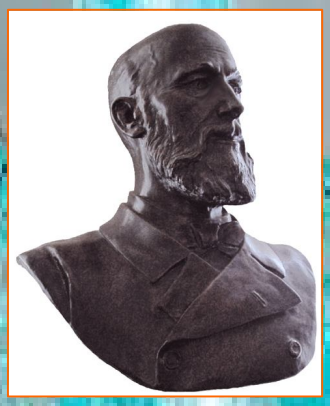
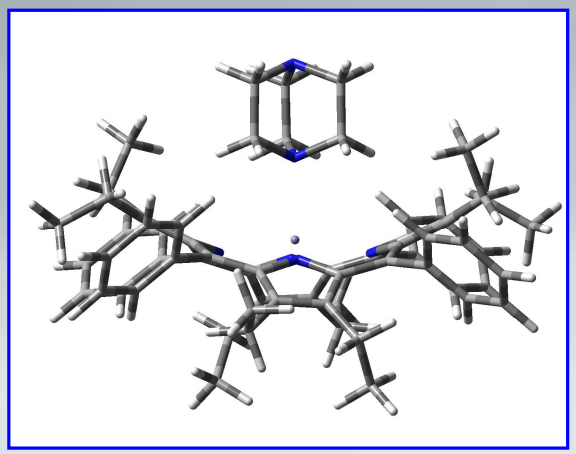
Butlerov Communications

No.9, Vol.47. 2016



ISSN 2074-0948



ISSN 2074-0212

National Edition in Russian:

Бутлеровские сообщения

The Innovative Publishing House "Butlerov Heritage" Ltd.
is Legal founder of the journal "Butlerov Communications".

The journal is the official publishing organ of the Butlerov Science Foundation (BSF) which also delegated the right to legally represent the interests of the journal.

The institute co-sponsorship exist for the journal and in the framework of which the treaty or agreement on scientific and technical, innovative and scientific publishing cooperation can be signed with co-founder.

Chief Editor: Prof. Yakov D. Samuilov
Executive Editor: Alexandre I. Kourdioukov

Editorial address:
Bondarenko St., 33-44. Kazan, 420066. Republic of Tatarstan. Russia.

Contact Information:
Phone: +7 917 891 2622

E-mail: butlerov@mail.ru or journal.bc@gmail.ru
Internet: http://butlerov.com/

The volume printed December 5, 2016

Full Paper _____ *Thematic Section:* Physicochemical Research.
Reference Object Identifier – ROI: jbc-02/16-47-9-58 *Subsection:* Chromatography.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Submitted on December 02, 2016.

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

© Sara Ali Kyzy Djabieva, **Christine A. Muzdina**,
Svetlana V. Kurbatova,*+ and **Elena A. Kolosova**
Physical Chemistry and Chromatography Division. Samara National Research University Named after Academician S.P. Korolev. Academic Pavlov St., 1. Samara, 443011. Russia.
Phone: +7 (846) 334-54-32. E-mail: curbatsv@gmail.com

*Supervising author; +Corresponding author
Keywords: topology, topological indices, indices Randič, benzotriazoles, correlation, retention factor hypercrosslinked polystyrene, a porous graphitized carbon.

Abstract

Benzotriazole derivatives chromatographic retention under conditions of high performance liquid chromatography on hypercrosslinked polystyrene and porous graphitized carbon (hypercarbia) surface from the water – acetonitrшle 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 Randič 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 hypercarbia. 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.

Introduction

Investigation of the organic compounds structure on a topological level is a promising direction of development of modern theoretical chemistry, as the mathematical modeling of chemical structures of the compounds allows them to predict the physical and chemical properties, biological activity, the value of chromatographic retention [1]. Topological indices (TI), and in particular Randič indices (or connectivity index – CI) are widespread as a correlated parameters for solving problems "structure – property" and "structure – retention." The main factor in the study of correlations "structure – property" is the choice of the molecular descriptors characterizing structural, topological, electronic, quantum, geometry and other parameters. Thus, quantum descriptors contain information about the charge of the atom, the dipole moment, the formation energy while other structural indices take into account only part of the molecule, but does not characterize the geometry and the electronic structure, which is determined by the order of atoms binding and the nature of

relationships, so often used topological indices taking into account the size and the degree of branching molecules [2-3].

