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SUPPLEMENTARY MATERIAL

A Computational Comparative Study for the Spectroscopic Evaluation of Triazine Derivative Dyes in Implicit Solvation Model Systems Using Semi-Empirical and Time-Dependent Density Functional Theory Approaches

Victor Akpe,[A,B] Timothy J. Biddle,[A] Christian Madu,[C] Christopher L. Brown,[A,B] Tak H. Kim,[A,B] and Ian E. Cock[A,B,D]

[A]School of Environment and Science, Griffith University, Nathan Campus, Nathan, Qld 4111, Australia.

[B]Environmental Futures Research Institute, Griffith University, Nathan Campus, Nathan, Qld 4111, Australia.

[C]Department of Chemistry, Collin College, Preston Ridge Campus, Frisco, TX 75035, USA.

[D]Corresponding author. Email: I.Cock@griffith.edu.au

Contents

Gaussian 16 reference

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Parameters used for defining the solvent, 2-methyltetrahydrofuran (2-MeTHF) in Gaussian 16 software

Eps=6.97
EpsInf=1.98
HBondAcidity=-1.68
HBondBasicity=1.34
SurfaceTensionAtInterface=17.06
CarbonAromaticity=0
ElectronegativeHalogenicity=0

Notes
Eps = Dielectric Constant (ε) [1]
EpsInf = The square of the index of refraction (n^2) [2]
HBond Acidity = Abraham's hydrogen bond acidity (α) [3]
HBond Basicity = Abraham's hydrogen bond basicity (β) [4]
SurfaceTensionAtInterface = Macroscopic surface tension at the liquid-air interface (298 K) (dyne/cm) (γ)[5]
Carbon Aromaticity = Aromaticity: fraction of non-hydrogenic solvent atoms that are aromatic carbon atoms (Φ)
Electronegative Halogenicity = Electronegative halogenicity: fraction of non-hydrogenic solvent atoms that are F, Cl, or Br (Ψ)

Refer to https://gaussian.com/smdtip/ for more information.

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