Thermodynamic parameters of adsorption of isomeric chloronaphthalenes on graphitized thermal carbon black

A. K. Buryak

Institute of Physical Chemistry, Russian Academy of Sciences,
31 Leninsky prosp., 117915 Moscow, Russian Federation.
Fax: +7 (095) 335 1778. E-mail: glazunov@lmm.phyche.msk.su

Henry's constants and the heats of adsorption of isomeric chloronaphthalenes on graphitized thermal carbon black were calculated by the semiempirical molecular statistical method. The calculated data were compared with experimental results. The best agreement was achieved when corrections for the interaction of the Cl atom with the C atom of the adjacent benzene ring and the presence of other Cl atoms in *ortho*-positions are introduced in calculations of the atom-atomic potential.

Key words: chloronaphthalenes, *ortho*-effect, semi-empirical molecular statistical calculations, heats of adsorption, Henry's constants.

The previously proposed[1] semi-empirical molecular statistical theory of adsorption is based on the atom-atomic approximation for the potential function of intermolecular adsorbate—adsorbent interaction on graphitized thermal carbon black (GTC).

$$\Phi = \sum_{A}\sum_{C(GTC)} \varphi_{A...C(GTC)} \qquad (1)$$

The potential function Φ is presented as the sum of atom-atomic potentials (AAP) of the intermolecular interaction of each atom (A) of the adsorbate molecule with each carbon atom (C) of the GTC adsorbent. The AAP of the interaction of the adsorbate atom with the adsorbent atom was chosen in the form of the Buckingham—Corner potential.

$$\varphi_{A...C(GTC)} = -C_1r^{-6} - C_2r^{-8} + B\exp(-qr) \qquad (2)$$

Henry's constant (K_1) is calculated on assumption of free motion along the mathematically uniform surface and harmonic oscillation perpendicular to the surface.

$$K_1 = \frac{1}{4\pi}\iint\left(\frac{2\pi kT}{\Phi''_z}\right)^{1/2}\exp\left(-\frac{\Phi_0}{kT}\right)\sin\Theta d\Theta d\psi \qquad (3)$$

Other thermodynamic parameters of adsorption (TPA) are calculated from Henry's constant. In particular, the differential molar change in the internal energy (heat of adsorption) is determined from the formula

$$\Delta U_1 = RT^2\mathrm{d}(\ln K_1)/\mathrm{d}T. \qquad (4)$$

In terms of this theory, the parameters of atom-atomic potential functions of the intermolecular adsorbate—adsorbent interaction (C_1, C_2, B) used for calculations of TPA are determined by approximate quantum-chemical formulas from the individual properties of the adsorbate and adsorbent. The AAP thus obtained for the interaction of atoms composing the adsorbate molecule with C atoms of graphite composing the adsorbent (GTC) are refined by comparison of the theoretically calculated and experimental values of Henry's constant for adsorption of one or several representatives of the class of molecules under study, so-called reference molecules. This refinement gives the correction factor β or simply the correction for AAP.

$$\varphi_{A...C(GTC)} = \beta\varphi^*_{A...C(GTC)} \qquad (5)$$

The initial and refined AAP differ only in the correction value, which results in an increase or decrease of numerical values of the parameters. To the present time, AAP for H and C atoms in different valence states for elements of the main subgroups of the VI and VII Groups[1—5] have been determined. The use of these potentials results in satisfactory agreement between experiment and calculation. At the same time, molecules whose TPA cannot be predicted with satisfactory accuracy are met more often as the experimental data accumulate and the scope of compounds under study extends. This concerns first molecules containing *ortho*-substituents, strained structural fragments, and heteroatoms in different valence states.[6] The inconsistency is explained by the differences in the parameters of AAP for atoms in the molecule under study and parameters refined by reference molecules. The differences in the AAP parameters are mainly due to a change in the nearest environment of the atom or its valent state, which appears as a change in its polarizability.

