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Reactions of polyhomofunctional organic compounds: 5: Kinetics of N-oxide-N-hydroxide tautomerism in a novel class of triazine-1-oxides

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Triazine-1-oxides are one among the well known classes of fungicides. Abundant reports are available on the functionality of these compounds. These compounds are feared because of their certain impact as they are among the most potent carcinogens in existence. The coordination chemistry of triazine-1-oxides has been well reported. It has been well argued that the monofunctional analogues of the triazine-1-oxides engage in tautomerism. The metabolic conversion of these compounds into safe products assume greater importance from agricultural and medicinal points of view and hence the hydrolysis of these compounds is of still greater importance. Herein, is reported the kinetics of hydrolysis of two isochemical triazine-1-oxide sites of a series of 3,3'-disubstituted 4,4'-bis(3-alkyltriazine-3-oxide)biphenyls (**1**) abbreviated as R-triaz-bp-X investigated at different concentrations of acids and at different temperatures. The studies reveal that the two triazine-1-oxide sites undergo N-oxide-N-hydroxyde tautomerism which is first order in [R-triaz-bp-X] and no dissociation at any of the reaction sites has been identified. Linear regression best fits of the kinetic plots are used to determine the rate constants of the reactions. The activation energy values and other thermodynamic parameters of the hydrolysis of R-triaz-bp-X have been evaluated by Arrhenius plots and Eyring equation.

Keywords: Triazine-1-oxides, Fungicides, Hydrolysis, Tautomerism, Isosbesticity, Thermodynamic parameters