Currently, for the construction of the correlation structure – property – the biological activity the indices of Wiener, Schultz, Shannon, Randič representing the encoded information on the size of the molecule, its cyclical nature, the presence or absence of hetero atoms in the structure [1]. It is possible to use two-dimensional or three-dimensional indices. Two-dimensional codes tend to ignore the metric relations in the molecule (bond angles, internuclear distance). When three-dimensional topological indices are based on the distance between atoms. This fact leads to an increase in their ability to discriminate and distinguish not only structural, but also rotational isomers. However, when calculating the three-dimensional codes must take into account not only real bond lengths and angles, but also the most possible conformation of the molecule, the change in the bond lengths, depending on the nearest atomic environment, making it more difficult calculations, even for relatively simple molecules. Therefore, to describe the topological structure of the molecules two-dimensional codes are used more often.

The aim of this study was to establish the role of the molecules topology in a chromatographic retention of benzotriazole derivatives on the surface of hypercrosslinked polystyrene (HCPS) and a porous graphite carbon (hypercarb), used as sorbents in a reversed-phase HPLC condition.

Experimental part

The experimental procedure. Studies carried out on a liquid chromatograph with UV detector *VARIAN ProStar 325* and plunger pump *ProStrar 210*. Detection was at 254 nm. As sorbents used hypercrosslinked polystyrene (HCPS) (column size 150h 4.6 mm, the diameter of the sorbent particles 5 microns) and a porous graphitized carbon (column size 50 h3 mm, the diameter of the sorbent particles 5 microns). Elution is performed in isocratic mode, using as eluent acetonitrile-water mixture in a ratio of 1: 3, 2: 3, 1: 1 and 3: 1 by volume, the flow rate was 0.5 ml/min. Sorbates individual solutions were prepared by dissolving the samples in a suitable mobile phase; sample was injected at 40 ml. The mobile phase was degassed before analysis to install and filtered. Sorbates solutions were prepared by dissolving the dry individual substances. The column temperature was kept constant with an accuracy of ±0.2 K by using a solid-state thermostat. The assay was performed at room temperature. Prior to the experiment column was thermostated and was washed by eluent for 1.5 hours. Retention of substances characterized by the value of the retention factor k, calculated by the formula [4]:

$$k = \frac{t_R - t_M}{t_M},$$

where t_R – the retention time of the test substance, t_M – retention time nonsorbent component. Values retention factor of benzotriazole derivatives shown in table. 1.

Method of calculation. Calculation of connectivity index was carried out using well-known formulas [1]:

$${}^0\chi = \Sigma(\delta_i)^{-1/2}, \quad {}^1\chi = \Sigma(\delta_i \delta_j)^{-1/2}, \quad {}^2\chi = \Sigma(\delta_i \delta_j \delta_k)^{-1/2}, \quad {}^3\chi = \Sigma(\delta_i \delta_j \delta_k \delta_m)^{-1/2}, \quad \delta_i = z_i - h_i,$$

where z_i – the number of valence electrons in the atom i; h_i – the number of hydrogen atoms at atom i.

Connectivity indices of higher orders was calculated by the same formulas.

Wiener Index, based on a matrix of distances, defined as half the sum of the elements of the matrix of distances:

$$W = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} d_{ij},$$

where d_{ij} – the shortest distance between vertices i and j (off-diagonal elements of the distance matrix), N – vertices number of molecular graph.

The off-diagonal elements of the distance matrix for vertex- and edge-weighted (multi-) graphs calculated as:

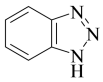
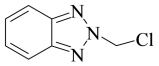
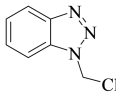
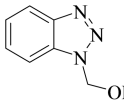
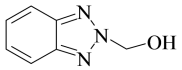
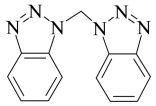
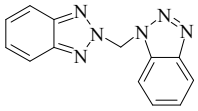
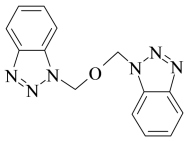
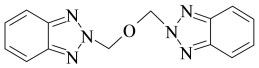
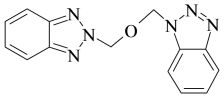
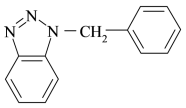
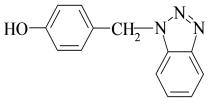
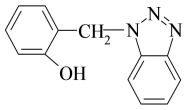
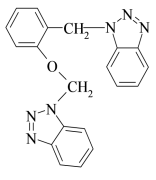
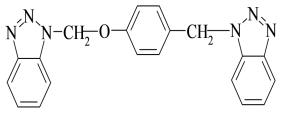
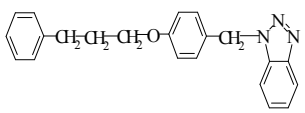
$$d_{ij} = \sum_r K_r,$$

