Synthesis, photoswitching and computational studies of multiple azobenzene connected photochromic system

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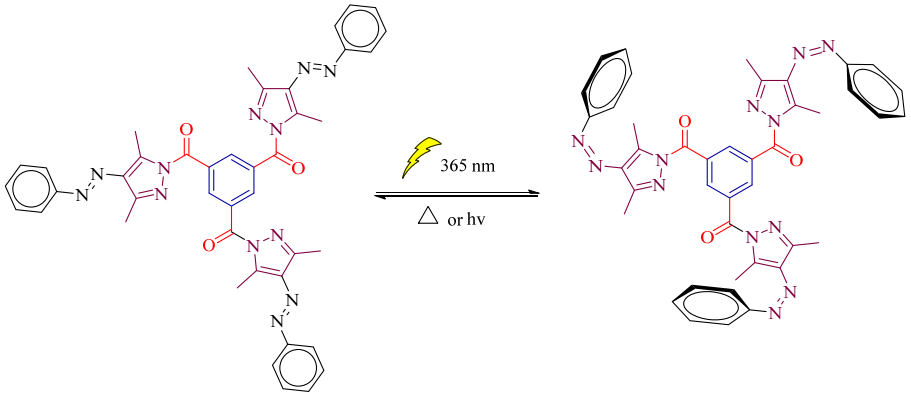
Abstract:
Photochromic molecules like azobenzenes are robust photoswitchable molecules that can switch reversibly between the thermodynamically more stable *trans* and less stable *cis* isomers.[1] Photoswitching often accompanies change in the molecular properties such as molecular structure, dipole moment etc. In azobenzenes, the forward switching (*E* to *Z*) is light induced, whereas the reverse isomerization can be induced by light or under thermal conditions. The light induced switching behaviour and thermal reverse isomerization kinetics largely depend on the substituents. The introduction of heterocycles in azobenzenes can be an alternate way to tune those properties and additional functions.[2]
Herein, we report a systematic investigation in developing a three step strategy on synthesis and studies of hetero azo-based photochromic compounds.[3] Our objective in this work is to connect multiple azobenzene units to a symmetric core moiety such as 1,3,5-substituted benzene through a linker, which can switch reversibly and efficiently.[4] After the synthesis of the target molecule, (**Scheme 1**) we tried to understand the *trans-cis* photoisomerization using UV-Vis and NMR spectroscopies. Apart from these, we also performed computational studies to understand the structural and thermochemistry aspects. Systematic design, synthesis, computational results, and photoswitching studies through spectroscopic studies will be presented through this contribution.



Scheme: Photoisomerization of benzenetriazopyrazole.

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