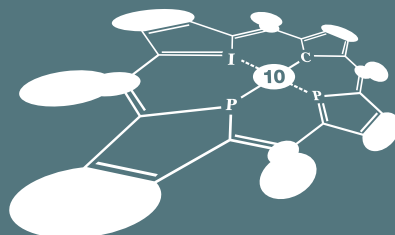
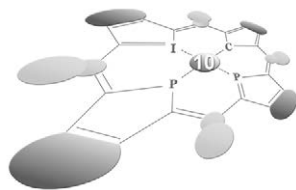




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Heterocyclic (Sub)Phthalocyanine Analogues

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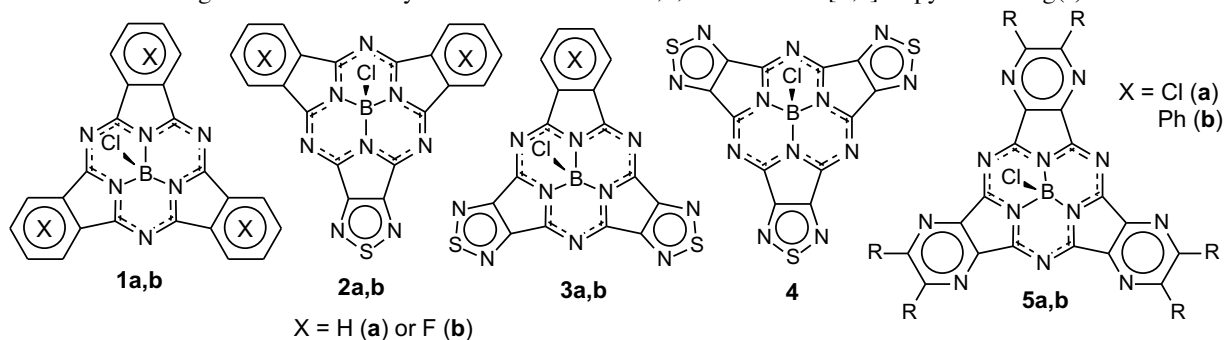
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Boron(III) subphthalocyanines are widely investigated as perspective *p*- or *n*-type materials for organic electronics (**1a,b**) [1]. To further develop this field, we have designed a series of heterocyclic subphthalocyanine analogues in which benzene 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 subporphyrines **2-5** have been characterized by LDI mass-spectrometry, ¹H, ¹¹B, ¹³C 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 subporphyrines 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 subporphyrines **1-5** has been also examined. The boron(III) complexes of other 1,2,5-thiadiazole fused porphyrinoids will be also discussed.

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REFERENCES

1. Morse GE, Bender TP. *ACS Applied Materials and Interfaces*, **2012**, *4*, 5055.
2. Hamdoush M, Ivanova SS, Pakhomov GL, Stuzhin PA. *Macromolecules*, **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. *Macromolecules*, **2017**, *10*, 548. DOI: 10.6060/mhc171038s.