Tetrazoles as versatile ligands establishing structure-property relationships in Fe(II) SCO chemistry

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Fe(II) spin crossover (SCO) materials based on N1-substituted ligands are very sensitive towards subtle modifications in the ligand design. Recently developed synthetic approaches towards systematically N1-functionalized tetrazoles gave access to a broad library of homologous ligands for a systematic study on the steric impact of the ligands' substitution pattern. In a series of 3-halogen substituted 1-propyl-*1H*-tetrazoles SCO-active Fe(II)-complexes were obtained, featuring a higher spin transition temperature than the parent compound (figure 1a).[1] Various analytical methods confirmed, that the halogen substitution had only an impact on the steric demand of the ligand but does not affect the electronic properties. A similar effect was observed for the methyl-substituted 1-([1,1'-biphenyl]-4-ylmethyl)-*1H*-tetrazoles (figure 1b), were the variation of the methyl-position had a notable impact on the crystal packing, affecting therethrough the SCO behaviour.[2] In the contribution is highlighted, how valuable information towards tuneable SCO materials is achieved based on such structure-property correlations.

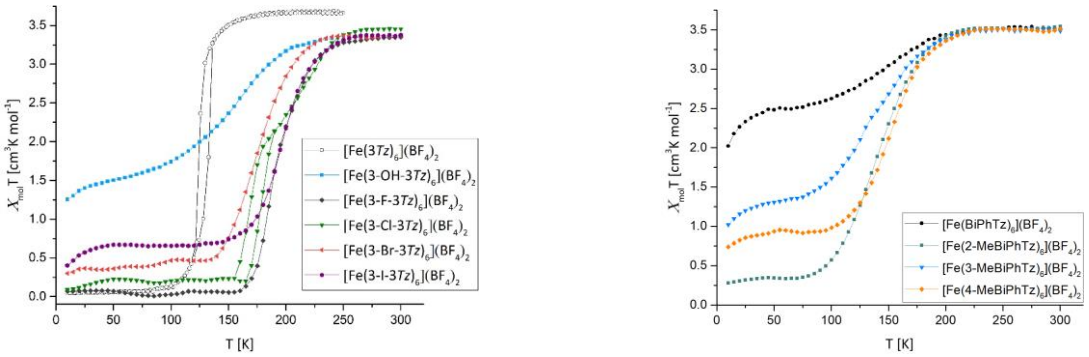

Figure 1 SCO in a series of a) 1-propyl-*1H*-tetrazoles b) 1-([1,1'-biphenyl]-4-ylmethyl)-*1H*-tetrazoles

1 D. Müller, C. Knoll, M. Seifried, J.M. Welch, G. Giester, M. Reissner, P. Weinberger, *Chem. Eur. J.,* **2018***, 24,1.*
2 D. Müller, C. Knoll, M. Seifried, J.M. Welch, G. Giester, M. Reissner, P. Weinberger, *Dalton Trans.,* **2018***, submitted*