The chemical and physical properties and the geometric and electronic structures of chloronaphthalenes and chlorobenzenes are close.[7—9] It can be assumed that

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the adsorption properties of these compounds are also similar. Therefore, AAP for the interaction of the Cl atom with the C atom of graphite and corrections for the *ortho*-effect introduced in this potential for the description of adsorption of *ortho*-substituted chlorobenzenes[10,11] could describe TPA of chloronaphthalenes. At the same time, the difference in the properties of the isomers substituted in positions 1 and 2 is known for naphthalene.[7—9] This difference is usually explained by the fact that when a bulky substituent, for example, the Cl atom, is introduced in position 1, its van der Waals radius and that of the C atom of the adjacent aromatic ring overlap. In the case where the naphthalene molecule contains two substituents in positions 1 and 8, not only van der Waals radii of the substituent atoms and C atoms of adjacent atomatic rings, but also van der Waals radii of the substituents overlap.[12] This overlapping can change the polarizability and, correspondingly, AAP of these atoms, and AAP can change by a value different from that observed for overlapping of *ortho*-arranged Cl atoms in chlorobenzenes.

It has been shown[10,11] that only introduction of corrections for the parameters of AAP allows one to correctly predict K_1 values; therefore, corrections determined from the retention values of 1-chloro- and 1,8-dichloronaphthalenes should be used for the calculation of Henry's constants of chloronaphthalenes with different degrees of substitution. Chloronaphthalenes are the simplest model for studying this interaction in more complex molecules as well, for example, in polychlorinated diphenyls, dibenzothiophenes, and dibenzothioanthrenes. It is especially important to theoretically predict TPA for molecules of this class belonging to dangerous contaminators of the dioxine type, because the number of isomers among polychlorinated aromatic hydrocarbons is very high, and experimental studies are difficult. For example, mixed tetrabromochlorine-containing dibenzothiophenes have 496 isomers.

The purpose of this work is the experimental and theoretical study of the influence of the substituents in positions 1 and 8 on the adsorption of chloronaphthalenes.

Experimental

Gas-chromatographic experiments were carried out on an LKhM-80 chromatograph with a flame-ionization detector. A micropacking column with an inner diameter of 1 mm and a length of 70 cm was packed with graphitized thermal carbon black (GTC, Sterling-MT trade mark) with a specific surface of 7.6 $m^2 g^{-1}$ and a grain diameter of 0.14—0.18 mm. The K_1 values were found as described previously.[1,2,6] Heats of adsorption were determined as in the earlier works[1,10,11,13] from the temperature dependence of experimental K_1 values using the following equations:

$$\ln K_1 = A + B/T, \tag{6}$$

$$q_1 = RB, \tag{7}$$

where R is the gas constant.

At low (zero) coverages of the surface corresponding to the conditions of chromatographic experiment, K_1 is accepted as numerically equal to the specific retention volume (retention value).[1,2]

$$K_1 = V_{A,1} \tag{8}$$

Molecular statistical calculations were performed by the known procedure.[1,2] The published[10,11] AAP parameters and corrections for *ortho*- and *ortho-ortho*-effects were used. The geometric parameters of the molecules were either taken from the electronographic data[9] or determined by combination of the known parameters for other molecules of this group.

Results and Discussion

The experimental and calculated Henry's constants obtained in this work and published previously[13] are compared in Table 1. The experimental K_1 values given in Tables 1 and 2 were determined by the known proce-

Table 1. Experimental and calculated Henry's constants ($\ln K_1$) for adsorption of monochloronaphthalenes on GTC at 575 K obtained in previous[13] (I) and this work (II)

Molecule	$\ln(K_1/cm^3 m^{-2})$				
	I		II		
	experiment	calculation	experiment	calculation 1^a	calculation 2^b
1-Chloronaphthalene	2.084	1.608	1.35	1.51	1.46
2-Chloronaphthalene	2.243	1.672	1.44	1.56	1.56

[a] Calculation was performed using the known AAP.

[b] The correction for the *ortho*-interaction of the Cl atom with the C atom of the adjacent benzene ring was introduced into AAP.

