# CALCULATIONS ON TRANSITION METAL COMPLEXES

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We report on DFT calculations on transition metal complexes which are designed as model complexes for nitrogenase activity. These complexes are characterized by iron centers surrounded by a sulfur-rich first ligand sphere. A typical example synthesized in Sellmann's group at Institute of Inorganic Chemistry in Erlangen is shown in the figure below. It features a trans diazene moiety which is conjectured to be an intermediate in the reduction of molecular nitrogen to ammonia. We discuss the importance of structural motifs like hydrogen bridges for the energetics of the metal complexes.

We present an approach based on shared electron numbers, which allows to estimate the contribution of intramolecular hydrogen bridges to complex stability from the charge distribution obtained from a DFT calculation, and discuss the problem of determining the relative energy of states with different multiplicity in the framework of DFT.

We discuss electronic structure and infrared spectra of certain Ru nitrosyl and HNO complexes and compare our results with the experiment, cf. Sellmann, Gottschalk-Gaudig, Häußinger, Heinemann, Hess, Chem. Eur. J. 7 (2001), 2099, Sellmann, Blum, Heinemann, Hess, Chem. Eur. J. 7 (2001), 1874.