



COST Action CM1305

ECOSTBIO

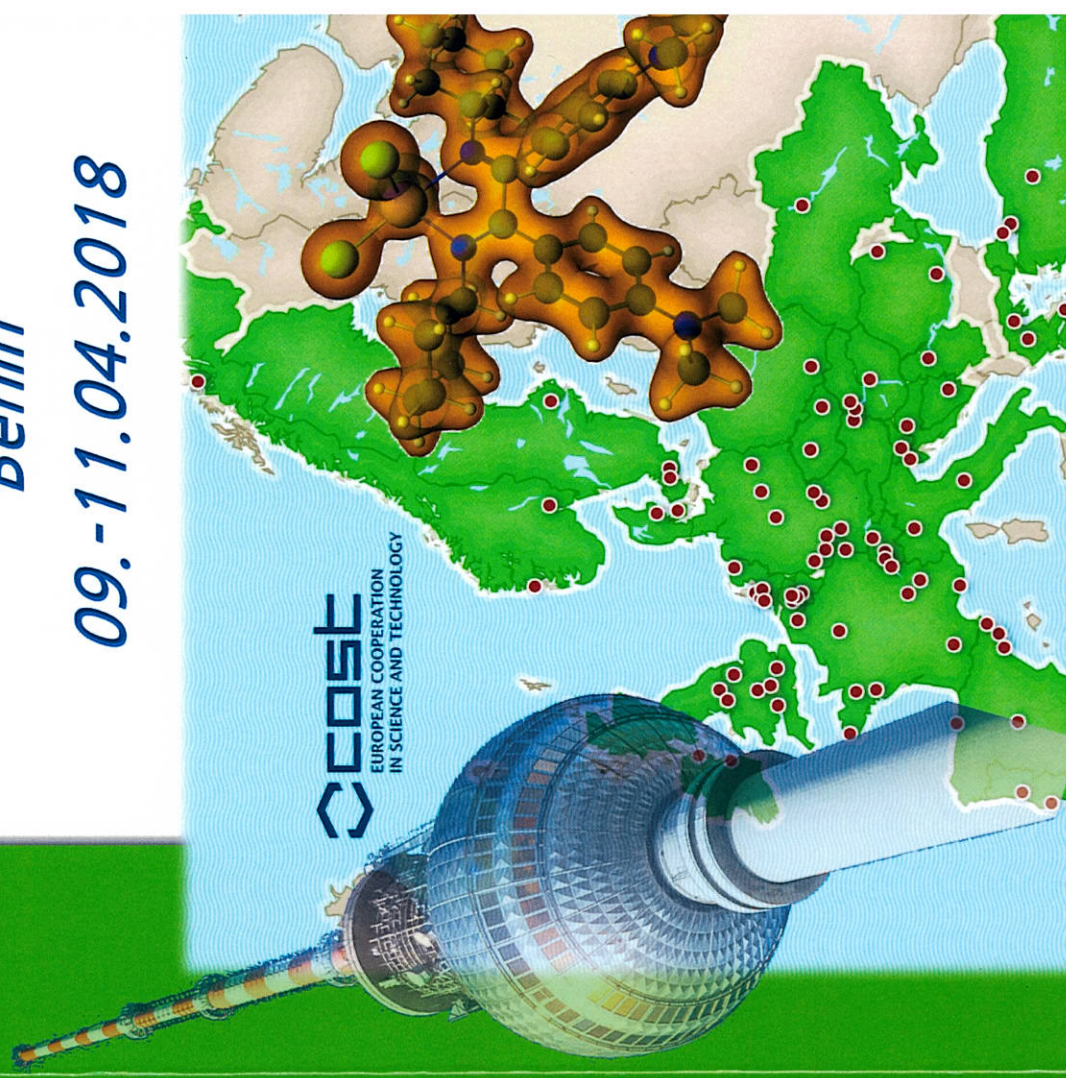
Explicit Control Over Spin-states
in Technology and Biochemistry

P. WEINBERGER

Final scientific workshop

Berlin

09.-11.04.2018



COST
EUROPEAN COOPERATION
IN SCIENCE AND TECHNOLOGY

PROGRAM

Sunday April 8

all day

Europe: Travel to Berlin

Monday April 9

Scientific sessions (Bildungszentrum Erkner)

08.00-08.30

Registration

08.30-08.50

Opening of Meeting (Chair and Local Organizers)