where K_r – parameter characterizing the interaction and connection of atoms in the molecule, defined as:

$$K_r = \frac{1}{b_r}\frac{36}{Z_i Z_j},$$

where Z_i , Z_j – the number of electrons in the atoms i and j, of the connected link, b_r – the bond order characteristic.

Table 1. Retention factor of studied substances

No.	Formula	k retention factor for different ratios of acetonitrile – water						
		SCPS			PGC			
		2:3	1:1	3:1	1:3	2:3	1:1	3:1
1		3.53	2.96	1.61	4.86	1.90	1.09	0.82
2		32.29	14.41	4.41	24.28	8.55	4.40	1.60
3		34.57	16.15	4.56	25.24	8.43	4.55	1.56
4		4.73	3.04	1.63	5.43	1.94	1.33	0.82
5		4.60	3.04	1.62	5.41	2.04	1.27	0.85
6		43.69	19.31	4.29	100.15	22.42	9.13	3.22
7		86.60	21.91	5.09	-	19.44	9.73	3.26
8		55.37	23.89	5.07	111.13	21.24	9.65	3.32
9		56.48	21.37	5.68	87.19	21.76	9.59	3.30
10		65.18	20.64	5.14	81.19	21.49	9.31	3.01
11		-	16.57	2.19	-	-	11.15	0.75
12		25.02	12.18	3.75	82.48	16.32	5.87	2.69
13		34.53	13.74	4.83	-	31.91	10.87	4.33
14		-	80.23	19.83	-	25.16	12.08	23.56
15		-	67.89	27.69	-	-	10.41	29.54
16		-	9.57	4.00	-	16.95	8.06	2.84

The diagonal elements of the distances matrix for vertex- and edge-weighted (multi-) graphs calculated as:

$$d_{ij} = 1 - \frac{6}{Z_i},$$

where Z_i – the number of electrons (valence and inner-shell electrons) i atom [1].

For the substances containing heteroatoms, calculation was performed by the formula:

$$W = \sum_i d_{ii} + \frac{1}{2}\sum_{i>j} d_{ij},$$

Calculation of the modified Wiener Index (Wmodif.) was carried out using real bond lengths as the distance between atoms [5] and using the computer program Marvin (W_{progr}). The obtained values are given in table 2.

Table 2. Topological indices of the studied substances

No.	$^0\chi$	$^1\chi$	$^2\chi$	$^3\chi$	$^4\chi$	$^5\chi$	$W_{calc.}$	$W_{modif.}$	$W_{progr.}$
1	4.704	2.725	1.829	1.232	0.789	0.492	49.62	110.14	79
2	6.562	3.842	2.442	1.668	1.075	0.768	91.92	209.04	147
3	6.562	3.842	2.458	1.830	1.343	0.771	91.03	204.19	143
4	5.805	3.307	2.219	1.604	1.022	0.646	94.60	200.88	143
5	5.805	3.307	2.202	1.454	0.968	0.653	95.50	206.11	147
6	10.009	5.981	4.056	3.107	2.171	1.483	471.49	985.89	698
7	10.716	6.482	4.334	3.260	2.347	1.464	475.98	1010.51	718
8	11.125	6.559	4.618	3.267	2.490	1.456	711.19	1450.14	1026
9	11.125	6.559	4.584	3.069	2.416	1.393	721.96	1510.52	1074
10	11.125	6.559	4.601	3.168	2.434	1.430	704.96	1480.20	1050
11	8.744	5.255	3.364	2.256	1.659	1.178	317.95	630.95	445
12	9.115	5.389	3.902	2.688	1.930	1.273	384.82	760.65	537
13	9.115	5.395	3.771	2.593	1.888	1.102	371.48	734.60	517
14	14.434	8.655	5.793	4.173	2.737	1.527	1416.99	2793.85	1972
15	14.434	8.649	6.256	3.468	2.596	1.416	1563.21	3099.91	2192
16	14.084	8.923	6.316	3.657	3.019	1.910	1634.27	3035.87	2122

Calculation of the benzotriazole derivatives values of the dipole moment (μ), polarizability (α), the surface area (S), volume (V) and the energy of hydration (Egidr) was performed using Spartan program version 1.1.0 by semiempirical method AM1. Lipophilicity (lgP) was performed using Marvin version 6.3.0 software.

