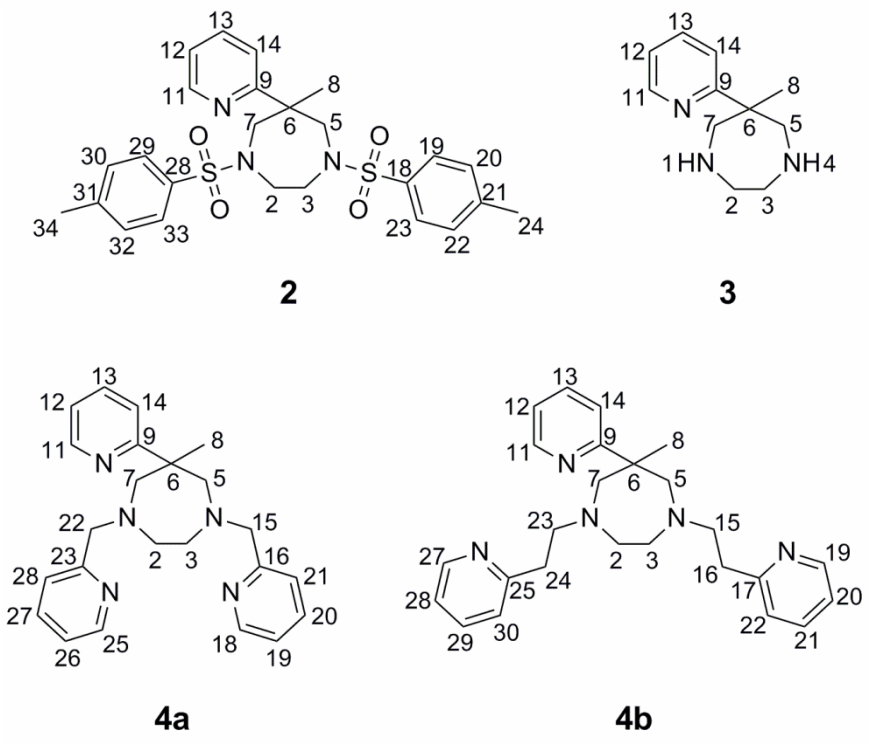
Eur. J. Inorg. Chem. **2013** · © WILEY-VCH Verlag GmbH & Co. KGaA, 69451 Weinheim, 2013 · ISSN 1434–1948

SUPPORTING INFORMATION

DOI: 10.1002/ejic.201201149
Title: Iron(II) Complexes of Two Amine/Imine N_5 Chelate Ligands Containing a 1,4-Diazepane Core – To Crossover or Not To Crossover
Author(s): Marc Schmidt, Dennis Wiedemann, Boujemaa Moubaraki, Nicholas F. Chilton, Keith S. Murray, Kuduva R. Vignesh, Gopalan Rajaraman, Andreas Grohmann*

Numbering schemes used for NMR assignments of compounds **2**, **3** and **4a/b**:



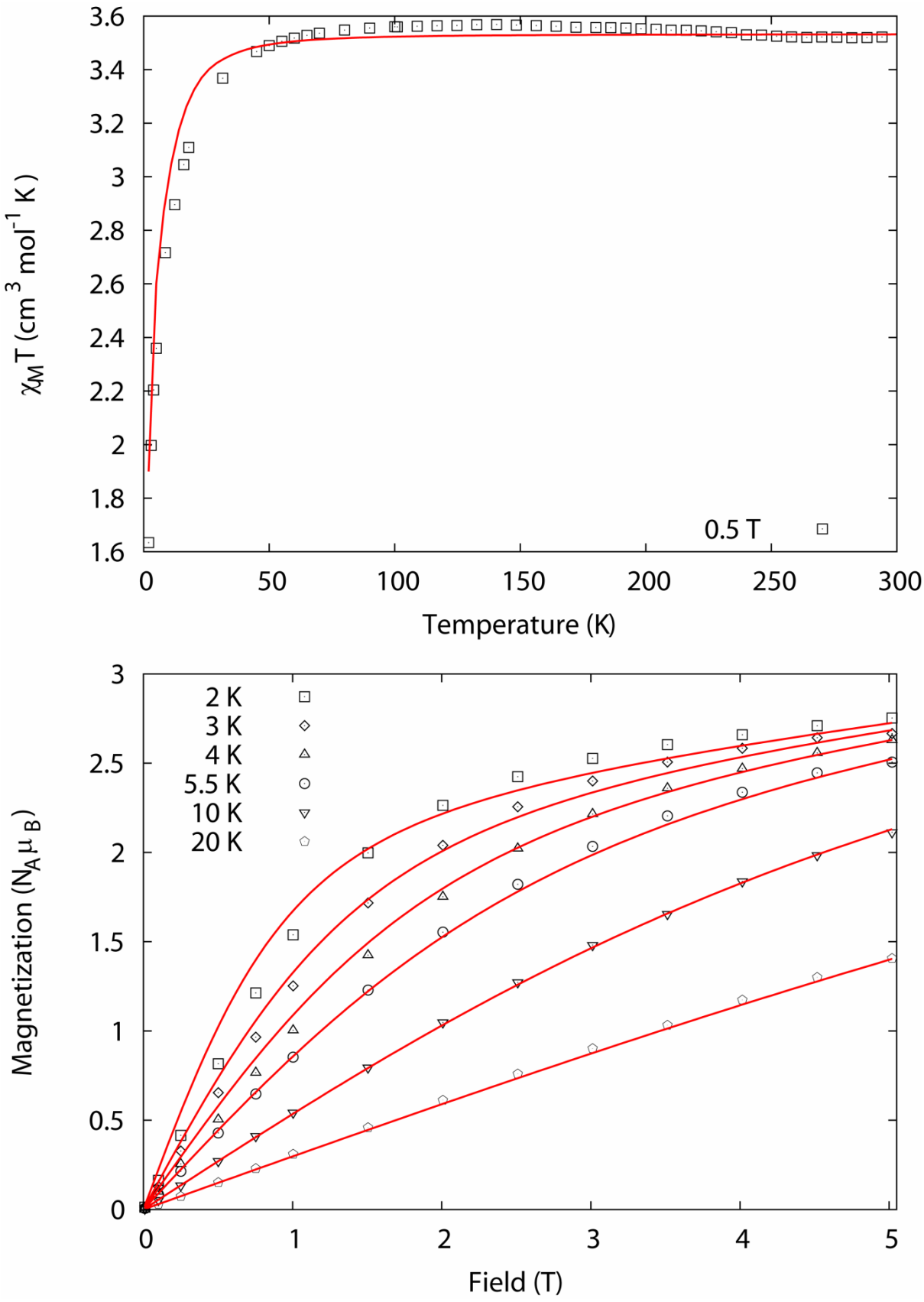


Figure S1. Plot of $\chi_M T$ *vs.* T for **7** in a field of 0.5 T (top). Magnetization isotherms for **7** at temperatures 2, 3, 4, 5.5, 10 and 20 K (bottom). The red lines are the best-fit calculated using the parameters given in the text.

