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| Title: | Understanding of the Kinetic Stability of cis- Isomer of Azobenzenes through Kinetic and Computational Studies |
| Authors: | Das, Dhiraj (/jspui/browse?type=author&value=Das%2C+Dhiraj)<br>Yadav, Manish K. (/jspui/browse?type=author&value=Yadav%2C+Manish+K.)<br>Singla, L. (/jspui/browse?type=author&value=Singla%2C+L.)<br>Karanam, M. (/jspui/browse?type=author&value=Karanam%2C+M.)<br>Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.) |
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| Abstract: | A library of halogen-substituted azobenzenes (ABs) have been synthesized and structurally characterized by single crystal X-ray diffraction technique. Azobenzenes studied 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. 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. Our results indicate that the fluorinated compounds display better kinetic stability of the cis- isomer compared to the corresponding chloro and bromo analogues. |
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