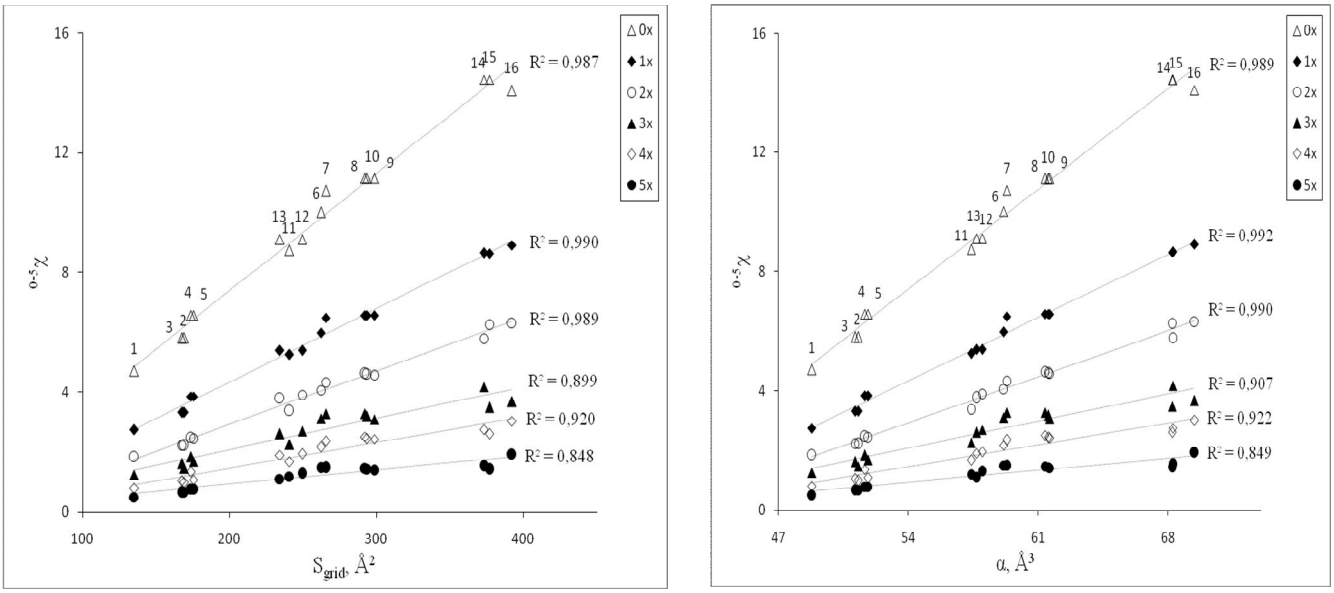
Results and discussion

The topological approach involves molecular structure study about the relationship and, as a consequence, the interaction of atoms in a molecule. This fact is the basis for most applications of graph theory for the study of molecular structure, which include, in particular, as a model theory of molecular orbitals by Huckel. Existence correlation between the physical and chemical properties chromatographic retention characteristics, in particulary, and the topological parameters of molecules is due, above all, the proportionality of the structural contribution of the interaction between the sorbate and sorbent in chromatographic system corresponding change in internal energy of the molecules of organic compounds with the variations in their structure. Simple linear dependence such as $I = a \cdot \chi + b$ cause from the same energy nature of the compared values.

The differences in the electronic and physical-chemical parameters of benzotriazole derivatives are due to their structural features associated with the presence of electron-donor nitrogen atoms and the presence of an extended conjugation system due to the interaction of nitrogen p -electrons with the π-electrons of the ring system. High delocalization energy of the system demonstrates distinct aromatic properties of nitrogen heterocycles. Thus, the main factors influencing the properties of these compounds are the nature of the substituents (electron acceptor or electron donor), its location (in the benzene ring, or a nitrogen atom), and the presence of one or two benzotriazole rings. These characteristics are largely determined by the topology of molecules. Table 2 shows a decrease in connectivity index values with increasing its order. This fact corresponds to literature data, of which it is known that with an increase in CI-order coherence values decrease monotonously due to less formal relatedness atoms per molecule. With the growth of CI-order atoms are geometrically and topologically more distant from each other [3]. In other words, a reduction $^n\chi$ actually reflects a decrease in the mutual influence of atoms in the molecule inside its topological space. For isomeric

compounds CI turns out and degenerate, but with increasing n degeneracy is lifted (mainly starting with n = 3), thereby increasing the discriminating ability of CI to the isomers of derivatives of benzotriazole.

