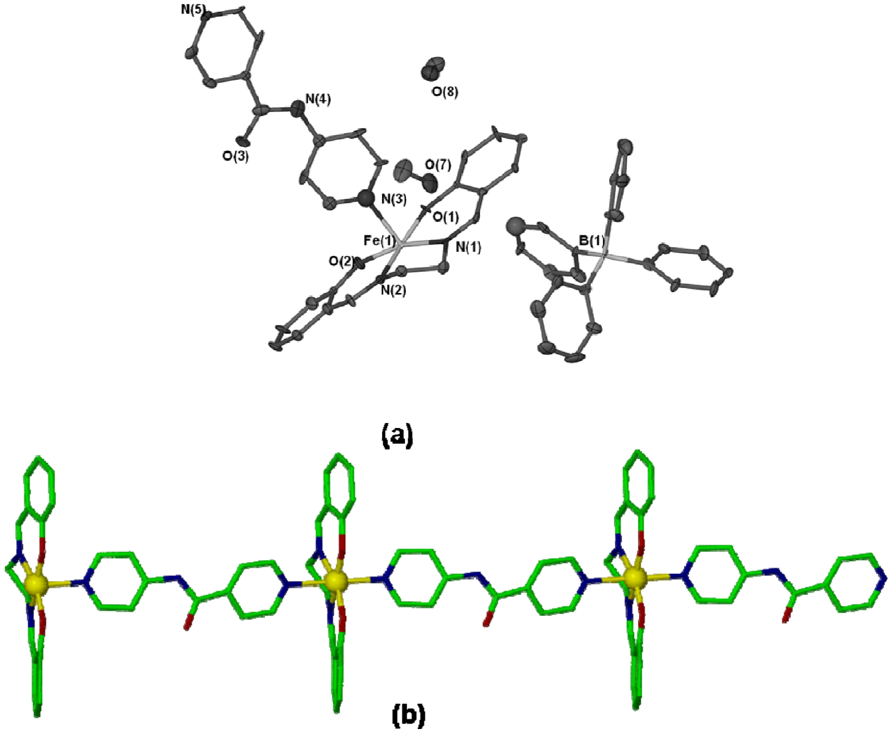

Figure S4: (a) Asymmetric unit and (b) the 1-D chain structure of **1d.** Hydrogen atoms and carbon labels omitted for clarity.

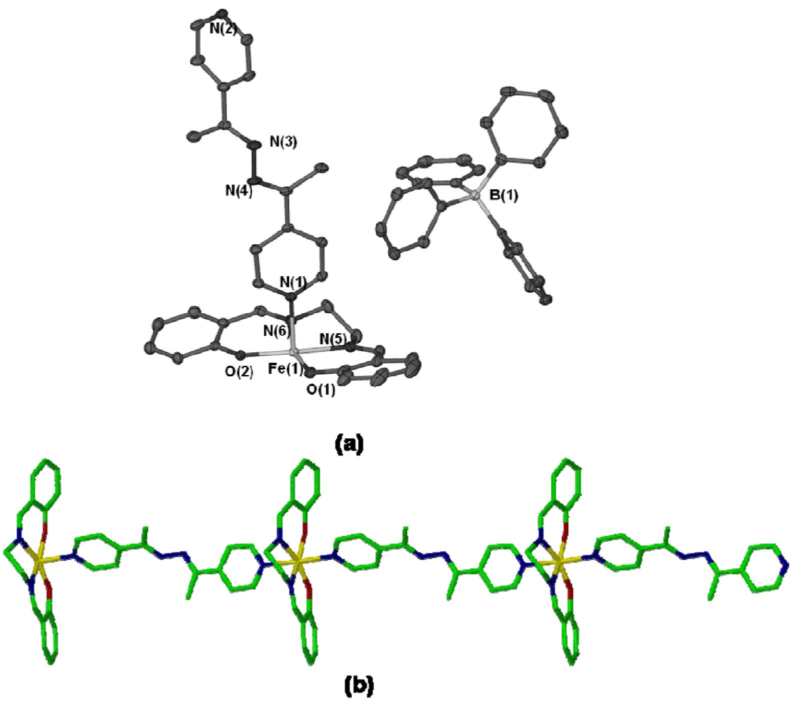

Figure S5: (a) Asymmetric unit and (b) the 1-D chain structure of **1e**. Hydrogen atoms and carbon labels omitted for clarity.