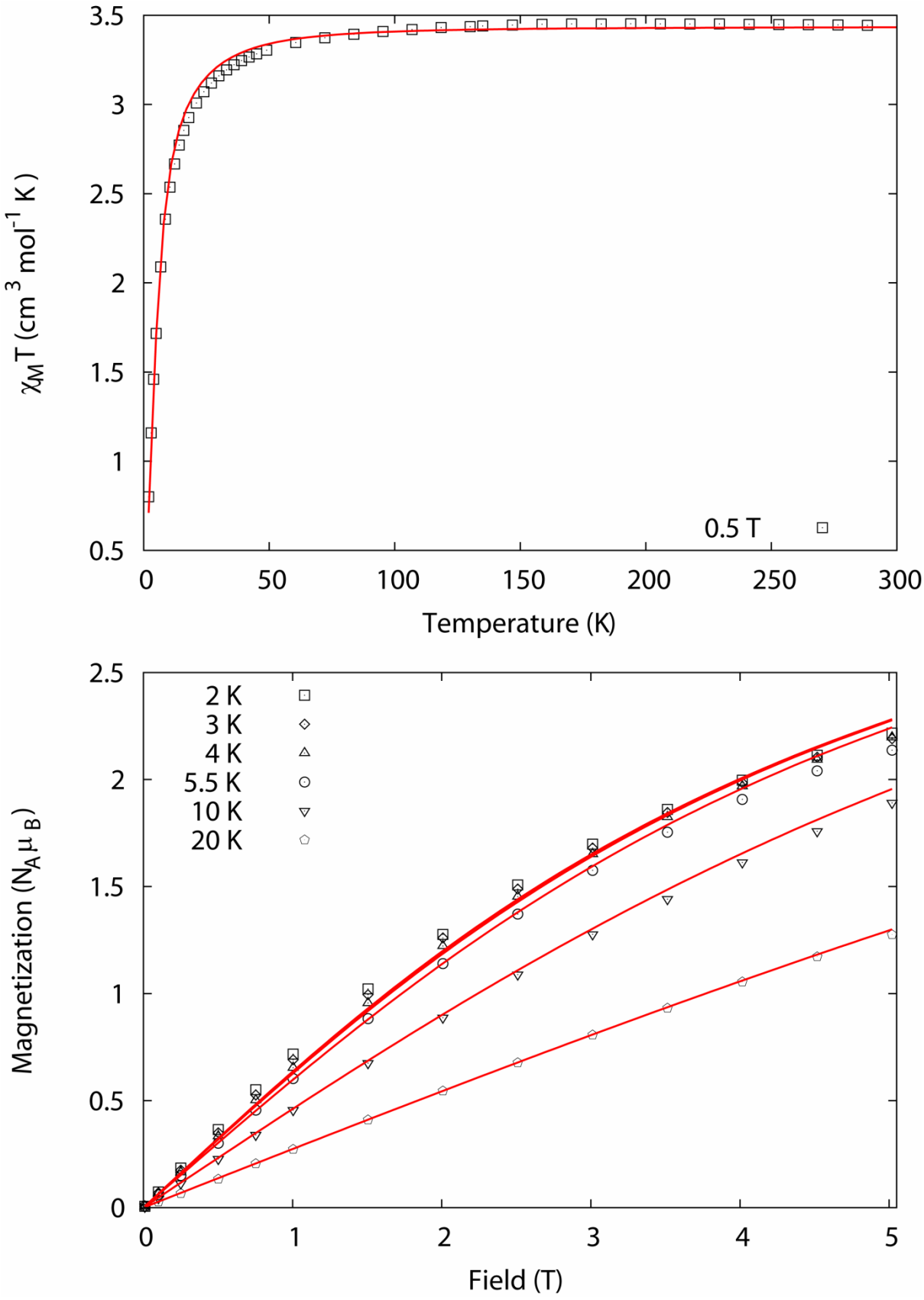
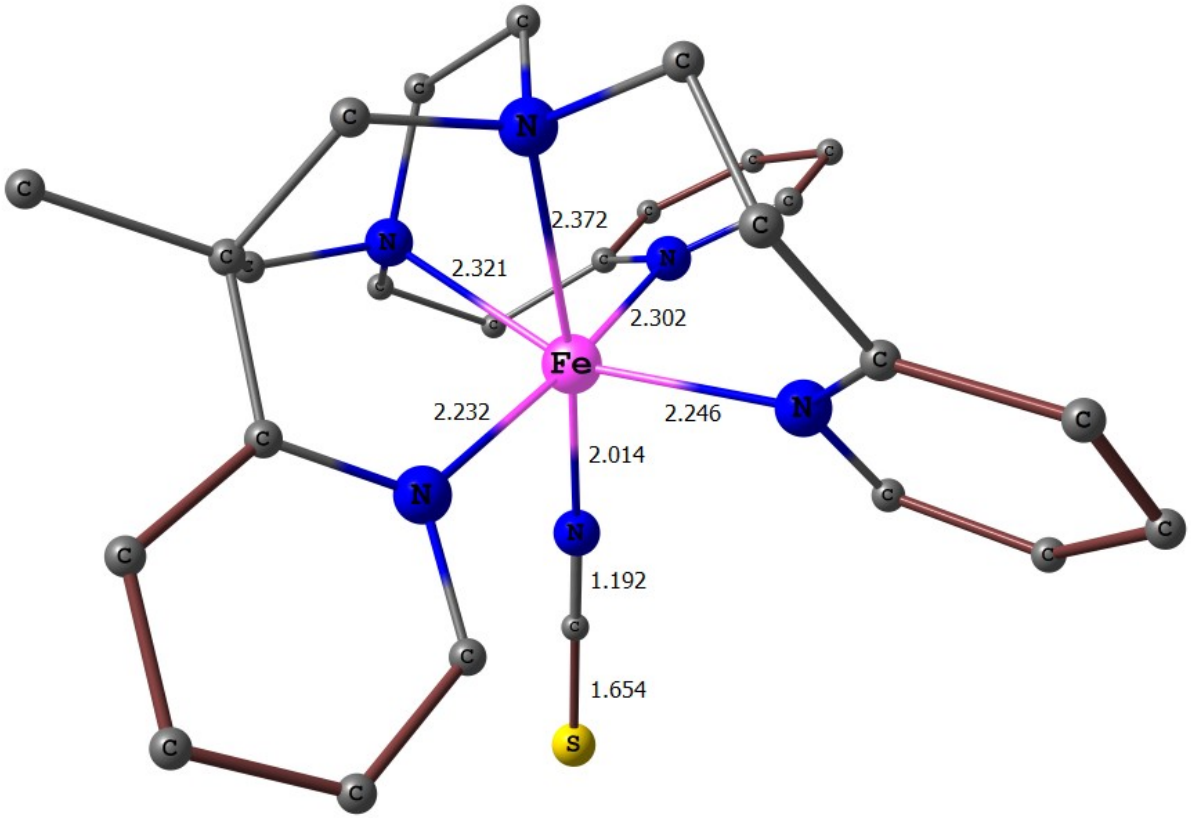


Figure S2. Plot of $\chi_M T$ *vs.* T for **9** in a field of 0.5 T (top). Magnetization isotherms for **9** at temperatures 2, 3, 4, 5.5, 10 and 20 K (bottom). The red lines are the best-fit calculated using the parameters given in the text.

a)



b)

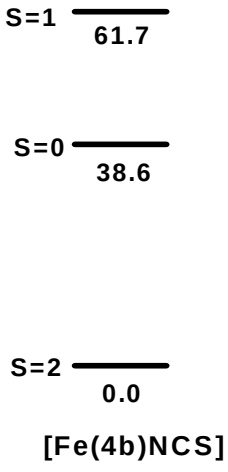


Figure S3: a) Optimized ground-state structure of [Fe(**4b**)NCS] and b) Energy level gaps (in kJ mol^{-1}) computed for different electronic configurations of complex [Fe(**4b**)NCS].