

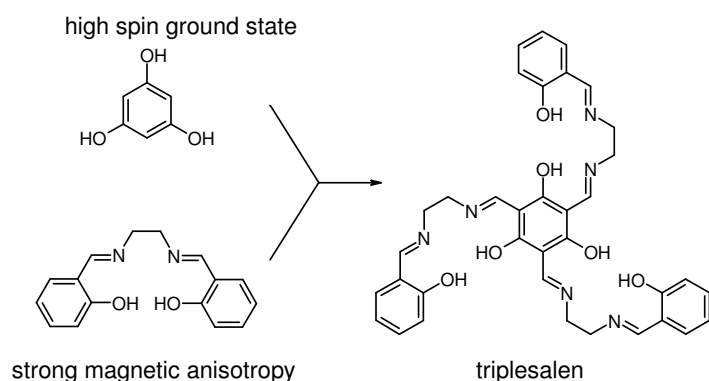
Rational Design of Single-Molecule Magnets

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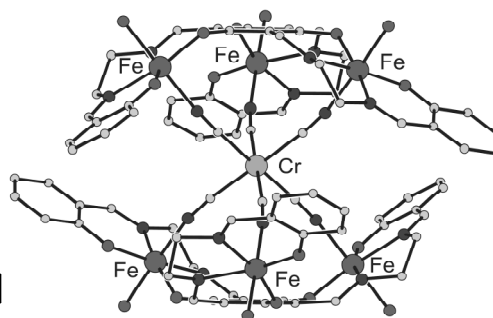
Single-molecule magnets (SMMs) are molecules that exhibit a magnetic bistability of pure molecular origin due to a slow relaxation of the magnetization. Thus, information can be stored in a single molecule with dimensions below 5 nm. The necessary prerequisites are a high spin ground state S_t along with a strong magnetic anisotropy of the easy-axis type which is described by a negative zero-field splitting D .

In order to rationally develop SMMs, we have designed the ligand triplesalen. This ligand combines the ferromagnetic coupler 1,3,5-trihydroxybenzene (phloroglucinol)^[1] for the generation of high spin ground states S_t with the coordination environment of a salen ligand to introduce magnetic anisotropy (Scheme 1).^[2,3] Spectroscopic and theoretical investigations on trinuclear copper complexes prove the successful ferromagnetic coupling by the spin-polarization mechanism.^[4,5]

Scheme 1.



Scheme 2.



The supramolecular assembly of two triplesalen complexes with one hexacyano-metallate results in real high spin molecules (Scheme 2). The complexes **Mn₆Cr** and **Fe₆Cr** exhibit high spin ground states of $S_t = 21/2$ and $S_t = 27/2$, respectively. AC susceptibility measurements and magnetization measurements on single-crystals demonstrate that **Mn₆Cr** is a SMM.^[6] This unprecedented supramolecular system based on the key-lock principle allows for the rational optimization of the SMM properties by the controlled variation of the molecular building blocks.

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[3] T. Glaser, M. Heidemeier, R. Fröhlich, P. Hildebrandt, E. Bothe, E. Bill, *Inorg. Chem.* **2005**, *44*, 5467-5482.

[4] T. Glaser, M. Heidemeier, S. Grimme, E. Bill, *Inorg. Chem.* **2004**, *43*, 5192-5194.

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[6] T. Glaser, M. Heidemeier, T. Weyhermüller, R.-D. Hoffmann, H. Rupp, P. Müller, *Angew. Chem.* **2006**, *118*, 6179-6183.