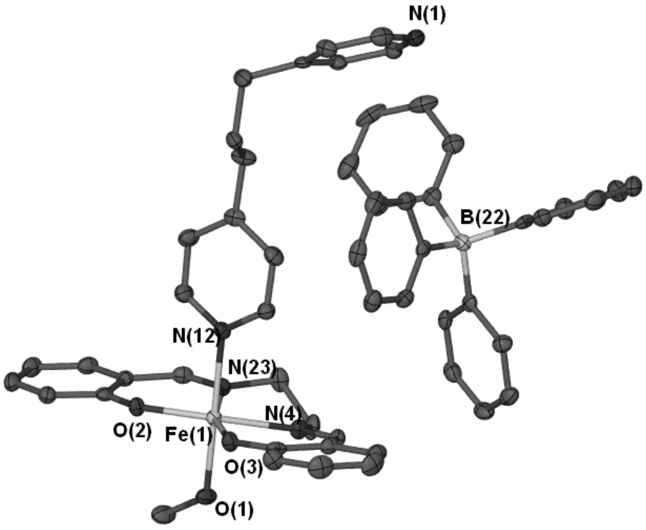

Figure S6: (a) Asymmetric unit of **2a**. Hydrogen atoms and carbon labels omitted for clarity.

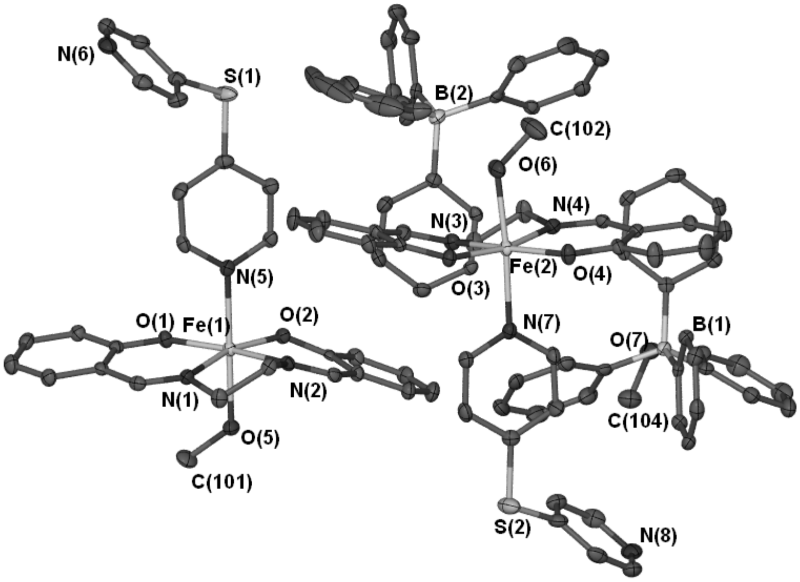

Figure S7: (a) Asymmetric unit of **2b**. Hydrogen atoms and carbon labels omitted for clarity.

