



Swiss Science Concentrates

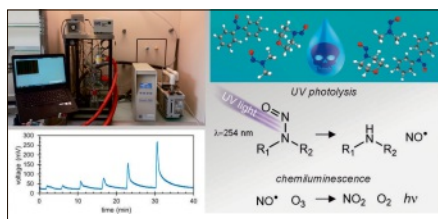
A CHIMIA Column

Short Abstracts of Interesting Recent Publications of Swiss Origin

Quantification of Total N-Nitrosamine Concentrations in Aqueous Samples via UV-Photolysis and Chemiluminescence Detection of Nitric Oxide

F. Breider and U. von Gunten*, *Anal. Chem.* **2017**, *89*, 1574. EPF Lausanne and Eawag, Dübendorf

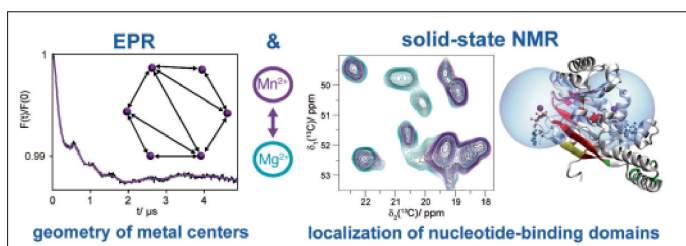
N-nitrosamines are potent mutagens and carcinogens that can be formed during water and wastewater treatment as well as in the gastric fluids by endogenous nitrosation. The analysis of the total N-nitrosamine concentration can indicate whether N-nitrosodimethylamine and other specific nitrosamines of current interest are dominant or minor components of the total N-nitrosamine pool. Breider and von Gunten now present a significant improvement of the measurement of total N-nitrosamines concentrations in aqueous samples by coupling photolytic cleavage of the N–N bond with chemiluminescence detection of nitric oxide. The method can be potentially used for numerous applications in the fields of water quality and treatment as well as in biomedical research.



Solid-state NMR and EPR Spectroscopy of Mn²⁺-Substituted ATP-Fueled Protein Engines

T. Wiegand, D. Lacabanne, K. Keller, R. Cadalbert, L. Lecoq, M. Yulikov, L. Terradot*, G. Jeschke*, B. H. Meier*, and A. Böckmann*, *Angew. Chem. Int. Ed.* **2017**, *56*, 3369. ETH Zürich

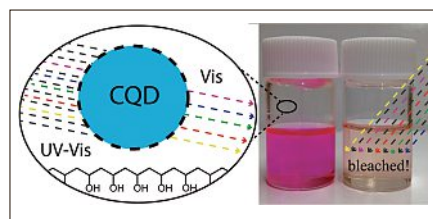
Paramagnetic metal ions deliver structural information both in EPR and solid-state NMR experiments, offering a profitable synergetic approach to study bio-macromolecules. Jeschke, Meier, Terradot, Böckmann and coworkers demonstrate the spectral consequences of Mg²⁺/Mn²⁺ substitution and the resulting information contents for two different ATP:Mg²⁺-fueled protein engines, a DnaB helicase from *H. pylori* active in the bacterial replisome, and the ABC transporter BmrA, a bacterial efflux pump. The research team shows that, while EPR spectra provide information on the geometry of the metal centers, NMR paramagnetic relaxation enhancements help localizing the residues at the binding site.



Direct Synthesis of Carbon Quantum Dots in Aqueous Polymer Solution: One-Pot Reaction and Preparation of Transparent UV-blocking films

S. C. Hess, F. A. Permatasari, H. Fukazawa, E. M. Schneider, R. Balgis, T. Ogi*, K. Okuyama, and W. J. Stark*, *J. Mater. Chem. A*, **2017**, *5*, 5187. ETH Zürich

There is a high demand for transparent UV-blockers as additives to polymers applied for food packaging. Due to their low toxicity, environmental sustainability, low synthesis costs, and simple synthesis routes, fluorescent carbon quantum dots (CQDs) are promising materials for the packaging industry. Herein, Stark, Ogi and coworkers present a one-pot CQDs reaction in an aqueous polyvinyl alcohol (PVA) solution. Transparent UV-protection films cast from CQDs–PVA solutions are obtained without purification. Applying CQDs–PVA films on commercially

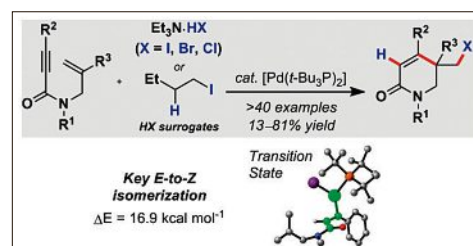


available PET bottle films resulted in high transparency of the composite film in the visible range (>80%) and UV absorption of over 90%.

Palladium-Catalyzed Hydrohalogenation of 1,6-Enynes: Hydrogen Halide Salts and Alkyl Halides as Convenient HX Surrogates

D. A. Petrone, I. Franzoni, J. Ye, J. F. Rodríguez, A. I. Poblador-Bahamonde*, and M. Lautens*, *J. Am. Chem. Soc.* **2017**, *139*, 3546. University of Geneva

While alkene and alkyne hydrohalogenation is a classic transformation that has been used broadly, reports of metal-catalyzed hydrohalogenations are scarce. This paucity can be partly attributed to the limited availability of practical hydrogen halide (HX) sources that ensure safe handling for laboratory use. The synthetic-computational synergy led by Lautens and Poblador-Bahamonde reports the use of ammonium halides as HX surrogates to accomplish the Pd-catalyzed hydrohalogenation of enynes. This work highlights that the use of safe and practical salts avoids many drawbacks associated with traditional HX sources including toxicity and corrosiveness. Their studies support a reaction mechanism involving a crucial E-to-Z vinyl–Pd isomerization and a carbon–halogen bond-forming reductive elimination.



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