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Biomimetic redox reactions of the Cu(II) μ -thiolate complex

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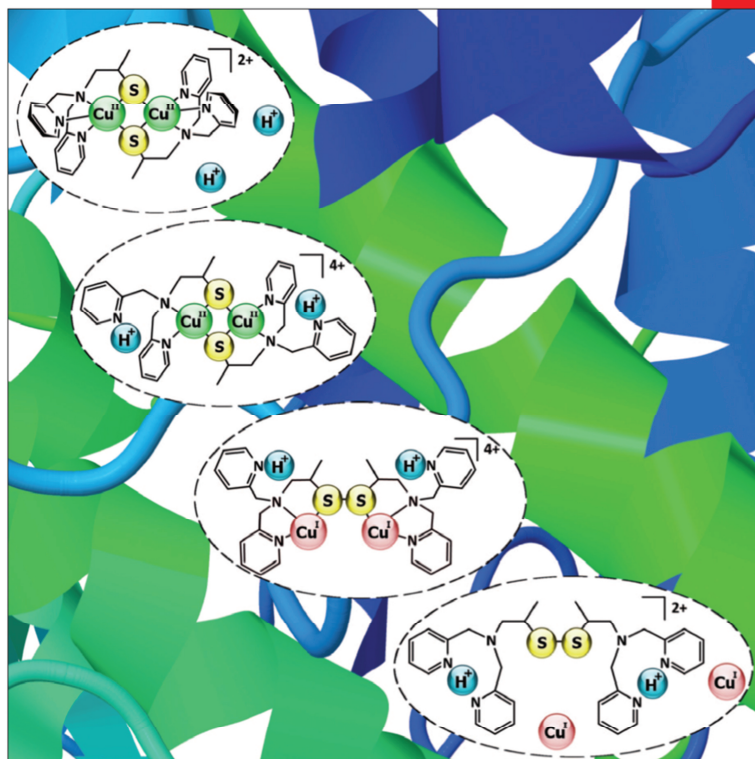
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Protonation of a Cu^{II} μ -thiolate complex ...

... induces an internal redox reaction by which a Cu^I disulfide compound is formed. The dinuclear Cu^I μ -thiolate species forms a model for the CuA site, which has been shown to be sensitive to pH changes. In their Full Paper on page 16913 ff., C. Fonseca Guerra, E. Bouwman et al. show, both experimentally and computationally, that, after addition of just one equivalent of acid per copper center, not only does this redox reaction occur, but ligand dissociation takes place as well. The results imply that pH can have a tremendous effect on the coordination environment of the metal center.

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List of Publications

‘The Quest for Cobalt-Free Alkyd Paint Driers’

J. W. de Boer, P. V. Wesenhagen, E. C. M. Wenker, K. Maaijen, F. Gol, H. Gibbs, R. Hage, *Eur. J. Inorg. Chem.* **2013**, 21, 3581-3591.

‘Homogeneous Hydrogenation and Isomerization of 1-Octene Catalyzed by Nickel(II) Complexes with Bidentate Diarylphosphane Ligands’

T. Mooibroek, E. C. M. Wenker, W. Smit, I. Mutikainen, M. Lutz, E. Bouwman, *Inorg. Chem.* **2013**, 52, 8190-8201.

‘Cu^I Thiolate Reactivity with Dioxygen: The Formation of Cu^{II} Sulfinato and Cu^{II} Sulfonate Species via a Cu^{II} Thiolate Intermediate’

E. C. M. Ording-Wenker, M. A. Siegler, M. Lutz, E. Bouwman, *Inorg. Chem.* **2013**, 52, 13113-13122.

‘Thermodynamics of the Cu^{II} μ -Thiolate and Cu^I Disulfide Equilibrium: A Combined Experimental and Theoretical Study’

E. C. M. Ording-Wenker, M. van der Plas, M. A. Siegler, S. Bonnet, F. M. Bickelhaupt, C. Fonseca Guerra, E. Bouwman, *Inorg. Chem.* **2014**, 53, 8494-8504.

