

Publication

Iron in a Cage: Fixation of a Fe(II)tpy₂ Complex by Fourfold Interlinking**JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)****ID** 4612189**Author(s)** Brandl, Thomas; Johannsen, Sven; Häussinger, Daniel; Suryadevara, Nithin; Prescimone, Alessandro; Bernhard, Stefan; Gruber, Manuel; Ruben, Mario; Berndt, Richard; Mayor, Marcel**Author(s) at UniBasel** [Mayor, Marcel](#) ; [Brandl, Thomas](#) ; [Prescimone, Alessandro](#) ; [Häussinger, Daniel](#) ;**Year** 2020**Title** Iron in a Cage: Fixation of a Fe(II)tpy₂ Complex by Fourfold Interlinking**Journal** Angewandte Chemie International Edition**Volume** 59**Number** 37**Pages / Article-Number** 15947-15952**Keywords** cage compounds, Fe terpyridine, hexadentate ligand, macrocyclic ligands, Wittig reactions

Abstract The coordination sphere of the Fe(II) terpyridine complex 1 is rigidified by fourfold interlinking of both terpyridine ligands. Profiting from an octa-aldehyde precursor complex, the ideal dimensions of the interlinking structures are determined by reversible Schiff-base formation, before irreversible Wittig olefination provided the rigidified complex. Reversed-phase HPLC enables the isolation of the all-trans isomer of the Fe(II) terpyridine complex 1, which is fully characterized. While temperature independent low-spin states were recorded with superconducting quantum interference device (SQUID) measurements for both, the open precursor 8 and the interlinked complex 1, evidence of the increased rigidity of the ligand sphere in 1 was provided by proton T₂ relaxation NMR experiments. The ligand sphere fixation in the macrocyclized complex 1 even reaches a level resisting substantial deformation upon deposition on an Au(111) surface, as demonstrated by its pristine form in a low temperature ultra-high vacuum scanning tunneling microscope experiment.

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