DEVELOPMENT OF A QUANTITATIVE SPIN FRUSTRATION VS SPIN SATISFACTION SCALE AND ITS APPLICATIONS TO Fe6 AND Fe7 CLUSTERS

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Polynuclear iron(III) clusters are the focus of numerous investigations not only because they mimic biological iron sites but also for their interesting magnetic properties. Some polynuclear iron clusters also behave as single-molecule magnets (SMM), a behavior that results from the combination of a large ground state spin, *S*, and a large zero-field splitting parameter, *D*. The presented work will describe Fe^{III} complexes that have an unusual $S = 3$ ground state spin. The unusual ground state has been rationalized on the basis of spin frustration effects; it will be shown how the ground state spin of these structures is extremely sensitive to the relative magnitude of the competing exchange interactions. In addition, a quantitative scale of spin compensation based on spin coupling that ranges from fully frustrated through fully satisfied and encompasses both partially frustrated and partially satisfied interactions has been developed and will be described.