Graphs in fig. 1 shows the relationship between the CI of different orders, surface area and molecular polarizability of benzotriazole derivatives.

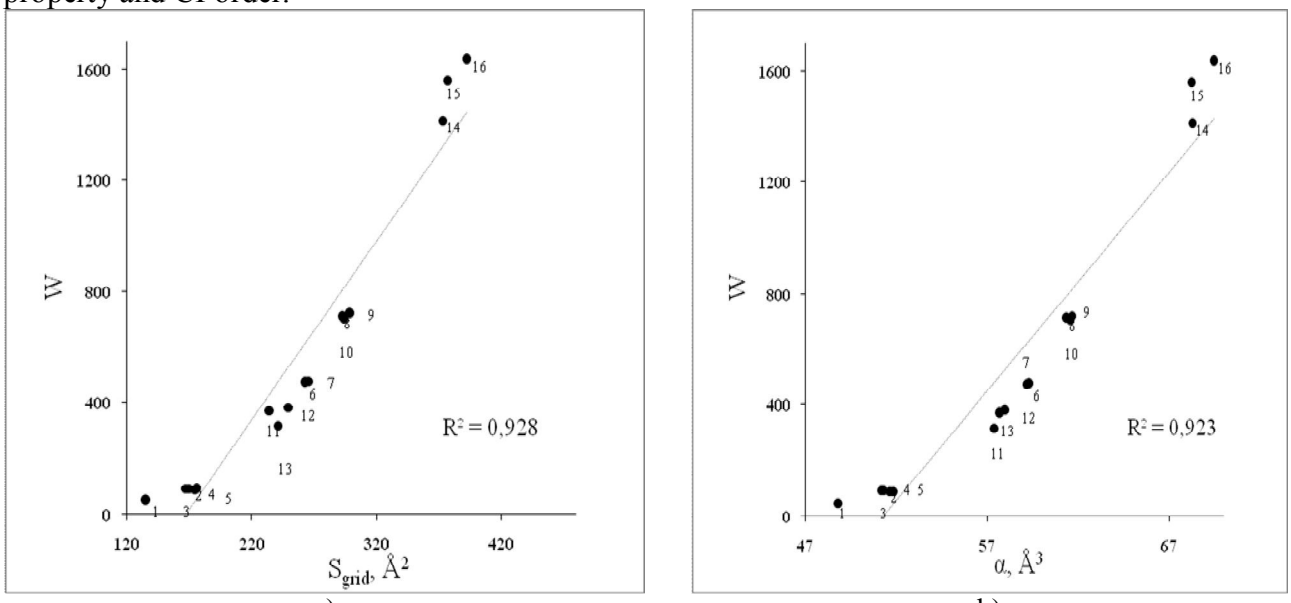


a) b)

Fig. 1. Correlation between $^{0-5}\chi$, surface area (a) and molecular polarizability (b) of benzotriazole derivatives

It should be noted that we have previously published data on the TI dependence of the electron and structural parameters for several smaller sample benzotriazole derivatives [6]. Substances characteristics were calculated in the HyperChem program version 7.0. In this study, as indicated in the experimental section, these characteristics we calculated using Spartan program and Marvin.

In general, as appears from the figure 1, the CI values with different orders vary symbatically to the physico-chemical parameters of molecules. In other words, the level of corresponding correlations is quite satisfactory, and the correlation coefficients are defined by correlated molecule property and CI order.



a) b)

Fig. 2. Correlation between W , surface area (a) and molecular polarizability (b)of benzotriazole derivatives

Wiener index (W) in the series studied nitrogen heterocycles vary monotonically, increasing with increasing molecular size. In this case, unlike the low-order CI, W are not degenerate for isomers. However, the correlation between the W and physico-chemical parameters of molecules is somewhat less strict (fig. 2).

For similar correlations, we used the W values, designed by well-known formulas [1]. A good level of correlation between the W values calculated by different methods described in the experimental section, shows the adequacy of all these types of TI (fig. 3).