‘Protonation of a Biologically Relevant Cu^{II} μ -Thiolate Complex: Ligand Dissociation or Formation of a Protonated Cu^I Disulfide Species?’

E. C. M. Ording-Wenker, M. van der Plas, M. A. Siegler, C. Fonseca Guerra, E. Bouwman, *Chem. Eur. J.* **2014**, 20, 16913-16921 (Inside Cover).

‘Coordination of New Disulfide Ligands to Cu^I and Cu^{II}: Does a Cu^{II} μ -Thiolate Complex Form?’

E. C. M. Ording-Wenker, M. A. Siegler, E. Bouwman, *Inorg. Chim. Acta* **2015**, *in press*.

‘Catalytic Catechol Oxidation by Copper Complexes: Development of a Structure-Activity Relationship’

E. C. M. Ording-Wenker, M. A. Siegler, M. Lutz, E. Bouwman, *submitted for publication*.

‘The Study of Unprecedented Cu^{II} Phenolate Redox Chemistry’

E. C. M. Ording-Wenker, M. J. B. Moester, M. A. Siegler, E. Bouwman, *manuscript in preparation*.

Curriculum Vitae

The author of this thesis was born in Hoorn, the Netherlands, on July 31st in 1986. In 2004, she graduated from the Gymnasium at the Etty Hillesum College in Den Helder. Later that year she started her BSc study Chemistry at Leiden University. She finished her propaedeutic year *cum laude* and was involved in several extracurricular activities during her studies like being a board member of the study association 'Chemisch Dispuut Leiden' and a board member of the PAC symposium foundation. She was also a student member of the Education Committee and the Faculty Council. Her BSc internship was carried out in the field of organic synthesis under supervision of dr. Amar Ghisaidoobe, prof. dr. Gijs van der Marel and prof. dr. Hermen Overkleef. After finishing her BSc studies she started the research master Chemistry in the track Design and Synthesis at Leiden University. During her masters she did an internship in homogeneous catalysis under supervision of dr. Tiddo Mooibroek and prof. dr. Lies Bouwman as well as an internship at the company Rahu Catalytics B.V. concerning paint-drying under supervision of dr. Ronald Hage. In addition, a summer internship at Occidental College in Los Angeles was done under supervision of prof. Tetsuo Otsuki in the field of organic chemistry. Based on the results obtained during her MSc study she was awarded the Unilever Research Prize in 2010 and the Oxford University Press Achievement in Chemistry Prize of 2010. She obtained her MSc degree in August 2010.

On the 1st of December in 2010, she started her PhD in the Metals in Catalysis, Biomimetics & Inorganic Materials group at Leiden University in the group of prof. dr. Lies Bouwman. During her PhD research she collaborated with dr. Sylvestre Bonnet (Leiden University), for the theoretical chemistry with dr. Célia Fonseca Guerra (VU University Amsterdam) and prof. dr. Matthias Bickelhaupt (VU University Amsterdam) and for Raman measurements with Miriam Moester, MSc (VU University Amsterdam). She has supervised several practical courses, a number of BSc students and two MSc students during the course of the research described in this thesis. Furthermore, she has participated in several courses like the NIOK course 'Catalysis – An Integrated Approach', the HRSMC course 'Molecular Modeling' and the Leiden Graduate school courses 'Time Management', 'Effective Communication', 'Scientific Integrity' and 'Communication in Science'.

The results reported in this thesis were presented at national conferences and meetings and at international conferences:

- Netherlands' Chemistry and Catalysis Conferences NCCC XIII – NCCC XV, 2012-2014 in Noordwijkerhout, 1x oral and 2x poster presentation
- NRSC-C Workshop, 2012 and 2014 in Utrecht, oral presentations
- Reedijk (LIC) Symposium, 2012 in Leiden, poster presentation
- HRSMC symposium, 2013 in Leiden, oral presentation
- Zing Coordination Chemistry Conference, 2013 in Playa del Carmen, Mexico, oral and poster presentation
- European Biological Inorganic Chemistry Conference EuroBIC 12, 2014 in Zürich, Switzerland, poster presentation

