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Prediction of octane numbers of substituted alkanes according to the topological characteristics of the molecules

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Abstract

There may occur a special mode of combustion of the fuel-air mixture called detonation, when using motor fuel with a low octane rating.

Methods of mathematical modeling are currently used to quickly determine octane numbers without using of expensive equipment. A nonlinear multidimensional QSPR regression model is proposed to predict the octane number of normal and substituted alkanes-gasoline components.

The model associates octane numbers with a set of descriptors (topological characteristics of molecular graphs): the Randic index, the Wiener index, and the functions of the eigenvalues of the topological matrix of the molecule, reflecting the main structural and chemical factors, such as branching, the length of the carbon structure and the energy parameters of the molecules, for example perturbation of Hückel spectrum of molecules, as well as affecting octane numbers.

The substituted alkanes were used as research objects. A studied sample included 36 hydrocarbons from the homolologus serious of substituted alkanes. The proposed model adequately describes the octane number of alkanes. The coefficient of determination of the model is 0.972. The model was tested on 19 substances which were not included in the base series. The average, absolute and relative error for the test sample of octane numbers were 1.5 units and 2.7% respectively.

The model is applicable for engineering and scientific forecasts of octane numbers of various alkanes in motor fuel.

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