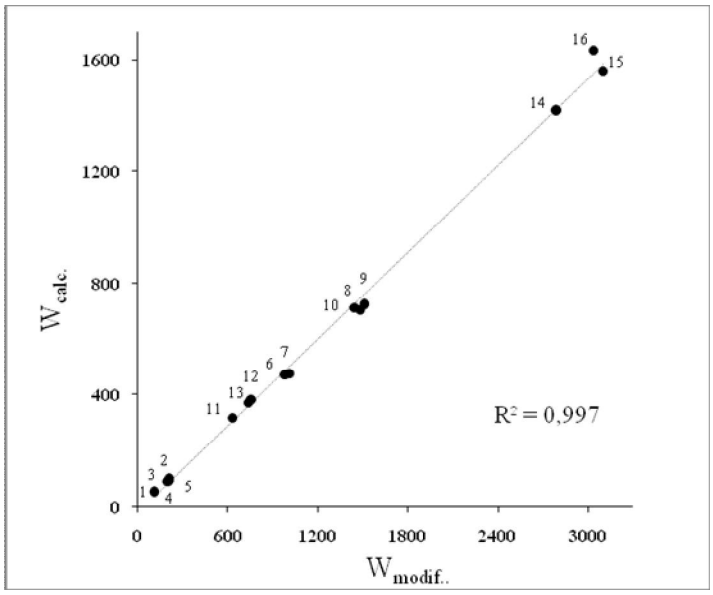
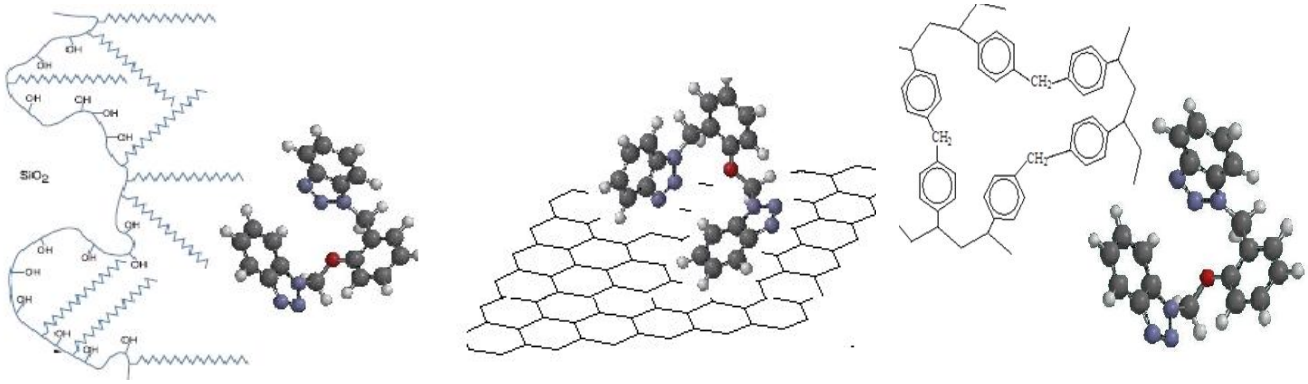


Fig. 3. The correlation between W, calculated in different ways

Features of the structure of molecules play an important role in the chromatographic retention, and the essential in the topology of molecules adsorbed on the flat surface of sorbents.

From the data represented in the table 1 follows that the retention factor values obtained by chromatography on various adsorbents, are significantly different. This fact is due to the specific interactions contribution of HCPS and carbon sorbent surface to the retention of the benzotriazole derivatives.

Thus, as noted above, topology play a decisive role on sorbate molecule adsorption on a flat surface when compared to the adsorption, for example on octadecylsilicagele. An illustration of manifestations of this kind of interactions can serve sorption of 1-[2-(1*H*-benzotriazol-1-ylmethoxy) benzyl]-1*H*-benzotriazol, value retention factor which (as well as some other substances) in the ODS, HCPS and hypercarb are significantly different (fig. 4).



k (ODS) = 5.79 k (hypercarb) = 12.08 k (HCPS) = 80.23

Fig. 4. 1-[2-(1*H*-benzotriazol-1-ylmethoxy)benzyl]-1*H*-benzotriazol retention on the ODS, HCPS and hypercarb

