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XIII International Conference "Synthesis and Application of Porphyrins and Their Analogues"



Kovkova U.P.a, Skvortsov I.A.a, Khodov I.A.a, Zhabanov Yu.A.b, Stuzhin P.A.a

PERHALOGENATED AZAANALOGUES OF SUBPHTHALOCYANINE AS A PERSPECTIVE ACCEPTORS FOR ORGANIC ELECTRONICS

^a Ivanovo State University of Chemical Technology, Ivanovo, Russia ^b Institute for Physics of Microstructures, Russian Academy of Sciences, Nizhny Novgorod, Russia e-mail: kovkova.ulya@mail.ru

Introduction of different substituents in a subphthalocyanine molecule leads to considerable modification of its properties [1]. While subphthalocyanines behave as donor p-layers in hybrid organic solar cells, perfluorinated subphthalocyanine analogs have n-type conductivity and can be used as electron acceptors [2]. Moreover, not only halogenation, but also aza-substitution in benzene rings of subphthalocyanine may be used to enhance its acceptor properties. In our work we combined both modification methods: halogenation and aza-substitution. Thus, by co-condensation of tetrafluorophthalonitrile and 5,6-dichloro-pyrazin-2,3-dicarbonitrle in the presence of BCl₃ in a p-xylene we have obtained a set of perhalogenated porphyrazines, containing dichloropyrazine and tetrafluorobenzene fragments.

The structure of obtained porphyrazines was characterized by MALDI-TOF mass spectroscopy and NMR-spectroscopy (¹¹B, ¹³C, ¹⁹F). Preliminary results of DFT calculations and electrochemical measurements indicate that obtained compounds are perspective acceptor materials for organic electronics.

This work was supported by Russian Science Foundation (grant №17-13-01522)

References

- [1] Claessens C.G. et al. Chem. Rev. 2014, 114, 2192.
- [2] Dearden C.A. et al. Phys. Chem. Phys. 2014, 16, 18926–18932.