Table 2. Experimental and calculated Henry's constants ($\ln K_1$) for adsorption of dichloronaphthalenes on GTC at 575 K obtained in previous[13] (I) and this work (II)

Molecule	$\ln(K_1/cm^3 m^{-2})$			
	I		II,	
	experiment	calculation	calculation 1^a	calculation 2^b
1,4-Dichloronaphthalene	3.432	2.847	2.69	2.61
1,3-Dichloronaphthalene	—	2.861	2.76	2.72
1,5-Dichloronaphthalene	3.404	2.870	2.71	2.63
1,6-Dichloronaphthalene	—	2.877	2.73	2.69
2,7-Dichloronaphthalene	3.666	2.928	2.79	2.79
1,7-Dichloronaphthalene	—	2.933	2.86	2.82
2,6-Dichloronaphthalene	—	2.985	2.80	2.80
2,3-Dichloronaphthalene	3.646	3.011	2.93	2.81
1,2-Dichloronaphthalene	3.575	3.043	2.99	2.79
1,8-Dichloronaphthalene	3.604	3.073	3.03	2.95 (2.79)[c]

[a] Calculation was performed using the known AAP.

[b] The corrections for *ortho*- and *ortho-ortho*-interactions of the Cl atoms were introduced into AAP.

[c] Calculation was performed taking into account the specific *ortho*-interaction of the Cl atoms in positions 1 and 8.

dure.[1,2,6] The published[13] experimental heats of adsorption were calculated from Eqs. (6) and (7), and molecular statistical calculations were performed[13] in terms of atom-atomic approximation using the semi-empirical molecular statistical theory of adsorption.[1,2,6] In calculations the authors[13] used AAP in the form of the Lennard-Jones potential, but did not refine its parameters and corrections for *ortho*-effects were not applied. It is seen in Table 1 that the differences in the previously determined[13] experimental K_1 values for the molecules studied and those in the present report are very high and exceed substantially the experimental error (~10%).[14] Other published data on retention of chloronaphthalenes on GTC are lacking; however, it is known that the order of elution of the isomers from a column with GTC corresponding to changing K_1 is independent of the absolute values of these constants.[10] This regularity was observed when experimental values for all isomers were obtained on the same column by the same author. Therefore, the order of elution of isomers from the column with GTC, *i.e.*, the sequence of changing Henry's constants (retention values), can be used to determine corrections for the *ortho*-arrangement of substituents. For quantitative determination of the correction, it is reasonablle to use the difference in the retention values of adjacent isomers, *i.e.*, the difference in K_1 values, for example, for 1- and 2-chloronaphthalenes. As follows from Table 1, the differences in K_1 values calculated for 1- and 2-chloronaphthalenes are 0.16 (see Ref. 13) or 0.09 (this work), whereas calculations without the correction to the *ortho*-interaction of the Cl and C atoms in positions 1 and 8 give 0.064 and 0.05, respectively. It can be assumed that the divergence between the experimental and calculated relative differences in retention of isomeric 1- and 2-chloronaphthalenes is due to the fact that the AAP used for calculations ignores the change in the parameters of this potential caused by the interaction of the Cl atom in position 1 with the C atom in position 8. A result coinciding with the experimental difference is obtained only when a correction is introduced into AAP. The considerable divergence of the experimental data for monochloronaphthalenes does not allow the refinement of the AAP parameters to be made using reference molecules by the known procedures.[1-5] Therefore, relative differences in retention were used in this work to determine corrections. The value of 0.09 obtained from the experimental Henry's constants that were determined in this work was used as the reference, because these values are close to the constants theoretically calculated previously[13] and in this work. The correction for AAP was determined by variation of the potential parameters for the interaction of the Cl atom with the C atom of graphite in such a manner that the differences in retention for 1- and 2-chloronaphthalenes coincided with the experimental value (0.09). The correction is 0.92, *i.e.*, the AAP parameters for the Cl atom in position 1 of the chloronaphthalene molecule is lower than those for the Cl atom in position 2. This correction for the Cl atom is close to that obtained[10,11] to take into account the effect of *ortho*-arrangement of Cl atoms in chlorobenzenes.

