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Adsorption of isomeric aryl- and diadamantane molecules on the surface of graphitized thermal carbon black

S. N. Yashkin,* D. A. Svetlov, and V. S. Sarkisova

Samara State Technical University,
244 ul. Molodogvardeiskaya, 443100 Samara, Russian Federation.
Fax: +7 (846) 278 4400. E-mail: physchem@samgtu.ru

The thermodynamic characteristics of adsorption of isomeric molecules of 1,1´-, 1,2´-, and 2,2´-diadamantanes, 1- and 2-phenyladamantanes, and 1-cyclohexyladamantane on the surface of graphitized thermal carbon black (GTC) were experimentally determined. The influence of the molecular structure of adsorbates on their adsorption on the basis face of graphite was considered. A high selectivity of the GTC surface for the gas chromatographic separation of mixtures of the considered structural isomers was shown.

Key words: aryladamantanes, diadamantanes, graphitized thermal carbon black, Henry´s constant, heat of adsorption, entropy of adsorption, model of dimeric ideal gas.

Interest in the chemistry of framework hydrocarbons is due to a great diversity of structures of these compounds, their unusual physicochemical properties, high biological activity, and an important role in the solution of various problems of theoretical chemistry.[1,2] Adamantane is the simplest representative of a large class of polyadamantane structures. The synthetic chemistry of these structure became especially popular in the recent years, because they are used for the directed synthesis and functional modification of precursors for various areas of nanoindustry.[3—5] Framework hydrocarbons are convenient building blocks, which possess the properties necessary for the production of nanomaterials. Among these properties are the high strength of the carbon framework and ease of formation of the three-dimensional structure; relative synthetic accessibility; the possibility of chemical modification to confer on framework a necessary set of physicochemical characteristics; the low toxicity; and stability at high pressures and temperatures and in diverse solvents.[1] However, in spite of the evident practical interest in these compounds, their physicochemical properties remain poorly studied.

This work continues a series of studies of a complex of adsorption chromatographic properties of adamantane and its derivatives on the surface of the graphite basis edge.[6—8] For example, the thermodynamic characteristics of adsorption (TCA) of molecules of alkyl-, halogen-, amino-, keto-, and hydroxy-substituted derivatives of adamantane and a large group of N-, O-, S-, and Se-containing heteroadamantanes on the surface of graphitized thermal carbon black (GTC) were determined under the conditions of equilibrium gas adsorption chromatography (GAC) in a wide temperature range. The theoretical calculations performed for the adsorption parameters made it possible to extend the molecular statistical theory of adsorption on uniform surfaces over the class of compounds of the framework structure. The specific features of adsorption of the molecular fragments of the adsorbate remote from the planar surface and the adsorption nonequilibrium of the bridging and nodal positions of the adamantane framework during the interaction with the graphite surface were taken into account.[6,8]

The studies of the adsorption behavior of the compounds containing several adamantane fragments on the GTC are of certain interest. However, there is only one published work in which the possibility was shown of using columns with this adsorbent for the efficient separation of a mixture of alkyl derivatives of 1,1´-diadamantane under the conditions of gas adsorption chromatography.[9] This mixture was also separated successfully on columns packed with molybdenum sulfide.[10] Mixtures of isomeric diadamantanes were separated at high temperatures on a capillary column with the dimethylsiloxane stationary liquid phase (SLP).[11] As compared to the classical SLP for GLC, the nonporous carbon adsorbents have a series of evident advantages for the separation of molecules of poorly volatile representative of the adamantane series (thermal stability, chemical inertness, structural selectivity, *etc.*).[12] The study of the adsorption properties of isomeric molecules of phenyladamantanes, which remain yet unseparated with the GTC under the gas chromatographic conditions, is also of interest.[13] The purpose of the present work is the experimental study of the adsorption of isomeric molecules of 1,1´- (**1**), 1,2´- (**2**), and 2,2´-diadamantanes (**3**), 1- and 2-phenyladamantanes (**4** and **5**, re-

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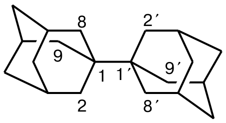
spectively), and 1-cyclohexyladamantane (**6**) on the GTC surface and the estimation of selectivity of the carbon black in the separation of the compounds considered.



