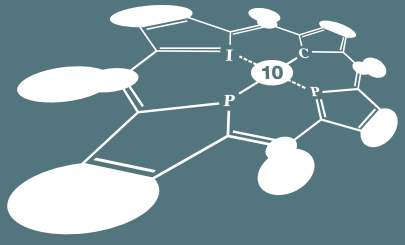
TENTH

INTERNATIONAL CONFERENCE on PORPHYRINS & PHTHALOCYANINES

ICPP-10 GERMANY Munich | JULY 1-6 2018

book of abstracts



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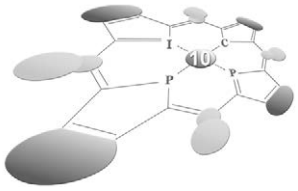

Heterocyclic (Sub)Phthalocyanine Analogues

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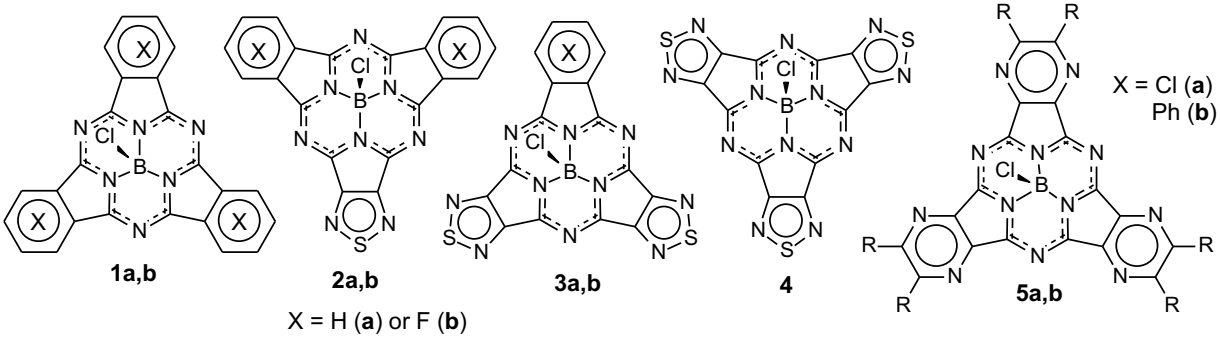
Boron(III) subphthalocyanines are widely investigated as perspective *p*- or *n*-type materials for organic electronics (**1a,b**) [1]. To further develop this field, we have designed a series of heterocyclic subphthalocyanine analogues in which benzene rings are substituted by π-electron-deficient 1,2,5-thiadiazole [2,3] or pyrazine ring(s):



All new 1,2,5-thiadiazole and pyrazine fused subporphyrazines **2-5** have been characterized by LDI mass-spectrometry, ^{1}H, ^{11}B, ^{13}C NMR spectroscopy, optical spectroscopy in the UV/Vis/NIR and IR domains and the structure of **2a**, **3a**, **4** and **5b** have been determined by single crystal X-ray diffraction study. DFT B3LYB calculations supported by the electrochemical characterisation and electronic absorption/emission experiments suggest that the synthesized subporphyrazines with fused 1,2,5-thiadiazole or pyrazine rings should behave as efficient acceptor materials. To prove their electron accepting and transporting properties, the prototype thin-film photovoltaic cells with a fully-subporphyrinoid planar heterojunction were fabricated, in which the donor layer is formed by subphthalocyanine **2a**, with its fluorinated 1,2,5-thiadiazole analogues **2b**, **3b** and **4** being used as the acceptor components [4]. The measured photovoltaic parameters reveal that due to a favourable combination of low sublimation temperatures, stability and high extinction in the solar activity range, some of these compounds win competition from C60 , the most popular acceptor in organic photovoltaics.
The effect of peripheral annulation on the photochemical properties of subporphyrazines **1-5** has been also examined. The boron(III) complexes of other 1,2,5-thiadiazole fused porphyrinoids will be also discussed.

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

REFERENCES

1. Morse GE, Bender TP. *ACS Applied Materials and Interfaces*, **2012**, *4*, 5055.
2. Hamdoush M, Ivanova SS, Pakhomov GL, Stuzhin PA. *Macroheterocycles*, **2016**, *9*, 230.
3. Hamdoush M, Skvortsov IA, Mikhailov MS, Pakhomov GL, Stuzhin PA. *J. Fluorine Chem*., **2017**, *204*, 31.
4. Pakhomov GL, Travkin V, Hamdoush M, Zhabanov Yu., Stuzhin PA. *Macroheterocycles*, **2017**, 10, 548. DOI: 10.6060/mhc171038s.

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