Journal Name

Supporting Information for

Iron(II) Spin Crossover Complexes with diaminonaphthalene-based Schiff base-like Ligands: Mononuclear Complexes.

Charles Lochenie, Julia Heinz, Wolfgang Milius and Birgit Weber*

Inorganic Chemistry II, Universität Bayreuth, Universitätsstraße 30, NW I, 95440 Bayreuth, Germany. Email: <u>weber@uni-bayreuth.de</u>



Temperature [K]



Figure S3: Powder diffraction patterns of sample 6 as bulk material (black line, room temperature and simulated powder diffraction pattern from the crystal structure of 6 (red line, 133 K).





Figure S5: Comparison of powder diffractograms of compound 12 (black line, calculated at 133 K), and compound 14 (blue line, measured at 133 K).





Figure S6: ORTEP drawing of 19 (left) and 20 (right). The thermal ellipsoids are shown at the 50% level. Hydrogen atoms and non-coordinating solvent molecules were omitted for clarity reasons.



Figure 57: left: crystal packing of 19 along [100], hydrogen atoms for clarity reasons. Right: crystal packing of 20 along [010], hydrogen atoms for clarity reasons.



Figure S8: Mössbauer spectrum of 15, hyperfine parameters: δ = 0.908(6), ΔE_Q = 2.066(12) and $\Gamma/2$ = 0.174(13).

Mössbauer spectrometry: ⁵⁷Fe Mössbauer spectra were recorded in transmission geometry on a constantacceleration using a conventional Mössbauer spectrometer with a 50 mCi ⁵⁷Co(Rh) source. The samples were sealed in the sample holder under an argon atmosphere. The spectra were fitted using Recoil 1.05 Mössbauer Analysis Software. The isomer shift values are given with respect to a α -Fe reference at room temperature.

Recoil Software: K. Lagarec and D. G. Rancourt, *Recoil, mössbauer spectral analysis software for windows 1.0*, Department of Physics, University of Ottawa, Canada, 1998.