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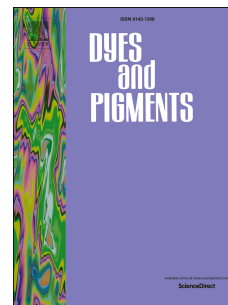
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1 Quinoidal bithiophene as disperse dye: Substituent effect on dyeing performance

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10 **Abstract:** A series of quinoidal bithiophene (QBT) dyes, namely **QBT1-QBT7**, which exhibit high
11 absorption coefficients in the red spectral region, were synthesized and used as disperse dyes to
12 examine their ability for dyeing poly(ethylene terephthalate) fabric. The dyeing properties, such as
13 color representation, dye exhaustion, dyeing rate, build-up and fastness properties were investigated.
14 Quantum chemical density functional theory (DFT) calculation suggested that there are much larger
15 QBT-benzene interaction energy and QBT-QBT interaction energy due to the high quinoidal
16 structural planarity. Substituent effect was also studied by DFT calculation. Suitable alkyl groups
17 with controlled steric hindrance were suggested to facilitate the formation of single dye molecule and
18 dye diffusion on the fiber surface and inside. As a result, **QBT6** with two *n*-butyl groups as end groups
19 gave the best overall dyeing performance. This study provides a preliminary suggestion for the
20 rational design of new disperse dyes based on quinoidal structure.

21 **Keyword:** Quinoidal bithiophene; Disperse dye; Dyeing property; Planarity; Substituent effect; DFT
22 calculation.

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