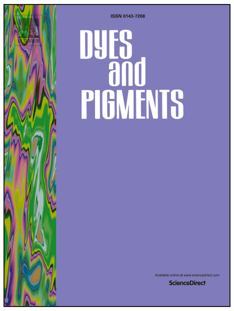

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PII: S0143-7208(17)32240-4

DOI: 10.1016/j.dyepig.2018.01.047

Reference: DYPI 6521

To appear in: *Dyes and Pigments*

Received Date: 1 November 2017

Revised Date: 21 January 2018

Accepted Date: 28 January 2018

Please cite this article as: Flamholc Rafał, Wrona-Piotrowicz A, Makal A, Zakrzewski J, Pyrenylpyrazole-based donor/acceptor fluorescent dyes: Synthesis and photophysical properties, *Dyes and Pigments* (2018), doi: 10.1016/j.dyepig.2018.01.047.

Pyrenylpyrazole-based donor/acceptor fluorescent dyes: Synthesis and photophysical properties

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Abstract. The reaction of 1-acetylpyrene phenylhydrazone with Vilsmeier reagent (DMF-$POCl_3$) afforded 1-phenyl-3-(pyren-1-yl)-1*H*-pyrazole-4-carbaldehyde in good yield. Condensation of this compound with a series of active methylene compounds (methyl ethyl ketone, diethyl ketone, malononitrile, 1,3-indandione and *N,N*-diethythiolbarbituric acid) gave a series of donor/acceptor dyes exhibiting fluorescence in the almost whole range of the visible spectrum. The electronic structure of the dyes was studied theoretically by the (TD) DFT method. Calculations elucidated the nature of intramolecular charge transfer (ICT) processes leading to emissive excited states of the synthesised compounds. It turned out that the electron acceptor ability influences the direction of ICT. For compounds with relatively weak acceptor groups, ICT from the pyrene moiety toward the remaining part of the molecule prevailed, whereas for those having stronger acceptor groups the main ICT pathway became that from the phenylpyrazole group to the acceptor group.

1. Introduction

Pyrene-based fluorophores continue to attract significant attention due to their interesting photophysical properties and numerous possibilities of structural modification [1-8]. They have found a plethora of applications in various branches of science, ranging from biology and medicine to materials science. We thought it would be of interest to synthesise and study