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Title:	Evaluation of Substituent Effect in Z-Isomer Stability of Arylazo-1H-3,5-dimethylpyrazoles: Interplay of Steric, Electronic Effects and Hydrogen Bonding
Authors:	Devi, Sudha (/jspui/browse?type=author&value=Devi%2C+Sudha) Saraswat, M. (/jspui/browse?type=author&value=Saraswat%2C+M.) Grewal, S. (/jspui/browse?type=author&value=Grewal%2C+S.) Venkataramani, Sugumar (/jspui/browse?type=author&value=Venkataramani%2C+Sugumar)
Keywords:	Z-Isomer Arylazo-1H-3 5-dimethylpyrazoles Electronic Effects
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Abstract:	The electronic and steric effects of aryl substituents and the influence of hydrogen bonding in Z-isomer stability of phenylazopyrazole derivatives have been investigated. In this regard, 38 substituted phenylazopyrazole derivatives and 6 N-methyl phenylazopyrazoles (with meta substitutions) have been synthesized. Their photoswitching behavior, photostationary states (PSS), and kinetics of thermal reverse isomerization were evaluated experimentally using UV-vis and NMR spectroscopic techniques. Furthermore, density functional theory (DFT) computations have been performed for more detailed insights. Despite the presence of substantial substituent effects inferred through Taft and Hammett relationships, the concentration dependency in controlling the isomerization rates has also been observed. Kinetics studies at different concentrations, solvent effects, and computations have confirmed the decisive role of hydrogen bonding and solvent-assisted tautomerism in this regard. Through this study, a complex interplay of steric, electronic effects and hydrogen bonding as factors in dictating the stability of Z-isomers in arylazo-1H-3,5-dimethylpyrazoles has been demonstrated.
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