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Relationship study of structurally – mechanical, quantum and structurally – chemistry characteristics of liquid aromatic hydrocarbons

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Abstract

The described approach allows to calculate the dynamic viscosity of liquid aromatic hydrocarbons by quantum and molecular parameters. This investigation is concerned with the benzene, naphthalene and substituted aromatic hydrocarbons. Based on Arrhenius-Frencel-Eyring equation, calculations of viscous flow activation energy and logarithms of pre-exponential factor have been performed. The value of the activation energy of viscous flow is an indirect characterization intermolecular interactions of the particles. Discovered kinetic compensation effect which is due to depedence logarithmic values of the pre-exponential constant in the Arrhenius equation on effective activation energy ($R^2 = 0.82$). In this paper, calculated topological indices Wiener, Randic and Harary for aromatic hydrocarbons. Topological index converts a chemical structure into a single number, useful in QSPR/QSAR studies. Assuming that the energy of the molecules of the same substance are equal, you can assume that equal and their energy (ionization potentials). The calculation of ionization potentials we used the method of density functional theory B3LYP/6-31G(d) level with full optimization of molecular geometry. Our theoretical values closely agreed with experimental values obtained by photoionization. Proposed dependence, in which the depends on two parameters (potential ionization & topological index). Dependence corresponds to the basic and common operation of the QAPR protocol. Furthermore, the method discussed here can also be used to analyse other experimental designs in which the size of the main sources of data variability are known. The calculated activation entropy of viscous flow. The results obtained with the simulations agree well with the experimental ones.

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