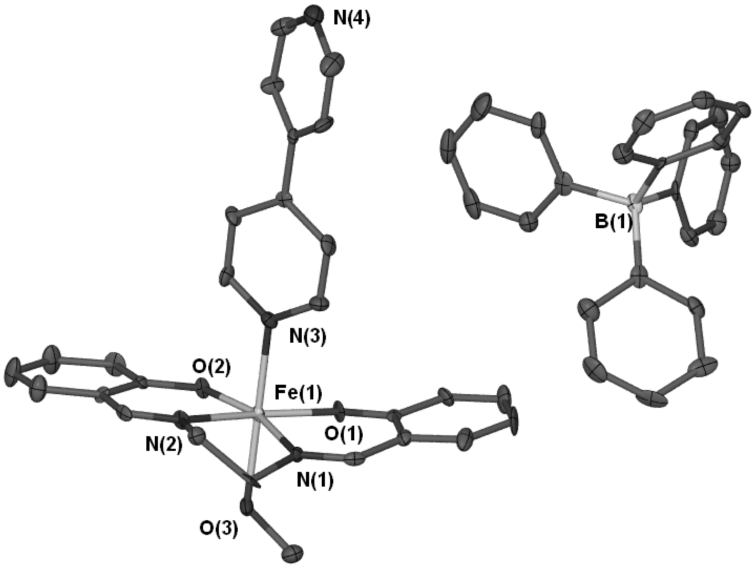

Figure S8: (a) Asymmetric unit of **2c**. Hydrogen atoms and carbon labels omitted for clarity.

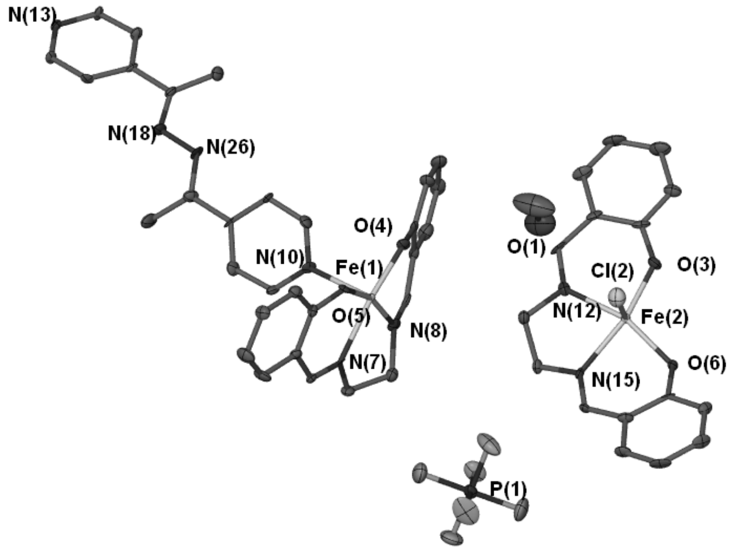

Figure S9: (a) Asymmetric unit of **3a**. Hydrogen atoms and carbon labels omitted for clarity.

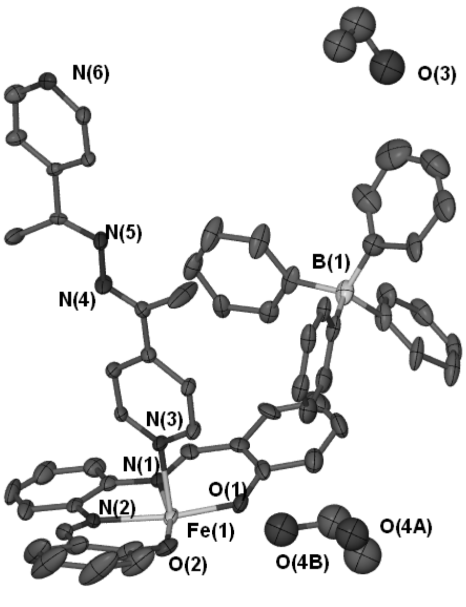

Figure S10: (a) Asymmetric unit of **4a**. Hydrogen atoms and carbon labels omitted for clarity