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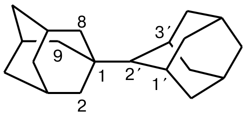

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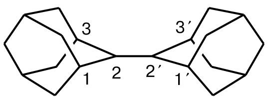

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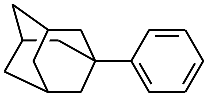

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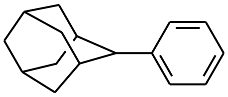

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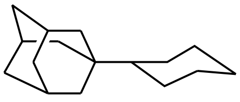

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Experimental

Some physicochemical characteristics of the studied compounds are given in Table 1.

Table 1. Normal melting (T_m) and boiling (T_b) points and the values of critical parameters (T_c and P_c) calculated by the Lidersen method**14** for molecules of studied compounds **1**—**6**

Compound	M /g mol^{-1}	T_m (see Ref. 2)	T_b (see Refs 2, 11)	T_c /bar	P_c
		K			
1	270.45	569	638.3	868.2	16.8
2	270.45	539—541	635.0	852.1	16.5
3	270.45	457—458	630.6	835.8	16.3
4	212.33	355	582.5	820.3	22.4
5	212.33	301—303	586.4	812.7	21.8
6	218.38	378	572.7	798.6	20.5

The TCA of molecules of isomeric diadamantanes, phenyladamantanes, and 1-cyclohexyladamantane were experimentally determined under the conditions of gas adsorption chromatography on a Kristallyuks-4000M instrument with a flame-ionization detector in the isothermal regime.

A glass micropacked column 0.25 m × 1.0 mm in size filled with the GTC (Carbopack C trade mark) treated with hydrogen with a diameter of carbon black particles of 60—80 mesh, a weight of 0.220 g, and a specific surface of 10 m^2 g^{-1} (Supelco) was used. Helium was used as a carrier gas, and methane served as a nonsorbed gas. The volume flow rate of the carrier gas ranged from 40 to 45 cm^3 min^{-1}. The high efficiency of the used micropacked column is confirmed by the values of the number of theoretical plates (N_i) determined for each of the studied isomers in particular (Table 2).

Dilute solutions of adsorbates in toluene were used in chromatographic measurements, which allowed us to perform experiments in the region of surface coverage close to zero. It is considered that only under these conditions the specific retention volume is equal to the adsorption equilibrium constant. This made it possible to obtain in the chromatograms symmetric peaks, whose retention times at a fixed temperature were independent of the amount of the adsorbate in the introduced sample (Fig. 1). The temperature of the column was varied in the range indicated for each adsorbate in Table 2 with an increment of 10 K, and the temperature of the injector was 20 K higher than that of the column. The inaccuracy of the experimental determination of

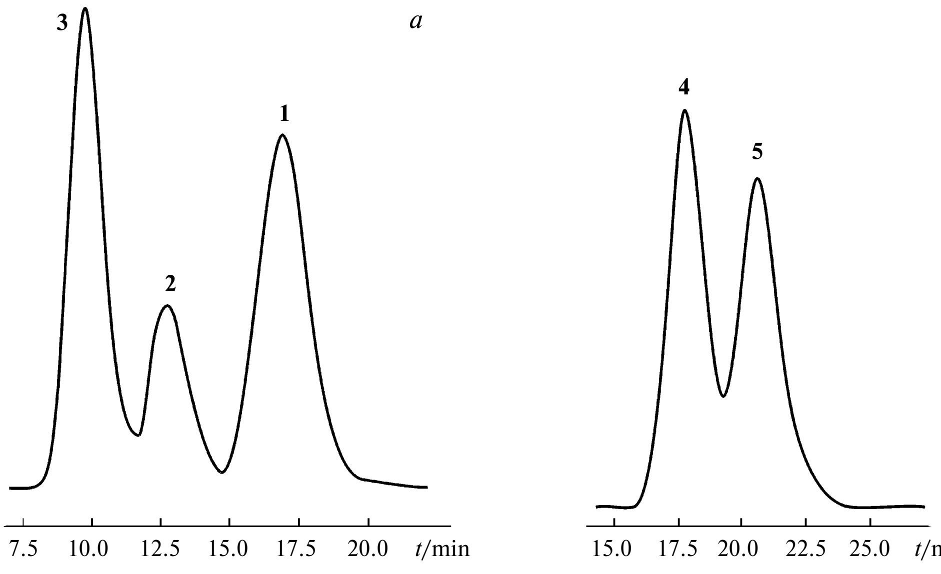

Fig. 1. Chromatograms showing separation of mixtures of the studied isomers on the micropacked column with Carbopack C: *a*, 1,1′- (**1**), 1,2′- (**2**), and 2,2′-diadamantanes (**3**) (T = 493 K; carrier gas consumption 45 cm^3 min^{-1}); *b*, 1- (**4**) and 2-phenyladamantanes (**5**) (T = 453 K; carrier gas consumption 40 cm^3 min^{-1}).

