THE ELECTRONIC STRUCTURE OF THE PLANARIZED BLATTER RADICAL AND ITS DERIVATIVES.

ANIKET HANDE, CLOVIS DARRIGAN, *Institute of Analytical Sciences and Physical Chemistry for the Environment and Materials, CNRS/ UNIV PAU0 & PAYS ADOUR/ E2S UPPA, Pau, France*; PIOTR KASZYŃSKI, *Department of Chemistry, University of Łódź, Łódź, Poland*; ANNA CHROSTOWSKA, *Institute of Analytical Sciences and Physical Chemistry for the Environment and Materials, CNRS/ UNIV PAU0 & PAYS ADOUR/ E2S UPPA, Pau, France*.

In recent years, derivatives of the 1,4 dihydrobenzo[e][1,2,4]triazin-4-yl radical (e.g. the Blatter1 radical [a]) are gaining much interest due to their properties, such as exceptional stability, spin Π-delocalization, narrow electrochemical window and low excitation energies. For these reasons, a rapidly increasing attention is given to these radicals as structural elements of advanced materials.[b] Their design requires, however, a good understanding of the electronic structure of these electro-, photo- and magnetically active molecular components.

Recent advances in the chemistry of the 1,4-dihydrobenzo[e][1,2,4]triazin-4-yl demonstrated access to the parent "planarized" Blatter radical, in which more effective spin delocalization onto the Ph ring at the N(1) position is observed.[c] In order to better understand the impact of electronic delocalization on properties of the radicals, a series of derivatives has been prepared and investigated by computational and spectroscopy methods.

Herein we present determination of the electronic structure of a series of substituted planar radical using UV photoelectron spectroscopy (UV-PES), EPR, and UV-vis spectroscopy.

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[b] Jasiński, M.; Szczytko, J.; Pociecha, D.; Monobe, H.; Kaszyński, P. "Substituent-dependent magnetic behavior of discotic benzo[e][1,2,4]triazinyls", J. Am. Chem. Soc. 2016, 138, 9421-9424. Kapuściński, S.; Gardias, A.; Pociecha, D.; Jasiński, M.; Szczytko, J.; Kaszyński, P. "Paramagnetic bent-core mesogens derived from the 1,4-dihydrobenzo[e][1,2,4]triazin-4-yl", J. Mater. Chem. C, 2018, 6, 3079–3088.

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