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ORIGINAL PAPER

Molecular modelling and spectral investigation of some triphenyltetrazolium chloride derivatives‡

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The molecular parameters of 2,3,5-triphenyl-2*H*-tetrazolium chloride (TTC) and some compounds based on triphenylformazans (TPFs) – resulting from the enzymatic transformation of TTC, were subjected to comparative investigation on the basis of semi-empirical quantum-chemical simulations, revealing some changes in dipole moment and polarisability in the TPFs in comparison with TTC. Chemical shift due to substituents was discussed using electronic absorption bands in the UV-VIS range recorded for diluted solutions in various solvents as well as the absorption spectra recorded in the infrared range for KBr dispersions. The correlation of the spectral shift of the electronic absorption bands with a specific function on the solvent refractive index, as recommended by theoretical studies focused on solute–solvent interactions, revealed the major role played by dispersive and induction forces. For several solvents, a different behaviour could be assigned to specific interactions overlapping with universal solute-solvent interactions.

Keywords: quantum-chemical approach, substituent influence, solvatochromic effect

Introduction

The 2,3,5-triphenyl-2*H*-tetrazolium chloride (TTC), synthesised by Pechmann and Runge (1894), is a colourless compound which turns red as a result of enzymatic action which leads to the formation of triphenyformazans (TPFs) that possess significant biological activity (Awasthi & Singh, 1982; Bharadwaj, 2002; Bačkor & Fahselt, 2005). Tetrazolium salts and their derivatives have found a wide range of applications, being in frequent use for analytical purposes, for instance in the assessment of antimicrobial activity in different media (Praveen-Kumar & Tarafdar, 2003; Piaru et al., 2012), as quantitative tests indicators for cell viability (Bhupathiraju et al., 1999; Ruf & Brunner, 2003), as well as in various technical applications due to their ability to form metal complexes (Sigeikin et al., 2006; Tezcan & Aksu, 2010).

In considering the dehydrogenation process of TTC biological transformation in living cells (Frederiks et al., 2006), some researchers also focused on the production of TTC derivatives and their characterisation (Gökçe et al., 2005; Tezcan, 2008; Mariappan et al., 2010; Pervova et al., 2010; Şenöz, 2012) in order to investigate their structures and their main physico–chemical properties. Tezcan and coworkers (Tezcan et al., 2002, 2008; Tezcan & Ozkan, 2003) reported on the synthesis and spectral and electrochemical characterisation of a series of TPF derivatives with possible use as dyes or dye precursors. A few theoretical studies also focused on the structural features of the TPFs compounds (King & Murrin, 2004; Erkoç et al., 2006). Other studies emphasised the importance of various controlling factors (i.e. pH, temperature, concentration, etc.) in the TTC reduction process (Jones & Prasad, 1969; Mahmoud & Ghaly, 2004; Burdock et al., 2011).

As the approach using the spectral behaviour of colour compounds entails consideration of their interaction with solvents, mathematical models for liquid-state could represent useful tools in the theoretical investigation. Among the theories developed at

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