Table 2. Experimental and calculated values of TCA and retention parameters on the surface of Carbopack C and SLP SE-30 (see Refs 11 and 15) for molecules of the studied compounds

Adsorbate	ΔT/K	$K_{1,C}$/cm^3 m^{-2}		I_i^T		H_i^{sorb}		N_i^a (T_{av}/K)	$\bar{q}_{dif,1}$ /kJ mol^{-1}		$-\Delta(S°_{1,c})^s$ /J mol^{-1} K^{-1}	
		T_{av}^b	473 K	I^c	II^d	I^c	II^d		Experiment	Calculation^e	Experiment	Calculation^f
1	453—543	226.78	529.62	1373^g	2266^g	−627	266	235	71.6	94.5	107.0	114.4
2	453—543	160.05	395.08	1340^g	2236^g	−660	236	227	71.0	93.6	108.8	114.4
3	453—543	124.42	299.20	1308^g	2200^g	−692	200	219	68.8	92.3	106.3	114.4
4	423—483	247.24	120.17	1211^h	1771^h	−389	171	306	66.2	77.3	108.5	113.0
5	423—483	277.54	128.10	1221^h	1796^h	−379	196	297	69.9	77.6	115.7	113.0
6	423—483	222.44	104.11	1200^h	—	−400	—	325	66.6	78.7	110.4	113.1

[a] The number of theoretical plates for the specific substance: $N_i = 5.545(t_R/\tau_{0.5})^2$, where $\tau_{0.5}$ is the peak width at the half-height expressed in time units (min).

[b] T_{av} is the middle of the studied temperature range (K).

[c] Data for Carbopack C.

[d] Data for the SLP SE-30.

[e] Calculated by the formula[16] $\bar{q}_{dif,1} = 0.446(T_c/P_c^{0.5})$.

[f] Calculated by the Lopatkin formula[17]: $-\Delta(S°_{1,c})^s = R\ln(MT_{av})^{0.5} + 56.95 + R$, where $R = 8.314$ J mol^{-1} K^{-1}.

[g] $T = 483$ K.

[h] $T = 453$ K.

$V_{A,1}$ did not exceed 4%. The experimental values of the adsorption equilibrium constants (Henry's constants, $K_{1,C}$ (cm^3 m^{-2})), molar differential heats $\bar{q}_{dif,1}$ (kJ mol^{-1}), and changes in the entropies of adsorption $\Delta(\bar{S}°_{1,c})^s$ (J mol^{-1} K^{-1}), and the logarithmic retention indices (I_i^T) were determined on the basis of the primary chromatographic data using the standard procedure.[7—9] The plots obtained in the work for the dependences of $\ln K_{1,C}$ on $1/T$ are presented in Fig. 2. The numerical values of the homomorphism factors (H_i^{sorb}) were calculated from the expression [9]

$$H_i^{sorb} = I_i^{sorb} - I_{n\text{-alkane}}^{sorb}, \quad (1)$$

where I_i^{sorb} is the logarithmic retention index of the hydrocarbon under study, and $I_{n\text{-alkane}}^{sorb}$ is the logarithmic retention index of reference *n*-alkane having the same number of carbon atoms as the hydrocarbon under study.

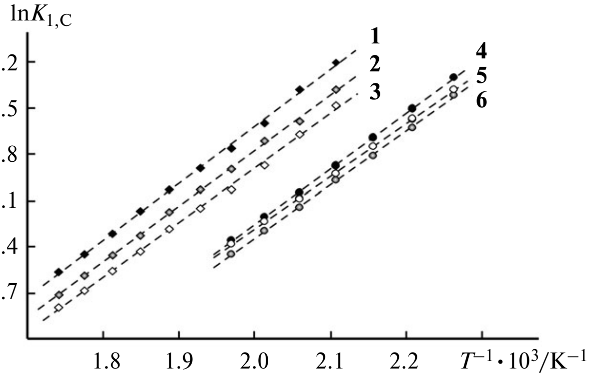

Fig. 2. Plots of $\ln K_{1,C}$ *vs* $1/T$ for the adsorption of molecules of isomeric diamantyls **1**—**3**, phenyladamantanes **4** and **5**, and 1-cyclohexyladamantane (**6**) on the Carbopack C surface.

