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Magneto-Structural Correlations of High-Spin Transition Metal Ions

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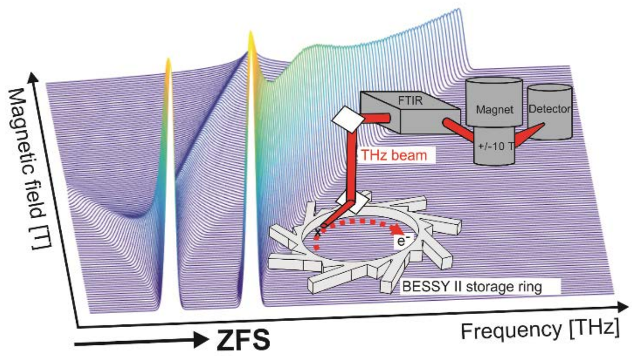
Paramagnetic transition metal ions (TMI) are crucial intermediates in important processes such as photosynthesis, mammal respiration or enzymatic small-molecule activation. Furthermore, they constitute function-determining units in many important artificial catalytic reactions as well as in single molecule magnets (SMM).

In high-spin (HS, $S > 1$) TMI, interactions among unpaired electron spins can induce zero-field splitting (ZFS) of the magnetic sublevels. ZFS probe the TMI coordination environment and electronic structure and can provide insight in their influence on chemical and magnetic properties. In addition, ZFS determine magnetic properties like *e.g.* SMM behavior.

The method of choice for studies in spin-coupling parameters, like ZFS, is electron paramagnetic resonance (EPR).



EPR-transition energy/magnetic-field map of an S = 1 state with very large rhombic ZFS. The insert shows the THz-EPR spectrometer at BESSY II. Reproduced after (2).

Yet, EPR-transition energies of HS TMI can spread over a very wide energy range. This range may even exceed the microwave energies applied in single-frequency EPR spectrometers, which renders EPR detection of these states notoriously difficult or even impossible.

Herein, we demonstrate how broadband high-field/high-frequency EPR can circumvent this limitation for mono- and multinuclear HS TMI complexes exhibiting ZFS parameters up to several THz (1, 2). It is demonstrated how spin-coupling parameters extracted from THz-EPR experiments can be employed to gain detailed insight into the electronic and magnetic structure of TMI complexes (3), metal proteins (4) and SMM (5-7).

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