

heptafulvenes into tropones is determined, future reaction mechanisms to be assayed in our research will be famous name reactions whose mechanism still remain obscure.

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Density Functional Theory characterisation of azobenzene derivatives

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Since the year 1937, when Harley published his work [1] about *cis* isomerization of azobenzene, this photochemical phenomena became widely studied. The idea behind it is photoisomerization of azobenzene under irradiation when non-polar *trans*-azobenzene can be photoisomerized into the polar *cis*-azobenzene. Due to relatively simple molecular structure and unique characteristics, azobenzene and its derivatives were investigated in different studies as photoswitchable substances, as dyes, as surface with controlable wettability.

The physical and chemical properties of azobenzene derivative depend on molecular groups used as ring substituents and stability of the configurations. In the present study, we have analyzed the effect of structural diversity on electronic and molecular properties. We have selected 10 derivatives with azobenzene as a parent compound. The first group is electron donating substituents: CH₃, C₆H₅, NH₂, SO₂-NH₂, N-(CH₃)₂. The second one is an electron acceptor substituents: OH, NO₂, CH₂-CH₂-OH. The last group contains derivatives with an electron-acceptor at the para-position and an electron-donor at the other para-position of another phenyl ring.

We performed density functional calculations in the GAUSSIAN03 [2] program with B3LYP functional and 6-31++G(d,p) basis set. For each molecule we have examined *trans* and *cis* forms and all possible configurations concerning spatial position of functional group. More details could be found in our previous works [3-5].

The planar *trans* structure has been obtained for all considered molecules. This configuration were found to be more stable than *cis*. The relative difference in the dipole moment between the *trans* and *cis* configurations was found to be lower than for azobenzene for all considered molecules except for molecule with N-(CH₃)₂ and NH₂ groups, for which the difference was obtained equal to 4.7 Debye. For this molecule, the largest polarizabilities have been obtained as well. The highest reactivities were found for this molecule and for molecule with NH₂ and NO₂ groups.

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