

Neutral Homoaromatic Hydrocarbons – a New Model Platform for Molecular Photoswitches

Trung Tran Ngoc,^{a,b} Niklas Grabicki,^c Elisabeth Irran,^b Oliver Dumele,^c and Johannes F. Teichert^a

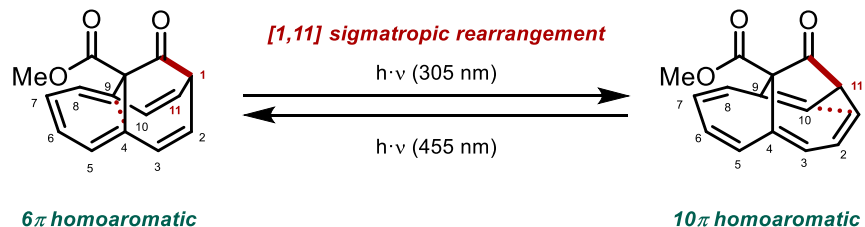
a Institut für Chemie, Technische Universität Chemnitz, Straße der Nationen 62, 09111 Chemnitz, Germany

b Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 115, 10623 Berlin, Germany

c Department of Chemistry & IRIS Adlershof, Humboldt Universität zu Berlin, Brook-Taylor-Straße 2, 12489 Berlin, Germany

The identification and characterization of homoaromatic compounds bearing an interrupted π -system are fundamental challenges for the understanding of electronic interactions in organic molecules.¹ This is further hampered by the fact that no stable neutral homoaromatic hydrocarbon is known. We present the preparation of a new class of neutral and stable homoaromatic compounds,² which is supported by experimental evidence (ring current observed by NMR spectroscopy, equalization of bond lengths through X-ray structure analysis) as well as computational analysis (NICS³ and ACID⁴).

Furthermore, we can show that one homoaromatic hydrocarbon of this class acts as a photoswitch through a reversible photochemical [1,11] sigmatropic rearrangement.² To the best of our knowledge, such a process involving the 10 π homoaromatic system has not been reported earlier. These results of stable and accessible homoaromatic neutral hydrocarbons and their photoswitching behaviour provide new insights for the understanding and study of homoconjugative interactions in organic molecules, and for the design of new responsive molecular materials.



[1] R. V. Williams, *Chem. Rev.* **2001**, *101*, 1185; DOI: 10.1021/cr9903149

[2] T. Tran Ngoc, N. Grabicki, E. Irran, O. Dumele, J.F. Teichert, *ChemRxiv*, DOI: 10.26434/chemrxiv-2022-6pc2z

[3] A. Stanger, *Eur. J. Org. Chem.* **2020**, *21*, 3120; DOI: 10.1002/ejoc.201901829

[4] D. Geuenich, K. Hess, F. Köhler, R. Herges, *Chem. Rev.* **2005**, *105*, 3758; DOI: 10.1021/cr0300901