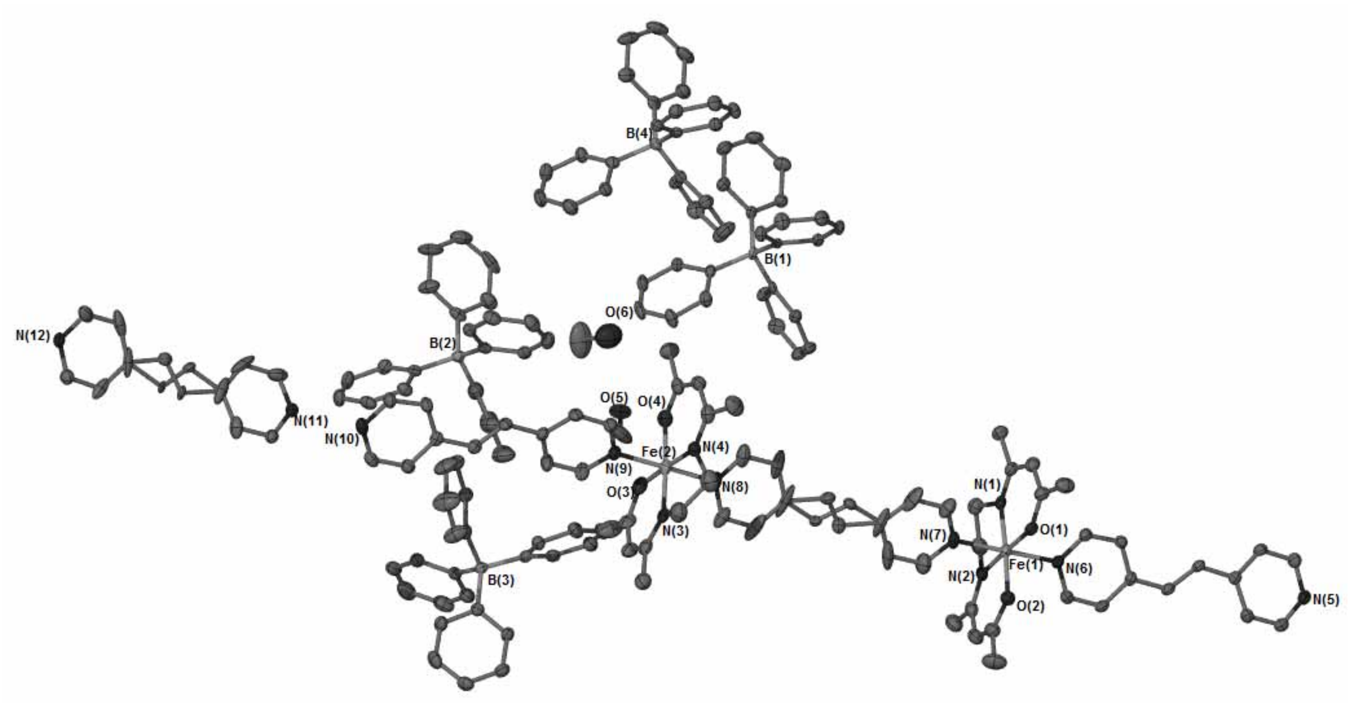

Figure S11: (a) Asymmetric unit of **5a**. Hydrogen atoms and carbon labels omitted for clarity

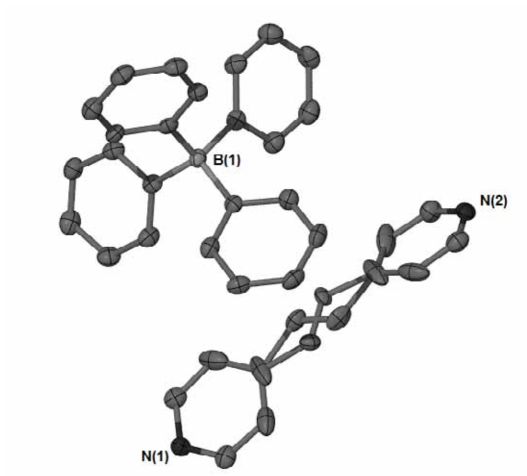

Figure S12 : Assymetric unit of **5a1**. Hydrogen atoms and carbon labels omitted for clarity.

Crystallographic Refinement Details

1a: The crystal was twinned, and the structure was refined using a HKLF5 file containing data for two twin domains, with a refined BASF of 0.54. No restraints were required in the model.

1b: Small residual peaks suggest disorder of the vinyl group, however this could not be accurately modelled.