The samples of the studied compounds were synthesized at the Chair of Technology of Organic and Petrochemical Synthesis at the Samara State Technical University. The procedures of the synthesis and identification of the synthesized compounds have previously been studied in detail.[11,15]

Results and Discussion

The data presented in Table 2 show that the values of Henry's constants and logarithmic retention indices for the series of the considered diadamantanes decrease in the order 1,1′-> 1,2′- > 2,2′-isomer. The differences in values of the free adsorption energy ($\delta(\Delta(\bar{F}°_{1,C})^s = -RT\ln(K_{1,C,i}/K_{1,C,j})$) at $T_{av} = 498$ K for the successively eluted 1,1′-/1,2′- and 1,2′-/2,2′-isomers are 1.443 and 1.043 kJ mol^{-1}, respectively, which is sufficient for their almost complete separation on the column packed with the GTC used in the work (see Fig. 1, *a*). Unlike diadamantanes, isomeric monophenyladamantanes exhibit an opposite behavior: the 1-isomer is eluted from the column with the GTC before the 2-isomer and the corresponding value of $\delta(\Delta(\bar{F}°_{1,C})^s$ at $T_{av} = 453$ K is only 0.436 kJ mol^{-1}. As a result, the degree of separation of isomeric phenyladamantanes (see Fig. 1, *b*) is lower than that of diadamantanes, which is also indicated by the close value of the TCA of phenyladamantanes (see Table 2). A 1-cyclohexyladamantane molecule is characterized by the lowest value of $K_{1,C}$ in the series of the compounds considered. It follows from the plots of $\ln K_{1,C}$ *vs* $1/T$ presented in Fig. 2 that the relative order of elution of the studied compounds from the column packed with the GTC remains unchanged in the whole temperature range considered. A comparison of the values of retention indices I_i^{T} on the GTC and the nonpolar SLP SE-30 (see Refs 11 and 15) (capillary column 50 m × 2 mm) shows that the order of elution of the compounds also remains unchanged on going from the GAC to GLC. At the same time, the distinction in the sorption mechanism under the conditions of GAC and GLC can easily be monitored by the numerical values of homomorphism factors H_i^{sorb}: in the case of the GTC, $H_i^{\mathrm{GTC}} < 0$; *i.e.*, the adamantane derivatives are adsorbed more weakly than the corresponding *n*-alkanes with the same number of C atoms, which is characteristic of the adsorption mechanism of retention.**9** Indeed, in the case of adsorption on the planar GTC surface, cyclane molecules, unlike *n*-alkanes, cannot touch the adsorbent surface by all units because of the rigid carbon framework and, therefore, they are retained more weakly than *n*-alkanes with the same number of C atoms. However, for the SLP SE-30, on the contrary, $H_i^{\mathrm{SE\text{-}30}} > 0$; *i.e.*, the cyclanes considered are retained more strongly than the corresponding *n*-alkanes, which is characteristic of the distribution mechanism of sorption under the GLC conditions. This is confirmed by the published results**18,19** on the application of the theory of generalized charges for the description of interatomic forces and adsorption, which showed that many electrons of internal bonds in the sorbate stop to be screened due to the surrounding of a sorbate molecule by the units of the SLP macromolecule (absorption of a sorbate molecule by the SLP) and are involved into the intermolecular interaction. In addition, it was assumed**18** that the effect of immobilization of the cycles on the fragments of the SLP molecules is observed upon the dissolution of cyclic molecules in the SLP, which results in the enhancement of the intermolecular interactions in the system cyclic sorbate—SLP compared to acyclic molecules that are not involved in similar interactions during sorption. Therefore, under the conditions of distribution GLC, *n*-alkanes are retained more weakly than the corresponding cyclic hydrocarbons with the same number of C atoms.