Henry's constants and the heats of adsorption for dichloronaphthalenes were calculated using this correction and the correction for the *ortho-ortho*-effect introduced for the Cl atom between two adjacent Cl atoms as, *e.g.*, the Cl atom in position 2 in 1,2,3-trichlorobenzene.[10,11] These compounds were chosen to verify reliability of the results obtained with the corrections proposed. The experimental and theoretical values of K_1 anf heats of adsorption for some dichloronaphthalenes have been published.[13] The experimental K_1 values for dichloronaphthalenes[13] are unusable for direct comparison with the calculation findings, because the values for monochloronaphthalenes and chlorobenzenes differ significantly from those of this and previous works.[10,11] A substantial overestimating of the obtained[13] K_1 values is also indicated by the extremely high K_1 value for naphthalene, which exceeds considerably the corresponding constants known from the literature.[15,16] At the same time, even at so high errors in absolute K_1 values, the experimentally observed order of elution of isomers from the column with GTC (see Table 2) confirms the reliability of the corrections introduced. The theoretical calculation[13] does not represent the experimental order of elution of isomers from the column with GTC, because it is based on the atom-atomic approximation only and does not contain corrections for *ortho*-effects. The experimental and calculated K_1 values for isomeric dichloronaphthalenes are compared in Table 2. It is seen that the values of Henry's constants calculated with corrections for *ortho*-effects describe correctly (within the experimental error) the experimental order of elution of isomers from the column with GTC. The K_1 value for 1,8-dichloronaphthalene, for which an anomalously high value is obtained, is the exception. The divergence between the experiment and calculation is explained by the fact that the Cl atoms in positions 1 and 8 interact with each other and with the C atoms in positions 8 and 1, respectively. This interaction results in a much higher change in AAP as compared to the potentials describing the standard *ortho*-interaction of the Cl atoms and *ortho*-interaction of the Cl and C atoms in position 8. Based on the experimental order of elution of isomers from the column with GTC, we determined the correction for AAP that brings the calculation and experiment into agreement. The correction by absolute value (0.89) is close to that for the *ortho-ortho*-arrangement of Cl atoms in chlorobenzenes (0.885), but it allows one to take into account the 1,8-arrangement of the Cl atoms in the naphthalene molecule. The K_1 value for 1,8-dichloronaphthalene calculated by the corrected AAP describes correctly the experimental order of elution of this isomer from the column with GTC (see Table 2).

It is of interest to estimate the influence of the corrections in AAP for *ortho*-effects on the absolute K_1 values of polychlorinated naphthalenes. The $\ln K_1$ values calculated with and without these corrections are pre-

Table 3. Henry's constants ($\ln K_1$) for adsorption of trichloronaphthalenes on GTC at 575 K calculated without (*1*) and with corrections for *ortho-* and *ortho-ortho*-effects (*2*)

Molecule	$\ln(K_1/\text{cm}^3\ \text{m}^{-2})$	
	1	*2*
1,3,6-Trichloronaphthalene	3.86	3.80
1,4,6-Trichloronaphthalene	3.94	3.82
1,3,5-Trichloronaphthalene	4.03	3.90
1,3,7-Trichloronaphthalene	4.07	4.01
2,3,6-Trichloronaphthalene	4.13	4.01
1,2,5-Trichloronaphthalene	4.15	3.91
1,2,6-Trichloronaphthalene	4.19	4.01
1,2,4-Trichloronaphthalene	4.20	3.95
1,4,5-Trichloronaphthalene	4.22	3.91
2,3,5-Trichloronaphthalene	4.25	4.06
1,3,8-Trichloronaphthalene	4.26	4.04
1,2,7-Trichloronaphthalene	4.35	4.16
1,2,3-Trichloronaphthalene	4.38	4.07
1,2,8-Trichloronaphthalene	4.51	4.21