1d: The crystal was twinned, and the structure was refined using a HKLF5 file containing data for two twin domains, with a refined BASF of 0.33 resulting in moderately high R-factors. No restraints were required in the model.

2c: We note that the theta max is rather low for this structure, many crystal were tested in the sample and they all diffracted poorly at high angle and thus is intrinsic to the material.

3a: The R-factors for this structure are relatively high (ca. 16% R1) owing to a combination of factors. Firstly, the crystals were only obtained via evaporation from solution under a stream of nitrogen and in general we find that this method does not produce high quality crystalline material. Secondly, the crystals were quite small and formed as thin plate morphology. Lastly, empirical absorption correction was used on the data in this case but owing to the plate-like crystal shape analytical absorption would have been more appropriate and indeed we observe satellite electron density peaks around the heavy metal atoms indicative of inappropriate absorption correction (further data collection was not possible).

4a: The lattice ethanol molecules showed signs of disorder and were refined using an isotropic model. One of the ethanol molecules was refined with the OH position disordered over two positions in fixed 50:50 occupancies.

5a: Two of the tvp C=C groups were disordered over two positions. These were refined using an anisotropic model with fixed 50:50 occupancies. One of the lattice methanol molecules (that containing O5) is refined at 50% occupancy, however there are signs of additional disorder, although these could not be accurately modelled. A DFIX command was applied to the N5 to H65 bond, and the N11 to H66 bond, to restrain both to 0.87Å. H65 and H66 attached to N5 and N11 respectively were located and assigned from the electron density difference map. Residual electron density around lattice solvent suggests disorder that could not be accurately modelled.

5a1: The C=C group of the tvp molecule is disordered over two positions, and these were refined using an anisotropic model with fixed 50:50 occupancies. A DFIX command was applied to the N2 to H2A bond, to restrain it to 0.87Å. H2A was located in the difference map. We note that the reflection count for these data is rather low (completeness is low), many crystals were tested in the sample and they all diffracted poorly.

S2: Magnetic Susceptibility Measurements

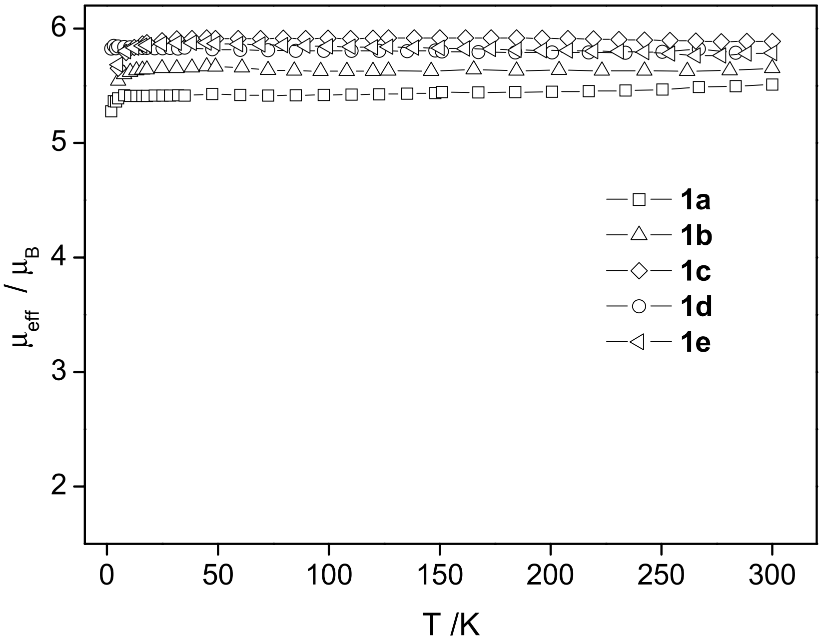

Fig. S13 Magnetic moment, per Fe, versus temperature over the temperature range 4-300 K for the salen containing 1-D chain materials **1a-e**.