Session Chair: C. McKenzie

08.50-09.30

Plenary lecture: S. Hammes-Schiffer

09.30-10.00

Keynote lecture: M. Driess

10.00-10.20

Scientific talk: T. Corona

10.20-10.40

Scientific talk: B. Weber

10.40-11.10

Coffee break

Session Chair: P. Weinberger

11.10-11.30

Scientific talk: L. Müller

11.30-11.50

Scientific talk: S. Realista

11.50-12.20

Keynote lecture: H. Schwarz

12.20-13.40

Light lunch

Session Chair: D. Pantazis

13.40-14.20

Plenary lecture: C. Cramer

14.20-14.40

Scientific talk: B. Cobeljic

14.40-15.00

Scientific talk: C. Van Stappen

15.00-15.30

Coffee break

Session Chair: M. Gruden

15.30-15.50

Scientific talk: L. González

15.50-16.10

Scientific talk: S. Xue

16.10-16.40

Keynote lecture: C. Duboc

16.40-17.20

Plenary lecture: T. Paine

17.20-18.00

Reports of WG leaders

TUNING PEROXIDE ACTIVATION BY NON-HEME COMPLEXES

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Employment of ethylenediamine-backed hexadentate aminopyridyl ligands successfully achieve biomimetic non-heme iron complexes, which can activate peroxides.^[1,2] Reactivity and stability of the FeO-OR species can be tuned by the *cis* donor of hexadentate ligand (figure 1a) and by the R-group of the peroxides (R = H, ^tBu, cumene, *m*-CPBA).^[3] The Fe^{II}/Fe^{III} redox potential of the precursor complexes work as a proxy for the fate of the FeOOH species towards either dissociation, homo- or heterolytic cleavage (figure 1b), and the spectroscopically characterized iron-based oxidants can be directed towards efficient substrate oxidation of alcohols, however destructive oxidation of the supporting ligand due to the release of the highly reactive hydroxyl radical, HO[•], from homolytic cleavage of the FeO-OH species will occur without the appropriate experimental design.^[2]

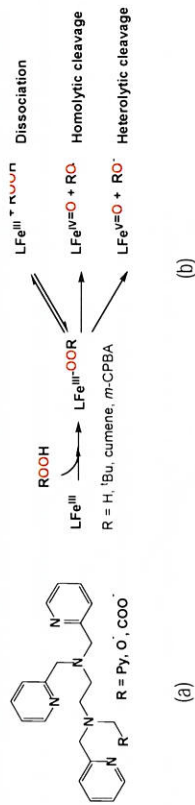


Figure 1: a) Schematic drawing of the hexadentate ligands used in this study b) Possible breakdown pathways for the LFe^{III}OOOR species depending on the supporting ligand.

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- 2) C. Wegeberg, F. R. Lauritsen, C. Frandsen, S. Morup, W. R. Browne, C. J. McKenzie, *Chem. Eur. J.* DOI: 10.1002/chem.201704615
- 3) C. Wegeberg, W. R. Browne, C. J. McKenzie, *In preparation*

N1-SUBSTITUTED TETRAZOLE LIGANDS AS VERSATILE BUILDING BLOCKS FOR Fe(II) SPIN CROSSOVER COMPOUNDS

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As the elucidation of the factors governing the spin transition properties of iron(II) spin crossover compounds shows a subtle interplay of electronic factors (*i.e.* the ligand field strength of the respective ligands used) and stereochemical impacts (*i.e.* the packing of the individual molecules and their intermolecular interactions and stabilizations via H-bonds, π - π stacking, anions and/or solvent molecules, etc...) we want to derive trends within homologous series of a ligand system based on the extremely versatile N1-functionalized tetrazoles aiming for comparative studies. In recent years we developed new synthetic pathways beyond the classical Franke synthesis^[1] such as a microwave assisted synthesis^[2] or via cross-coupling methods^[3] thus allowing the preparation of a synthetic library of tetrazole ligands and their respective iron(II) spin crossover compounds. Starting off from a homologous series of Fe(II) complexes of *n*-alkyl N1-substituted tetrazoles^[4], synthetic strategies towards Fe(II) complexes of iso-^[5] and cyclo-alkyl^[6] N1-substituted tetrazoles are presented as well as bridging ligand systems of α,ω -ditetrazoles with different alkyl-^[7-10] and aryl spacer^[11]. Furthermore, the impact of side-chain halogenation^[12,13] or substitution with main group (IV) elements^[14] are discussed.

References

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