# Bio-inspired nonheme iron oxygen activation

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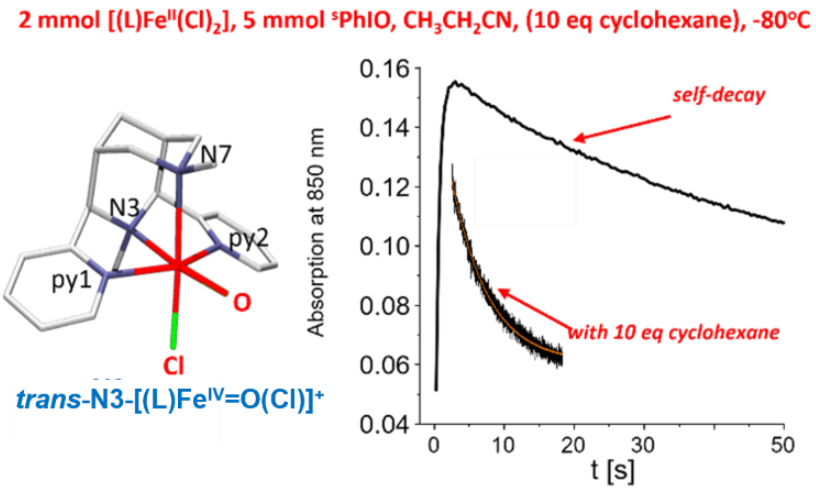
The lecture will start with a short discussion of a range of current projects in the Comba group from various areas of bioinorganic and coordination chemistry, also involving medicinal applications, where iron complexes might be of importance. The main part will concentrate on high-valent nonheme iron chemistry, and one possible application that will be shortly described is in the area of environmental chemistry.

In the main part the iron(IV)oxido species *trans*-N3-[(L)$Fe^{IV}$=O(Cl)]$^+$ with a tetradentate bispidine as supporting ligand (see Figure) will be discussed in detail. This species has an $S$ = 1 electronic ground state (in contrast to enzymes with an $S$ = 2 ground state), is the most reactive nonheme iron model system known so far, with a reactivity similar to nonheme iron enzymes (C-H abstraction at cyclohexane, -90°C (propionitrile), $t_{1/2}$ = 3.5 sec), and with 100% selectivity produces cyclohexyl chloride.[1-3] In absence of organic substrates, there are various self-decay pathways, one leading to an oxido-bridged diiron(III) species. The reactivity of this "resting state" as well as reasons for the unprecedented reactivity of *trans*-N3-[(L)$Fe^{IV}$=O(Cl)]$^+$ are discussed on the basis of temperature-dependent kinetics, a spectroscopic analysis of the ferryl complex, also involving a ligand-field-based analysis of the electronic ground state.




*References*

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2) Abu-Odeh, M.; Bleher, K.; Britto, N. J.; Comba, P.; Gast, M.; Jaccob, M.; Kerscher, M.; Krieg, S.; Kurth, M. Chem. Eur. J. **2021**, *27*, 11377-11390. 'Pathways of the extremely reactive iron(IV)-oxido complexes with tetradentate bispidine ligands.'
3) Bleher, K.; Comba, P.; Faltermeier, D; Gupta, A.; Kerscher, M.; Krieg, S.; Martin, B.; Velmurugan, G.; Yang, S. Chem. Eur. J., **2022** ,e202103452.'Non-heme-iron-catalyzed selective halogenation of unactivated carbon-hydrogen bonds.'