In the series of the adsorbates studied, the values of $\bar{q}_{\mathrm{dif},1}$ change in the same sequence as the values of Henry´s constants. A comparison of the values of $\bar{q}_{\mathrm{dif},1}$ isomeric diadamantanes ($C_{20}H_{30}$) and adamantane ($C_{10}H_{16}$) ($\bar{q}_{\mathrm{dif},1}$ = 39 kJ mol^{-1})**20** shows that the contribution of the second adamantyl radical to the heat of adsorption is 6.4—9.2 kJ mol^{-1} lower than that from a molecule of unsubstituted adamantane. At the same time, a comparison of the values of $\bar{q}_{\mathrm{dif},1}$ for molecules of cyclohexane (29.3 kJ mol^{-1})**20** and dicyclohexyl (58.0 kJ mol^{-1})**21** suggests the equal contributions of two cyclohexane rings to the heat of adsorption of a dicyclohexyl molecule. Therefore, in the field of adsorption forces of the GTC, diadamantane molecules take such an equilibrium configuration that excludes a contact of the molecule with the surface through two cyclohexane rings. The scheme of the equilibrium orientations of molecules of dicyclohexyl and 1,1´-diadamantane during adsorption on the basis face of graphite is shown in Fig. 3. The equilibrium geometry of dicyclohexyl and 1,1´-diadamantane molecules in the state adsorbed on graphite agrees well with the known data on the structure of these compounds in the free state.**22,23** The results obtained clearly indicate a substantially smaller adsorption potential of the atoms that are far from the graphite-like surface in diadamantanes compared to the C and H atoms in cyclohexane and dicyclohexyl molecules. An addition proof for this assumption is given by the values of $\bar{q}_{\mathrm{dif},1}$ (theor.) (see Table 2) calculated from the critical parameters (T_c and P_c) for the adsorbate molecules. In the case of adsorption of molecules with the linear or planar structure, when all atoms that form the molecule contact with the planar graphite surface, there is a good agreement between the experimental and calculated values of $\bar{q}_{\mathrm{dif},1}$, which is valid for all cases of non-specific interaction of gases and vapors with various adsorbents.**16** However, for the adsorbates studied, the values of $\bar{q}_{\mathrm{dif},1}$ (theor.) are noticeably higher than $\bar{q}_{\mathrm{dif},1}$ (exp.). This is explained by the fact that the values of critical parameters used in the calculation of $\bar{q}_{\mathrm{dif},1}$ (theor.) take into account intermolecular interactions of the adsorbate in the gas phase volume, whereas the main contribution to $\bar{q}_{\mathrm{dif},1}$ (exp.) is made only by the atoms or atomic groups that are situated in the direct vicinity to the adsorbent surface. The difference in the values of $\bar{q}_{\mathrm{dif},1}$ for isomeric phenyladamantane molecules can analogously be explained. It should be mentioned that the data obtained provide only qualitative con-

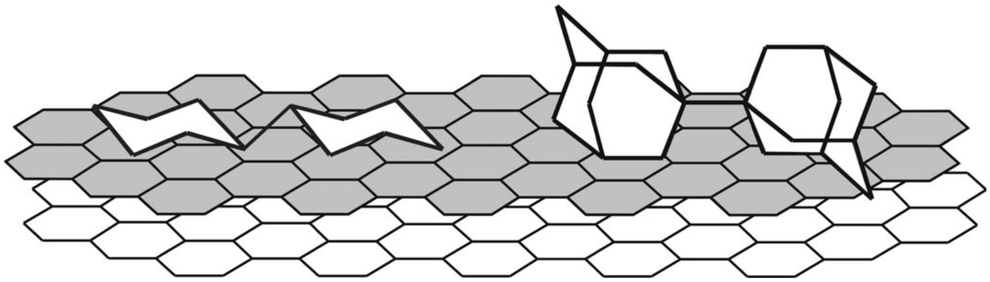

Fig. 3. Scheme of equilibrium orientations of dicyclohexyl and 1,1´-diadamantane molecules during adsorption on the basis face of graphite.

clusions about the configuration of the adsorbed diadamantane molecules on the GTC. The quantitative estimation of the contributions from various conformers to the values of TCA is possible using molecular statistical calculations. The latter for the compounds considered represent a particular independent task.

