

Magnetic response and its relation to the keto-enol tautomerism of 3,3'-(1,4-phenylene)bis(pentane-2,4-dione): Experimental and theoretical insights

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A direct correlation between aromaticity and the thermodynamic stability in the tautomeric equilibrium of 3,3'-(1,4-phenylene)bis(pentane-2,4-dione) is studied using experimental methods and theoretical approaches. According to the results, the most abundant tautomer corresponds to the bis- β -keto-enol tautomer when conditions such as temperature, solvent polarity, and pH are deliberately changed. Theoretical results of aromaticity analysis showed good concordance with the experimental results, using rigorous computations such as induced magnetic field (Bind) and free of in-plane component NICS (FIPC-NICS). © 2020 Wiley Periodicals LLC

aromaticity

induced magnetic fields

tautomerism

Solvents

Experimental methods

In-plane components

Induced magnetic fields

Keto-enol tautomerism

Magnetic response

Solvent polarity

Tautomeric equilibria

Theoretical approach

Paraffins