

Propargyl-1*H*-tetrazole as promising ligand for post-functionalization of spin switchable iron(II) complexes

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Spin crossover complexes with ligands suitable for a further functionalization after coordination could allow for an easy access to various multifunctional switchable materials. Within this context we recently characterized Fe(II) SCO complexes of propargyl-1*H*-tetrazole.¹ The carbon-carbon triple bond provides a well-known motif for a possible post-functionalization via standard protocols like alkyne-metathesis or click reaction. Although the design of the ligand shows similarities to the well-known propyl-1*H*-tetrazole,^{2,3} the spin transition behaviour is notably different.

Due to the potential instability of those complexes, especially of the perchlorate complex, further investigations regarding their sensitivity towards thermal and mechanical stress were made. These experiments led to the conclusion that upon proper handling no enhanced risk of an explosive decomposition has been found.

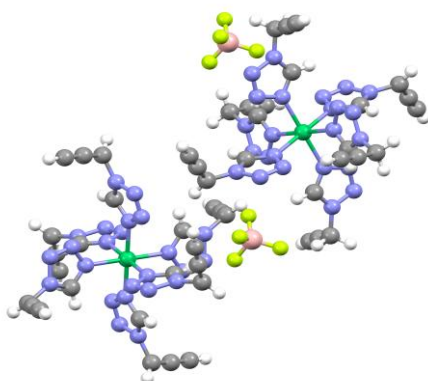


Figure 1 Molecular structure of the isotypic $[\text{Ni}(\text{prgTz})_6](\text{BF}_4)_2$ complex

1 M. Seifried, C. Knoll, G. Giester, M. Reissner, D. Müller, P. Weinberger, *Magnetochemistry*, submitted.

2 P. Gülich, *Struct Bond*, **1981**, *44*, 83-195.

3 P.L. Franke, J.G. Haasnoot, A.P. Zuur, *Inorganica Chimica Acta*, **1982**, *59*, 5-9.