Table 4. Henry's constants ($\ln K_1$) for adsorption of tetrachloronaphthalenes on GTC at 575 K calculated without (*1*) and with corrections for *ortho-* and *ortho-ortho*-effects (*2*)

Molecule	$\ln(K_1/\text{cm}^3\ \text{m}^{-2})$	
	1	*2*
1,3,5,7-Tetrachloronaphthalene	5.36	5.23
1,3,6,7-Tetrachloronaphthalene	5.41	5.21
1,3,6,8-Tetrachloronaphthalene	5.42	5.17
1,2,4,7-Tetrachloronaphthalene	5.43	5.18
1,2,5,7-Tetrachloronaphthalene	5.45	5.20
1,2,4,6-Tetrachloronaphthalene	5.46	5.21
1,4,6,7-Tetrachloronaphthalene	5.47	5.21
2,3,6,7-Tetrachloronaphthalene	5.49	5.24
1,2,3,6-Tetrachloronaphthalene	5.50	5.19
1,2,5,6-Tetrachloronaphthalene	5.60	5.23
1,3,5,8-Tetrachloronaphthalene	5.62	5.21
1,2,5,8-Tetrachloronaphthalene	5.63	5.25
1,2,3,5-Tetrachloronaphthalene	5.66	5.29
1,2,3,7-Tetrachloronaphthalene	5.69	5.38
1,2,4,8-Tetrachloronaphthalene	5.70	5.33
1,2,6,7-Tetrachloronaphthalene	5.71	5.40
1,2,6,8-Tetrachloronaphthalene	5.72	5.41
1,2,4,5-Tetrachloronaphthalene	5.72	5.29
1,4,5,8-Tetrachloronaphthalene	5.73	5.24
1,2,3,4-Tetrachloronaphthalene	5.83	5.34
1,2,3,8-Tetrachloronaphthalene	5.91	5.48
1,2,7,8-Tetrachloronaphthalene	6.07	5.63

sented in Table 3. It is seen that the introduction of the corrections leads to a decrease in the absolute values of the constants, especially for the *ortho*-substituted isomers. Due to this, the interval of changing the constants decreases and the order of elution of isomers changes. The calculated data suggest that the complete chromatographic separation of all isomeric trichloronaphthalenes on a micropacking column with GTC cannot be achieved in practice.

Table 5. Henry's constants ($\ln K_1$) for adsorption of penta-, hexa-, hepta-, and octachloronaphthalenes on GTC at 575 K calculated without (*1*) and with corrections for *ortho-* and *ortho-ortho*-effects (*2*)

Molecule	$\ln(K_1/\text{cm}^3\ \text{m}^{-2})$	
	1	*2*
1,2,3,7,8-Pentachloronaphthalene	7.37	6.87
1,2,3,4,5-Pentachloronaphthalene	7.35	6.73
1,2,4,5,8-Pentachloronaphthalene	7.20	6.65
1,2,3,5,8-Pentachloronaphthalene	7.16	6.66
1,2,4,5,6-Pentachloronaphthalene	7.15	6.65
1,2,4,7,8-Pentachloronaphthalene	7.13	6.63
1,2,3,5,6-Pentachloronaphthalene	7.10	6.60
1,2,3,4,6-Pentachloronaphthalene	7.08	6.59
1,2,3,6,8-Pentachloronaphthalene	7.07	6.63
1,2,3,6,7-Pentachloronaphthalene	7.05	6.61
1,2,4,5,6-Pentachloronaphthalene	7.02	6.65
1,2,4,5,7-Pentachloronaphthalene	7.01	6.57
1,2,3,5,7-Pentachloronaphthalene	6.99	6.61
1,2,4,6,7-Pentachloronaphthalene	6.98	6.98
1,2,3,4,5,8-Hexachloronaphthalene	8.84	8.10
1,2,3,4,5,6-Hexachloronaphthalene	8.78	8.09
1,2,3,6,7,8-Hexachloronaphthalene	8.73	8.10
1,2,4,5,6,8-Hexachloronaphthalene	8.71	8.08
1,2,4,5,7,8-Hexachloronaphthalene	8.70	8.07
1,2,4,6,7,8-Hexachloronaphthalene	8.67	8.10
1,2,3,4,5,7-Hexachloronaphthalene	8.67	8.04
1,2,3,5,6,8-Hexachloronaphthalene	8.66	8.03
1,2,3,5,6,7-Hexachloronaphthalene	8.63	8.00
1,2,3,4,6,7-Hexachloronaphthalene	8.62	7.99
1,2,3,4,5,6,8-Heptachloronaphthalene	10.36	9.54
1,2,3,4,5,6,7-Heptachloronaphthalene	10.32	9.49
Octachloronaphthalene	12.01	11.00

