16th Blue Danube Symposium on Heterocyclic Chemistry

June 14-17, 2015
Balatonalmádi, Hungary

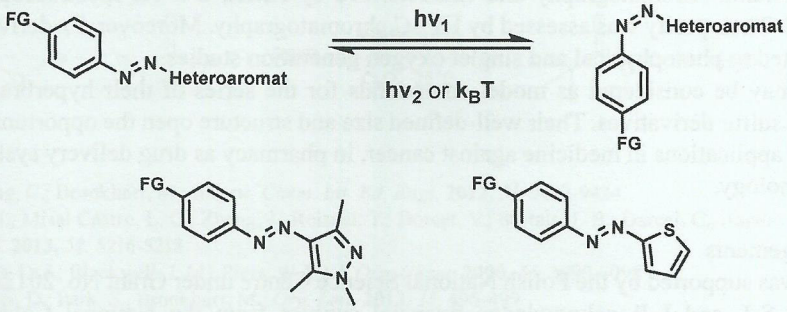
Programme & Book of Abstracts

AZOHETEROARENE PHOTOSWITCHES – EFFECTS OF HETEROAROMATICS AND FUNCTIONAL GROUP DECORATION ON THEIR PHOTOPHYSICAL PROPERTIES

D. Dreier; C. Cziegler; H. Kalaus; E. Horkel; M. Schnürch; M. D. Mihovilovic

Institute of Applied Synthetic Chemistry, TU Wien
Getreidemarkt 9/163-OC, A-1060 Vienna, Austria
dominik.dreier@tuwien.ac.at

Azobenzenes as molecular photoswitches have found great applications in numerous fields including data storage[1], optochemical genetics[2] and material sciences[3]. When irradiated with suitable wavelengths the naturally more stable E-isomer is converted into its Z-isomer causing a major change in molecular geometry. The E-isomer features a π-π* absorbance typically in the range of 300 – 400 nm, which is reponsible for the E to Z isomerization. The back-isomerization can be triggered thermally or by light irradiation using higher wavelengths. While the light induced isomerzation in both directions is a very fast process, the half life time of the thermal back-isomerization varies between μs and years. Spectral properties can be tuned by decorating the phenyl rings with functional groups. In this context, azoheteroarenes are significantly less studied. Variations on the heterocyclic scaffold might enable an even deeper influence on the spectral properties. Regarding the influence on the half life times no principle guidelines can be found in the literature and there is still some debate on the mechanism of the back-isomerization. Recently, arylazopyrazoles were presented as photoswitches featuring remarkably long half life times.[4] Inspired by this work we sought to investigate the influence of functional groups in the para position of the phenyl ring on the spectral properties as well as on the half life times. One series of arylazopyrazoles and one series of arylazothiophenes were synthesized, characterized and compared. Theoretical predictions of the spectral properties were performed at density functional theory level for comparison with the experimental data.



1. Kawata, S.; Kawata, Y. *Chem. Rev.* **2000**, *100, 1777 - 1788*
2. Fehrentz, T.; Schönberger, M.; Trauner, D. *Angew. Chem. Int. Ed.* **2011**, *50, 12156 – 12182.*
3. Koshima, H.; Ojima, N.; Uchimoto, H. *J Am. Chem. Soc.* **2009**, *131, 6890 - 6891*
4. Weston, C. E.; Richardson, R. D.; Haycock, P. R.; White, A. J. P.; Fuchter, M. J. *J Am. Chem. Soc.* **2014**, *136, 11878 - 11881*