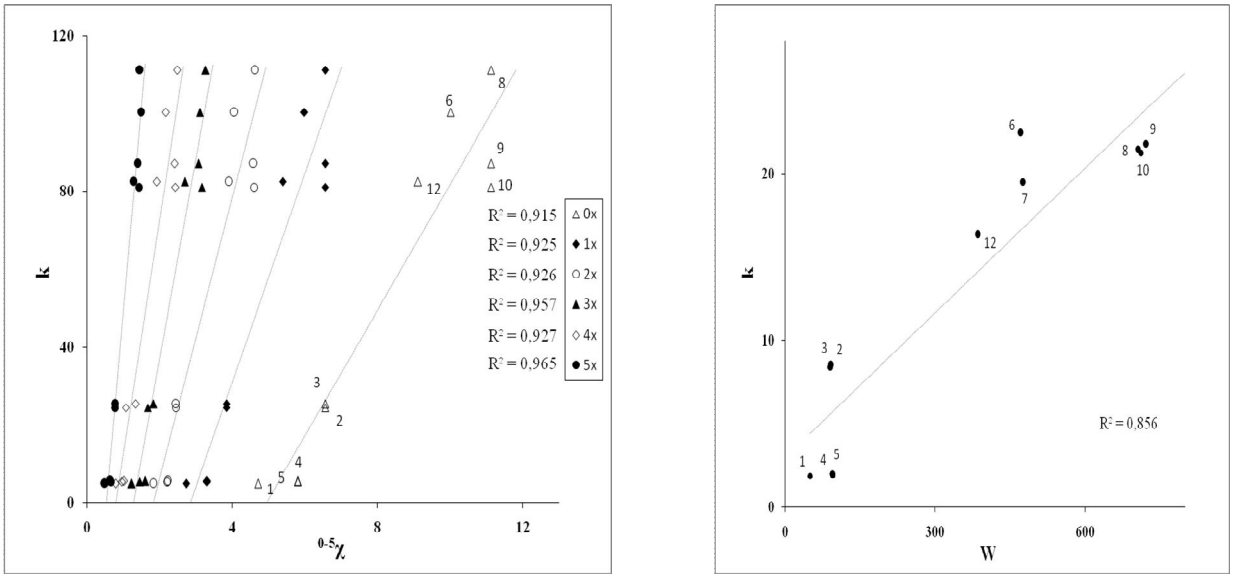
Fig. 5 shows graphs of the benzotriazole derivatives retention factor of topological indices, and table 4 – relevant parameters of correlation equations.

From these data it follows that the maximum value of the correlation coefficient R^2 corresponds to the relationship between TI and the retention factor in HCPS and hypercarb when the concentration of acetonitrile in the eluent is less than 50%. Increasing the concentration of the modifier greatly degrades the quality of the correlation.

Less than a strong correlation between TI and retention on HCPS sorbent is probably due to the fact that the decisive role in the sorption on hypercrosslinked polystyrene, as mentioned above, plays a significant contribution π-interactions of aromatic systems sorbate molecules and the adsorbent as compared to the contribution of the topology of molecules, while the absence of such interactions on a flat surface enhances the effect of hypercarb topological factor. Similar dependences were obtained earlier for imidazole derivatives [7]. We can assume that in general topology plays an important role in the sorption-azotso holding heterocycles in a high performance liquid chromatography, even though the competitive impact of the polar eluent component that reduces retention.

Table 4. Correlation coefficients depending on the type k = aTI + b for sorption of benzotriazole derivatives at HCPS and hypercarb at different ratios of acetonitrile-water eluent

