


Flame-made Pt/K/Al₂O₃ NO_x storage-reduction catalysts

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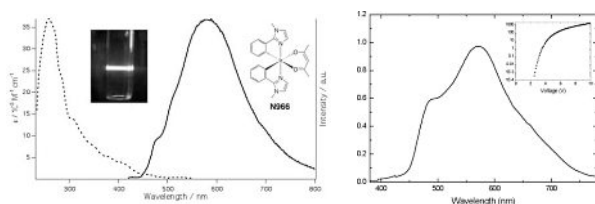
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Panchromatic Phosphorescence Emission from a Single Molecule

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To date organic white light-emitting devices (WOLEDs) are obtained by combining multiple emission which requires complex device architectures, which has so far greatly hindered their market entry. Therefore, the development of a white light-emitting phosphorescent single transition metal complex is very much desired.



We obtained an iridium complex exhibiting very broad photo- and electro-luminescence. Theoretical calculations rationalize the reasons behind such broad emission, opening the way for generalization of this new strategy for WOLEDs development. Our result demonstrates that low cost white light-emitting OLEDs with a single emitting component can be achieved.

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Novel thiocyanate free cyclometalated ruthenium sensitizers upon anchoring to nanocrystalline TiO₂ films exhibit remarkable incident monochromatic photon-to-current conversion efficiency 83%, and the solar cell employing a liquid based electrolyte exhibited a short circuit photocurrent density of 17.10 mA/cm², the open circuit voltage was 802 mV and a fill factor of 0.74, corresponding to an overall conversion efficiency of 10.08% at standard AM 1.5 sunlight.[1] To understand the structural, electronic and optical properties of the cyclometalated ruthenium sensitizers we have investigated using both density functional theory (DFT) and time dependent DFT (TDDFT). Our results show that the HOMO is located mostly on ruthenium and cyclometalated ligand where as the LUMO is on 4-carboxylic acid-4'-carboxylate-2,2'-bipyridine. Molecular orbitals analysis confirmed the experimental assignment of redox potentials, and TDDFT calculations allowed assignment of the visible absorption bands. The present findings provide new design criteria for the next generation of ruthenium sensitizers, which foster widespread interest in engineering of new sensitizers that allow an interaction with the I/I₃⁺ redox couple.

[1] T. Bessho, E. Yoneda, J.-H. Yum, M. Guglielmi, I. Tavernelli, H. Imai, U. Rothlisberger, M. K. Nazeeruddin and M. Grätzel, *J. Am. Chem. Soc.*, **2009**, *131*, 5930.

Flame-made Pt/K/Al₂O₃ NO_x storage-reduction catalysts

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NO_x storage-reduction (NSR) catalyst can trap exhaust NO_x under fuel lean conditions on an alkali- or alkaline earth metal in the form of metal-nitrates. Here Pt/K/Al₂O₃ was prepared using flame spray pyrolysis (FSP)[1]. Raman investigations showed amorphous K₂CO₃ to be the active storage compound. The K-based NSR material showed better NO_x storage performance than the classical Ba based system, during the lean period and the switch from fuel lean to fuel rich conditions (Figure 1). This superior performance was attributed to good K distribution in the sample as evidenced by STEM combined with EDX analysis.

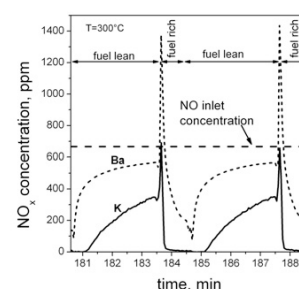


Figure 1: Comparison of K/Pt/Al₂O₃ and Ba/Pt/Al₂O₃ during NSR testing.

[1] R. Strobel, L. Madler, M. Piacentini, M. Maciejewski, A. Baiker, S.E. Pratsinis, *Chem. Mater* **2006**, *18*, 2532.

Cu(II) Complexes with 5'-GMP and poly d(GC): Structure Determination with the Help of Pulsed EPR Spectroscopy

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Z-DNA is a higher energetic form of DNA. In contrast to the normally prevailing right-handed form of DNA (B-DNA), Z-DNA presents a left-handed helix.¹ Substoichiometric amounts of dicopper and dinickel complexes were able to convert poly d(CG) from the right- to the left-handed conformation.²

In this work, we have used Cu(II)-GMP (GMP: 5'-guanosine monophosphate) as an entry system to understand the interactions between copper and polynucleotides with the help of EPR. The first aim of the present work was to carry out a detailed analysis of the electronic and geometric structure of the CuGMP complex.³ In addition, we have studied the interaction of copper with poly d(GC). Here, always two copper species were found. Despite the additional challenge in form of extensive signal overlap, it was possible to describe the coordination environment of the two copper species, both bound to poly d(GC). Continuous-wave and pulse EPR methods like ENDOR and HYSCORE provided unique information about the structure of these copper centers through an elaborate mapping of the hyperfine interactions between the unpaired electron of the Cu(II) ion and the magnetic nuclei of the nucleotide ligand.

[1] B. Spingler, F. Zobi, P. M. Antoni, A. Medina-Molner, R. Alberto, *Chimia* **2005**, *59*, 826. B. Spingler, C. Da Pieve, A. Medina-Molner, P. M. Antoni, M. G. Santangelo, *Chimia* **2009**, *63*, 153
[2] B. Spingler, P. M. Antoni, *Chem. Eur. J.* **2007**, *13*, 6617.
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