The comparative analysis of the values of $\Delta(\bar{S}^{\circ}_{1,c})^{s}$ (exp.) performed in the present work showed that for isomeric diamantane molecules the characteristics considered almost coincide. This indicates that molecules of these adsorbates lose the same number of the degrees of freedom on going from the gas phase to the adsorbed state. The values of $\Delta(\bar{S}^{\circ}_{1,c})^{s}$ for isomeric 1- and 2-phenyladamantanes differ to a greater extent (~7 entropy units). The increased values of $\Delta(\bar{S}^{\circ}_{1,c})^{s}$ and $\bar{q}_{\mathrm{dif},1}$ for 2-phenyladamantane compared to those of 1-phenyladamantane indicate a more favorable arrangement of the isomer molecule in position 2 on the planar GTC surface. The values of $\Delta(\bar{S}^{\circ}_{1,c})^{s}$ (theor.) were calculated (see Table 2) in terms of the model of dimeric ideal gas, according to which the molecule completely loses one translational degree of freedom upon adsorption. It is seen that $\Delta(\bar{S}^{\circ}_{1,c})^{s}$ (theor.) > > $\Delta(\bar{S}^{\circ}_{1,c})^{s}$ (exp.) in all cases, except for the 2-phenyladamantane molecule, and the difference in the values of $\Delta(\bar{S}^{\circ}_{1,c})^{s}$ does not exceed 8 entropy units. The latter is comparable with the inaccuracy of experimental determination of $\Delta(\bar{S}^{\circ}_{1,c})^{s}$ and can serve as a reliable argument in favor of the validity of the model of dimeric ideal gas as applied to the description of adsorption of isomeric aryl- and diadamantane on the GTC. In the case of other adamantane derivatives studied earlier in our group (in particular, methyladamantanes, halogenadamantanes, and others),[6,7] the model of dimeric ideal gas had considerable restrictions.

The correlation between the enthalpy ($\bar{q}_{\mathrm{dif},1}/RT$) and entropy ($(\Delta(\bar{S}^{\circ}_{1,})^{s} + R)/R$) contributions to the adsorption equilibrium constant on the GTC at T = 473 K is shown in Fig. 4 for compounds **1—6** considered in this work, as well as for molecules of dicyclohexyl[21] (**7**), phenylcyclohexane[21] (**8**), and diphenyl[21] (**9**). It is seen that the enthalpy factor makes the main contribution to adsorption of the considered compounds, and its role increases on going from isomeric phenyladamantanes to diadamantanes. It follows from this that the distinctions observed in the adsorption behavior of the considered compounds are mainly caused by the difference in the adsorption heats and are almost independent of the influence of the internal and external degrees of freedom on the mobility of adsorbate molecules in the field of adsorption forces of the GTC.

Thus, the values of TCA were determined for the first time for isomeric molecules of aryl- and diadamantanes on the GTC surface. It was concluded that this adsorbent is highly selective to representatives of the studied class of compounds. The applicability of the model of dimeric ideal gas to the description of adsorption of the compounds studied on the planar uniform surface was shown.

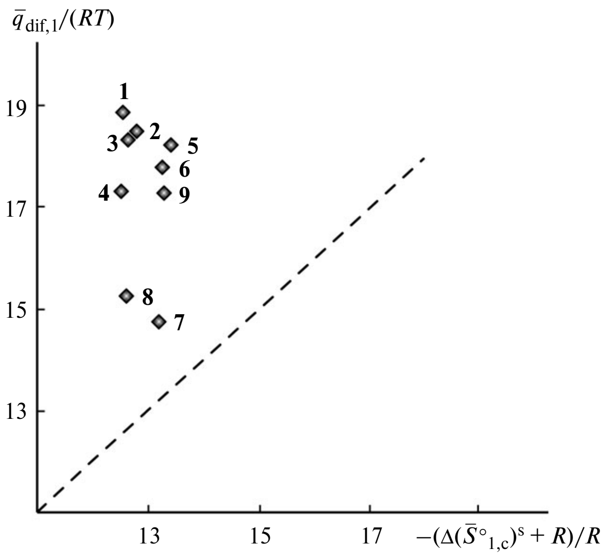

Fig. 4. Correlation between the enthalpy ($\bar{q}_{\mathrm{dif},1}/RT$) and entropy [$(\Delta(\bar{S}^{\circ}_{1,c})^{s} + R)/R$] contributions to the adsorption equilibrium constant on Carbopack C for molecules of isomeric diadamantanes **1—3**, phenyladamantanes **4** and **5**, 1-cyclohexyladamantane (**6**), dicyclohexyl[21] (**7**), phenylcyclohexane[21] (**8**), and diphenyl[21] (**9**) at T = 473 K (dashed line corresponds to the equality of the enthalpy and entropy contributions to the value of $K_{1,\mathrm{C}}$).

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