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The Use of Polar Substituent Groups for Promoting Azo Disperse Dye Solubility and Reactivity for More Economic and Environmental Benign Applications: A Computational Study

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Abstract : The economic and environmental challenges associated with azo disperse dyes applications are due to poor aqueous solubility and low degradation tendency which stems from low chemical reactivity. Poor aqueous solubility property of this group of dyes necessitates the use of dispersing agents which increase operational costs and also release toxic chemical components into the environment, while their low degradation tendency is due to the high stability of the azo functional group (-N=N-) in their chemical structures. To address these problems, this study investigated theoretically the effects of some polar substituents on the aqueous solubility and reactivity properties of disperse yellow (DY) 119 dye with a view to theoretically develop new azo disperse dyes with improved solubility in water and higher degradation tendency in the environment using DMol^3 computational code. All calculations were carried out using the Becke and Perdew version of Volsko-Wilk-Nusair (VWN-BP) level of density functional theory in conjunction with double numerical basis set containing polarization function (DNP). The aqueous solubility determination was achieved with conductor-like screening model for realistic solvation (COSMO-RS) in conjunction with known empirical solubility model, while the reactivity was predicted using frontier molecular orbital calculations. Most of the new derivatives studied showed evidence of higher aqueous solubility and degradation tendency compared to the parent dye. We conclude that these derivatives are promising alternative dyes for more economic and environmental benign dyeing practice and therefore recommend them for synthesis.

Keywords : aqueous solubility, azo disperse dye, degradation, disperse yellow 119, DMol^3, reactivity
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