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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 [2]. Moreover, azobenzene derivatives have vivid colors, which caused them to be used as dyes. Due to the formation of polar *cis*-isomer, the contact angle can be significantly decreased. This feature can be used to control wettability of surface [2]. Furthermore, changes in dipole moment cause changes in the surface potential, which can be used to create a surface with the controlled motion and net mass transport [2].

The physical and chemical properties of azobenzene derivative depend on both different molecular groups used as ring substituents and stability of the *trans/cis* configurations. In the present study, we have analyzed the effect of structural diversity on electronic properties. We have selected 10 molecules with different types of activating groups with azobenzene as a parent compound:

1. Azobenzene's derivatives of the type of aminoazobenzene, i.e., azobenzene substituted with an electron donating groups CH₃, C₆H₅, NH₂, SO₂-NH₂, N-(CH₃)₂;
2. Azobenzene's derivatives substituted with an electron acceptor group OH, NO₂, CH₂-CH₂-OH;
3. Azobenzene's derivatives of the pseudostilbene type, i.e., substituted with an electron acceptor at the *para*-position of a phenyl ring and an electron-donating group at the other *para*-position of another phenyl ring. This type is also known as push-pull azobenzene.

For this purpose we performed density functional calculations in the GAUSSIAN03 [3] program. All properties have been obtained using the B3LYP functional and 6-31++G(d,p) basis set, which were selected as the most appropriate in terms of time, accuracy, and cost of computer resources for the structural, electronic, molecular and vibrational properties determination [4]. 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 [4-6].

The planar *trans* structure has been obtained for all considered molecules. On both configurations, an asymmetry in structural parameters was obtained for all molecules. The *trans* configurations 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. Concerning molecular properties, the highest reactivities were also found for this molecule and for the molecule with NH₂ and NO₂ groups as well.

1. Hartley G. Nature, 1937, **140**: 281.
2. Halabieh El. et al. Pure Appl.Chem., 2004, **76**: 14453.
3. Frisch, M. J., et al. "Gaussian 03, revision c. 02; Gaussian." Inc., Wallingford, CT, 2004, **4**.
4. Minisini B. et al. J.Mol.Model., 2007, **13**: 1227-1235.
5. Piyanzina I. et al. J.Mol.Model., 2015, **21**: 34.
6. Minisini B. et al. J.Str.Chem., 2014, **5**: 843-851.

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The program of the Second Kazan Summer School on Chemoinformatics includes 12 plenary lectures, 7 key-note lectures, 4 oral reports, 4 tutorials and 23 presentations.

OFFICIAL LANGUAGE

The official School language is English. No translation will be provided.

OFFICE OF THE ORGANIZING COMMITTEE

The office of the organizing committee is located at A.M. Butlerov Chemical Institute building, Auditorium No. 218. Participants will be able to use telephonic Internet and printing facilities there.

