Title:	Understanding of the kinetic stability of cis- isomer of halogenated azobenzene through structural, kinetic and computational studies
Authors:	Yadav, Manish K.
Keywords:	Kinetic stability Computational studies
Issue Date:	May-2020
Publisher:	IISERM
Abstract:	As we know that Azobenzene (AB) derivatives are widely used as photo switchable systems for various applications. Aromatic azobenzenes are excellent candidates as molecular switches, their capability to undergo fast, efficient, and reversible photo-isomerization (trans□cis). Our study focuses on synthesis of symmetrically as well as unsymmetrically halogen substituted AB derivatives with the focus on the kinetics of spontaneous cis- to trans- isomerization in the presence of visible light. A library of halogen-substituted azobenzenes (ABs) have been synthesized and structurally characterized by single crystal X-ray diffraction technique and various other spectroscopic technique like IR, NMR, PXRD, DSC after that their solid-state interactions has been studied. Halogenated azobenzenes studies herein display fast photo switching properties. Kinetics of cis- □ trans- isomerization has been studied using UV-VIS spectroscopy and the rate constant for this transformation were determined. Theoretical studies like Intrinsic Reaction Coordinate (IRC) was followed to establish the transformation TS to trans- and TS to cis- isomers. The optimizations of the trans-, cis- isomers and the probable transition states were conducted using DFT/B3LYP level of theory and 6-311++G(d,p) as basis set. The effect of the solvents (DMSO) were modelled with the polarizable continuum model (PCM). Optimization of probable conformers of the cis- isomer and the corresponding transition state (TS) were carried out to determine the energy of activation. The Time- Dependent Density Functional Theory (TD-DFT) calculations were also performed to gain insight into the photo-isomerization by comparing the wavelength and the nature of transitions observed in the experimental UV-Vis spectra. Our results indicate that the fluorinated compounds display better kinetic stability of the cis- isomer compared to the corresponding chloro and bromo analogues.
URI:	http://hdl.handle.net/123456789/3681
Appears in Collections:	MS-14

Files in This Item:

File	Size	Format	
MS14055_Manish.pdf	9.45 MB	Adobe PDF	View/Open

Show full item record