

## Influence of molecules topology on the benzotriazole derivatives sorption on the hypercarbe and hypercrosslinked polystyrene surfaces

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### Abstract

Benzotriazole derivatives chromatographic retention under conditions of high performance liquid chromatography on hypercrosslinked polystyrene and porous graphitized carbon (hypercarb) surface from the water – acetonitrile solution were studied. It was suggested a possible role of topology sorbate molecules in their sorption on the flat surface of these sorbents. To determine the effect of topology on chromatographic retention values the topological indices (connectivity indices, or Randić indices and indices of Wiener) for the 16 benzotriazole derivatives were calculated. The Wiener index calculation performed in different ways – according to known equations and using real bond lengths in the molecule and a computer program. We analyzed the patterns of change in the index with the change of topological structure of molecules benzotriazole derivatives. A decrease in the values of the connectivity indices with the growth of their order, caused by geometrical and topological removal of atoms from each other with increasing order of relatedness was demonstrated. It was found that connectivity indices of isomeric compounds are singular, but with the growth of the order of topological index degeneracy is lifted, increasing thus discriminating ability of connectivity indices to the benzotriazole derivatives isomers.

Physicochemical characteristics of these compounds, determining retention under reverse phase high performance liquid chromatography (such as polarizability, volume, surface area, dipole moment) were received by quantum chemical calculations. The interrelation between the physical and chemical parameters and topological indices were investigated. It is shown a simultaneous change in the topological indices and dimensional characteristics of molecules – the volume and surface area. Correlations between the topological indices and retention factors values of the compounds were studied on hypercrosslinked polystyrene and hypercarb. The correlation coefficients of the corresponding equations and established the relationship between the physical and chemical properties, topological and chromatographic characteristics of some derivatives of benzotriazole were analysed. It is shown that the correlation level is determined by the order of connectivity indices used, the type and composition of the parameter correlated and eluent used in the chromatographic system.