Iron(II) spin-crossover complexes with chiral ligands – towards a non-destructive read-out of spin states

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Aiming for novel approaches towards a technologically simple, non-destructive read-out of the spin state of an Fe(II) spin crossover (SCO) material, halogenation of 1-propyl-*1H*-tetrazole in the β-position resulted a series of monodentate, *per-se* chiral, SCO-ligands. For all materials, SCO-active Fe(II) compounds were obtained and structurally characterized (figure 1).[1] The enantiopure Fe(II) SCO-materials featured a higher SCO temperature than the unsubstituted derivative, with the $T_{1/2}$ increasing with the size of the halogens, in good agreement with previous results.[2] To derive a correlation between spin-state and optical activity, the materials were analyzed by various chiroptical methods. Especially in the electronic spectra (figure 2), the direct correlation between the chiroptical information and the Fe(II) spin state became apparent. Quantum chemical calculations were used to support the experimental results. The contribution highlights how enantiomerically pure, chiral ligands may enable a novel non-destructive read-out of the spin-state of Fe(II)-SCO materials.[1]

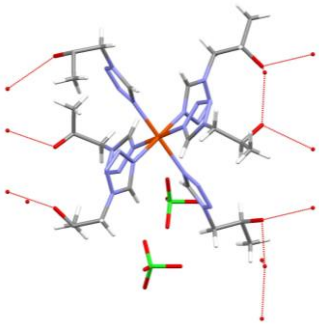

Figure 1 Molecular structure of HS-$[Fe(2\text{-}OH\text{-}3Tz)_6](ClO_4)_2$

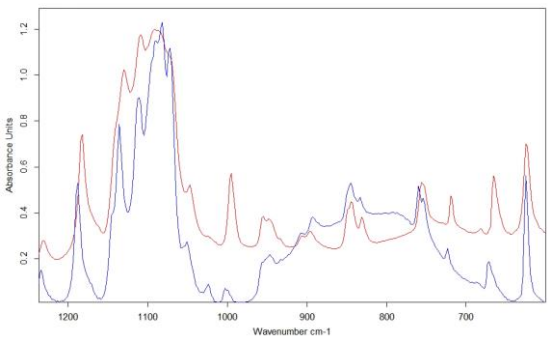

Figure 2 Polarized MIR of $[Fe(2\text{-}OH\text{-}3Tz)_6](ClO_4)_2$ in the HS (red) and LS (blue)

1 D. Müller, C. Knoll, M. Seifried, J.M. Welch, G. Giester, M. Wildner, M. Reissner, P. Weinberger, *manuscript under preparation*
2 D. Müller, C. Knoll, M. Seifried, J.M. Welch, G. Giester, M. Reissner, P. Weinberger, *Chem. Eur. J.,* **2018***, 24, 1.*