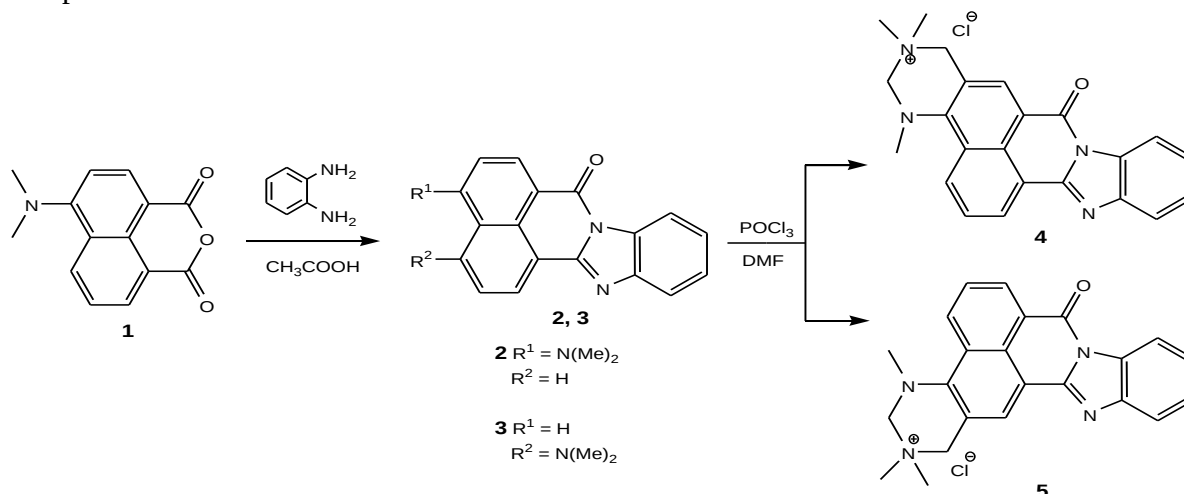


WATER-SOLUBLE NAPHTHOYLENE-BENZIMIDAZOLE DERIVATIVES AND THEIR SPECTRAL PROPERTIES

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The Vilsmeier-Haack reaction was used to obtain water-soluble quaternary salts of naphthoylene-benzimidazole derivatives. Spectral properties of the products were studied and compared.



Condensation of 4-dimethylaminonaphthalic anhydride (1) and ortho-phenylenediamine in acetic acid results in a mixture of isomers 2 and 3 that contain benzimidazole moiety. The isomers were isolated and purified by column chromatography. Each of the dimethylamino derivatives 2 and 3 reacts with complex POCl_3 —DMF to form water-soluble products 4 and 5, respectively, which contain quaternized 1,3-diazine cycle.

Spectral properties of dyes 2-5 were studied in toluene, methanol, and water. The position of dimethylamino group in compounds 2, 3 and 1,3-diazinium cycle in products 4, 5 greatly affects their spectral properties. Derivatives 2 and 4 absorb at 410–440 nm and emit light at 483–515 nm in methanol. Absorption and emission maxima of products 3 and 5 are red-shifted in comparison to dyes 2 and 4, respectively. This effect is much more pronounced in emission spectra.

Positive solvatochromic (15 nm) and solvatofluorochromic (30 nm) effects were observed for compounds 2 and 3 when the solvent was changed from non-polar (toluene) to more polar (methanol). Due to their highly polar structure, the quantum yields of these products are dramatically decreased in methanol as compared to toluene solutions.

Introduction of the 1,3-diazinium cycle into compounds 2 and 3 leads to a blue-shift of the absorption and emission maxima by 20–30 nm. Fixation of the dimethylamino group with the diazine cycle formation in product 2 leads to a 56-fold increase of quantum yield in methanol.

Considering that compounds 2 and 3 exhibit significant Stokes shifts and bright fluorescence in a non-polar environment, they can be used as light shifters in polymeric matrixes. Water-soluble derivatives 4 and 5 can be further modified to include reactive groups for covalent labelling of biomolecules.