STABILITY OF TRIARYLAMINE RADICAL CATIONS STUDIED BY IN-SITU VOLTAMMETRY WITH ELECTRON PARAMAGNETIC RESONANCE (EPR)

Ján Tarábek, Denisa Hidasová, Tomáš Slanina

Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo náměstí 542/2, Prague, Czech Republic
jan.tarabek@uochb.cas.cz

Triarylamines are one of the most prominent group in organic electronic applications such as light-emitting diodes or solar cells in which they usually act as a hole-conducting/transporting material.[1] They can undergo one-electron oxidation (chemically, electrochemically or even photochemically) forming relatively stable radical cation, that can serve as an oxidant in the additional reactional pathways.[2,3] The crucial role of radical cation is affected by the follow-up reactions like dimerization. Substituents like *tert*-butyl on aromatic rings may dramatically hinder the dimerization via σ-bond character. Moreover, the propeller-conformation of aromatic rings suppress the stacking of radical cationic species (e.g. π-dimerization). Otherwise, with planar structure stacking appears to be very likely present. However, also radical cations with almost planar configuration or slightly helical can exhibit quite high stability, even higher than those for propeller-shaped triarylamines. This will be shown by the results obtained via combined *in-situ* voltametric EPR technique as the dimerization gives rise to quenching of the radical cations (see Figure 1) and intensity decline of the corresponding EPR spectra. Therefore, the stability/reactivity can be characterized by the kinetic rate constants, accordingly.

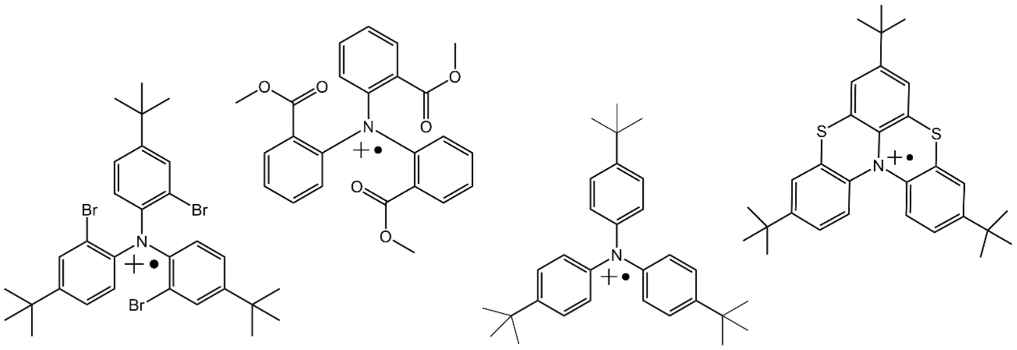

Figure 1. Structure of triarylamine radical cations as a subject of the combined in-situ voltametric EPR (Electron Paramagnetic Resonance) stability studies.

Acknowledgements. This work has been supported by the Czech Science Foundation Project 19-20467Y and by the Czech Academy of Sciences RVO-61388963

REFERENCES

[1] J. Wang, K. Liu, L. Ma, X. Zhan, *Chem. Rev.* **2016**, *116*, 14675–14725.

[2] S. Liu, M. Klussmann, *Org. Chem. Front.* **2021**, *8*, 2932–2938.

[3] S. M. Bonesi, M. Mella, D. Merli, S. Protti, *Photochem. Photobiol.* **2021**, *97*, 1278–1288.