Correlated parameters		R^2	a	-b
k HCPS (eluent AN – water 2:3, vol.)	$^0\chi$	0.757	9.308	40.94
	$^1\chi$	0.775	15.4	38.95
	$^2\chi$	0.705	20.05	30.44
	$^3\chi$	0.747	28.38	30.51
	$^4\chi$	0.748	34.3	21.74
	$^5\chi$	0.708	56.89	23.72
	W	0.600	0.075	-10.75
k HCPS (eluent AN – water 1:1)	$^0\chi$	0.524	4.994	26.22
	$^1\chi$	0.487	7.662	22.1
	$^2\chi$	0.452	10.1	17.95
	$^3\chi$	0.468	16.75	22.8
	$^4\chi$	0.331	17.59	12.28
	$^5\chi$	0.206	24.32	7.147
	W	0.493	0.028	-5.232
k hypercarb (eluent AN – water 1:3)	$^0\chi$	0.915	16.2	80.04
	$^1\chi$	0.925	26.87	76.45
	$^2\chi$	0.926	36.1	66.08
	$^3\chi$	0.957	51.71	66.66
	$^4\chi$	0.927	60.45	47.85
	$^5\chi$	0.965	105.9	57.07
	W	0.835	0.135	-6.32
k hypercarb (eluent AN – water 2:3)	$^0\chi$	0.950	3.351	15
	$^1\chi$	0.956	5.497	14.03
	$^2\chi$	0.943	7.447	11.98
	$^3\chi$	0.953	10.29	11.43
	$^4\chi$	0.947	12.4	8178
	$^5\chi$	0.965	21.34	9.726
	W	0.856	0.028	-2.985
k hypercarb (eluent AN – water 1:1)	$^0\chi$	0.658	0.947	1.943
	$^1\chi$	0.639	1.529	1.333
	$^2\chi$	0.597	2.021	0.521
	$^3\chi$	0.703	3.572	2.082
	$^4\chi$	0.673	4.37	1.03
	$^5\chi$	0.644	7.484	1.464
	W	0.387	0.004	-4.866



а) б)

Fig. 5. Correlation between retention factor and TI (hypercarb sorbent; eluent AN – water 2:3)

Conclusions

1. The calculated and analyzed values of the five orders connectivity indices , and the Wiener indices for some derivatives of benzotriazole. It was shown, that connectivity index values decrease with an increasing in their order, caused by geometrical and topological removal of atoms from each other with increasing order of relatedness.

2. It was found that for the isomeric substances CI are singular, but with the growth of the TI order degeneracy is lifted, increasing thus discriminating ability CI for isomers benzotriazole derivatives.

3. Correlation relationship between topological indices, physical-chemistry characteristics and chromatographic retention of a benzotriazole derivative were obtained. 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.

References

[1] Chemical applications of topology and graph theory. Ed. By R. King. Trans. from English. *Moscow: World.* **1987**. 550p. (russian)
[2] V.I. Minkin, B.J. Simkin, R.M. Minyaev. The theory of molecular structure. *R.-D.: Phoenix*. **1997**. (russian)
[3] M.G. Vinogradova, Y.G. Papulov, V.M. Smolyakov, M.N. Saltykov. *Journal of Physical Chemistry*. **1996**. Vol.70. No.4. P.675-680. (russian)
[4] V.D. Shatz, O.V. Sahartova. High performance liquid chromatography. *Riga: Zinatne*. **1988**. 390p. (russian)
[5] Yu.A. Malysheva, Yu.G. Papulov, M.G. Vinogradova, A.B. Botov, V.M. Smolyakov. *Journal of Structural Chemistry.* **1998**. Vol.39. No.3. P.484-492. (russian)
[6] S.A. Dzhabieva, I.V. Skvortsova, S.V. Kurbatova, E.A. Kolosova, E.E. Finkelshtein. Topology of benzotriazole derivatives. *Butlerov Communications*. **2014**. Vol.38. No.6. P.8-14. ROI: jbc-02/14-38-6-8
[7] O.V. Kharitonova, A.S. Paramonova, S.V. Kurbatova. Acid-base equilibria in water-acetonitrile solutions of nitrogen-containing heterocycles. *Butlerov Communications.* **2009**. Vol.16. No.4. P.31-35. ROI: jbc-01/09-16-4-31 (russian)

In the English version of this article, *the Reference Object Identifier* – ROI: jbc-02/16-47-9-58

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

© **Sara Ali Kyzy Dzabieva**, **Christine A. Muzdina**,
Svetlana V. Kurbatova,*+ and **Elena A. Kolosova**
Physical Chemistry and Chromatography Division. Samara National Research University Named after Academician S.P. Korolev. Academic Pavlov St., 1. Samara, 443011. Russia.
Phone: +7 (846) 334-54-32. E-mail: curbatsv@gmail.com

*Supervising author; +Corresponding author

Keywords: topology, topological indices, indices Randič, benzotriazoles, correlation, retention factor hypercrosslinked polystyrene, a porous graphitized carbon.

Abstract

Benzotriazole derivatives chromatographic retention under conditions of high performance liquid chromatography on hypercrosslinked polystyrene and porous graphitized carbon (hypercarbia) surface from the water – acetonitrıle 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 Randič 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 ivestigated. 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 hypercarbia. 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.