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BORON(III) COMPLEXES OF HETEROCYCLIC (SUB)PHTHALOCYANINE ANALOGUES: 1,2,5-THIADIAZOLE FUSED (SUB)PORPHYRAZINES

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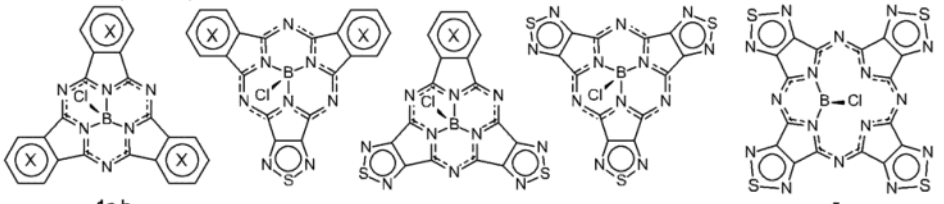
Boron(III) subphthalocyanines (**1a**) are widely investigated as perspective materials for organic electronics [1]. Usually they behave as *p*-type materials; their perfluorinated derivatives (**1b**) exhibit the *n*-type conductivity. Another way to enhance the electron acceptor properties of subporphyrazine core is annulation of π-deficient heterocycles instead of benzene rings. Thus, fusion of 1,2,5-thiadiazole rings strongly increases π-electron-deficiency of porphyrazine core [2] and tetra(1,2,5-thiadiazolo)porphyrazines were used as *n*-type layers in the prototypes of photovoltaic cells and other electronic devices [3]. Recently, we have prepared the first heterocyclic subphthalocyanine analogue with strongly electron deficient 1,2,5-thadiazole rings (**4**) [4]. In order to reveal the influence of these heterocycles on the electronic properties of boron(III) subporphyrazines we have synthesized the series of macrocycles combining 1,2,5-thiadiazole and benzene rings (**2a**, **3a**) and their perfluorinated derivatives (**2b**, **3b**).



1a,b **2a,b** **3a,b** **4** **5**

X = H or F

The electronic absorption and emission spectra, electrochemical properties, conductivity of the sublimed thin films have been studied and the results are compared with the properties of boron(III) subphthalocyanine **1a** and perfluorosubphthalocyanine **1b**.

The evidence have been obtained that reaction of 1,2,5-thiadiazole-3,4-dicarbonitrile with BCl_3 along with boron(III) subporphyrazine **4** affords also boron(III) porphyrazine complex **5** as a cyclotetramerization by-product.

The influence of the 1,2,5-thiadiazole annulation on the electronic properties and geometrical features of subporphyrazine complexes as well as possible structures of boron(III) porphyrazines is discussed an the basis of DFT calculations results.

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