SEKTIONEN FOR UORGANISK KEMI
**KEMISK FORENING**
Universitetsparken 5
DK-2100 København Ø

# SUK-MØDE

Onsdag den 17. maj 2006, kl. 17.30 i auditorium 8, H.C.Ørsted Instituttet.

Sektionen indbyder til to foredrag:

**Marina Yu. Kustova**
Center for Sustainable and Green Chemistry
Department of Chemistry
Technical University of Denmark

taler om

**Hierarchical Nanoporous Materials: Synthesis and Catalysis.**

I aftenens hovedforedrag taler

**Dr. Peter Weinberger**
Institute of Applied Synthetic Chemistry
Vienna University of Technology

om

**New Experimental and Theoretical Insights into the Spin Transition Behaviour of Iron(II) Complexes with 1-Substituted Tetrazole Ligands**

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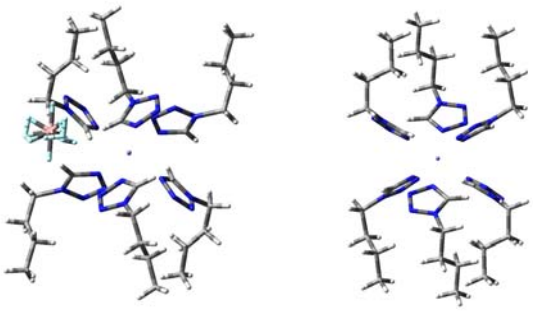
Efter mødet er der spisning. Pris: 40,- pro persona, studerende: 20,- pro persona.
**Tilmelding SENEST mandag d. 15. maj til Line Schwarner Nielsen, tlf: 35321822 / e-mail: line@kiku.dk**

# NEW EXPERIMENTAL AND THEORETICAL INSIGHTS INTO THE SPIN TRANSITION BEHAVIOUR OF IRON(II) COMPLEXES WITH 1-SUBSTITUTED TETRAZOLE LIGANDS

Peter Weinberger

Institute of Applied Synthetic Chemistry, Vienna University of Technology, Getreidemarkt 9/163-AC, A-1060 Vienna, Austria.
e-mail: weinberg@mail.zserv.tuwien.ac.at

Based on the extremely versatile ligand system of 1-substituted tetrazoles several iron(II) spin crossover compounds are presented. Recent research on mono- and polynuclear complexes yielded new insight into their spin transition behaviour[1]. To further elucidate the influence of the factors governing the spin transition properties $T_{½}$ and abruptness of transition high level DFT calculations on the series of mononuclear $[Fe(ntz)_6](BF_4)_2$ complexes (*ntz* = tetrazol-1-yl-alkane with n=1-4, *i.e.* methyl – butyl) have been preformed reproducing the X-ray structure extremely well (see fig.) and yielding a full vibrational analysis.



Furthermore, based on our experience with α,ω-bis(tetrazol-1-yl)alkanes as bridging ligands[2,3] a homologous series of iron(II) spin crossover coordination polymers has been prepared featuring a fascinating spacer length and parity dependence of the magneto-optic properties[4]. But despite of the obvious impact of the ligand used the influence of the non-coordinating anion and of the solvent used will be discussed.

1. P.J. van Koningsbruggen, M. Grunert and P. Weinberger, invited review**,** *Monatsh. Chem.*, **134 (2)** (2003) 183-198.
2. J. Schweifer, P. Weinberger, K. Mereiter, M. Boca, C. Reichl, G. Wiesinger, G. Hilscher, P.J. van Koningsbruggen, H. Kooijman, M. Grunert and W. Linert; *Inorg. Chim. Acta*, **339** (2002) 297-306.
3. M. Grunert, J. Schweifer, P. Weinberger, W. Linert, K. Mereiter, G. Hilscher, M. Müller, G. Wiesinger, P.J. van Koningsbruggen, *Inorg. Chem.*, **43 (1)** (2004) 155-165.
4. A. Absmeier, M. Bartel, C. Carbonera, G.N.L. Jameson, P. Weinberger, A. Caneschi, K. Mereiter, J.-F. Letard and W. Linert; *Eur. J. Chem.*, **12** (2006) 2235-2243.