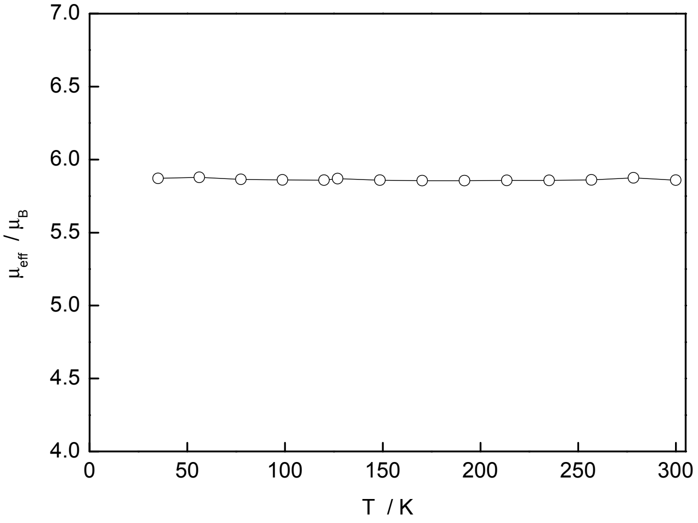

Figure S14: Temperature dependence of the magnetic moment per Fe(III) for **2a**.

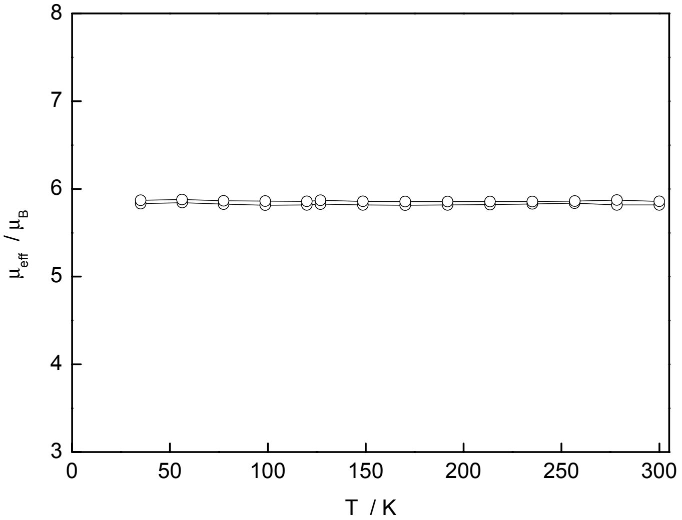

Figure S15: Temperature dependence of the magnetic moment per Fe(III) for **2b**.

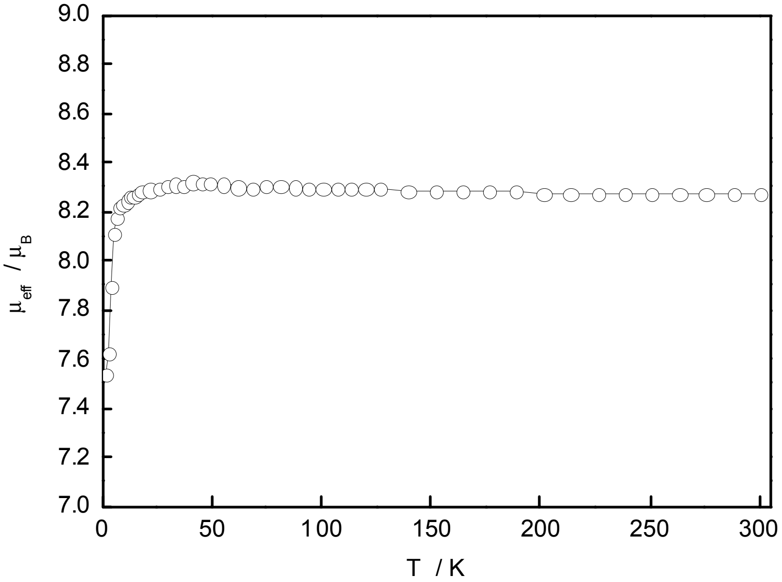

Figure S16: Temperature dependence of the magnetic moment per 2 Fe(III) for **2c**.