Similar results were obtained for tetrachloronaphthalenes (Table 4). The introduction of corrections for *ortho*-effects decreases the absolute K_1 values and the differences in retention of the isomers. For penta-, hexa-, and heptachloronaphthalenes, the differences in the constants calculated with and without corrections for *ortho*-effects increase regularly, reaching the maximum value for octachloronaphthalene (Table 5). The introduction of corrections for the *ortho*-effect should result in a change in the expected order of elution of the majority of isomers from the column with GTC. The decrease in the interval of changing the absolute K_1 values due to *ortho*-effects suggests that mixtures of polychloronaphthalenes can be separated on the column with GTC to homologous groups based on the degree of substitution.

As compared to Henry's constants, the heats of adsorption are less sensitive to changes in AAP; however, they correspond more rigidly to the atom-atomic approximation and, hence, they are an important criterion of reliability of experimental and calculated values. The previously obtained data[13] and the results of this work (Table 6) show that the differences in the calculated heats of adsorption do not exceed the experimental error. The introduction of the corrections for *ortho*-effects results in an insignificant decrease in the heats of

Table 6. Experimental and calculated heats of adsorption (q_1) of dichloronaphthalenes on GTC at 575 K obtained in previous[13] (I) and this work (II)

Molecule	q_1/kJ mol^{-1}			
	I		II, calculation	
	experiment[a]	calculation	*1*[b]	*2*[c]
1,4-Dichloronaphthalene	68	78.5	77.3	76.9
1,3-Dichloronaphthalene	—	78.8	77.7	77.6
1,5-Dichloronaphthalene	68	78.4	76.9	76.4
1,6-Dichloronaphthalene	—	78.5	77.3	77.2
2,7-Dichloronaphthalene	68	78.7	77.7	77.7
1,7-Dichloronaphthalene	—	79.1	78.1	78.1
2,6-Dichloronaphthalene	—	78.5	77.3	77.3
2,3-Dichloronaphthalene	66	79.1	78.1	77.7
1,2-Dichloronaphthalene	67	79.2	78.5	77.3
1,8-Dichloronaphthalene	73	79.2	78.5	77.7 (77.3)[d]

[a] The experimental error is ±1 kJ mol^{-1}.

[b] Calculation was performed using the known AAP.

[c] The corrections for *ortho*- and *ortho-ortho*-interactions of the Cl atoms were introduced into AAP.

[d] Calculation was performed taking into account the specific *ortho*-interaction of the Cl atoms in positions 1 and 8.

Table 7. Intervals of changing the heats of adsorption (q_1) of chloronaphthalenes on GTC at 575 K calculated without (*1*) and with corrections for *ortho*- and *ortho-ortho*-effects (*2*)

Homologous group	q_1/kJ mol^{-1}	
	1	*2*
Monochloronaphthalenes	69.7	69.6—69.7
Dichloronaphthalenes	76.9—78.5	76.9—77.7
Trichloronaphthalenes	86.5—87.4	85.3—85.7
Tetrachloronaphthalenes	94.5—94.9	93.2—93.7
Pentachloronaphthalenes	103.3—104.2	100.8—101.0
Hexachloronaphthalenes	112.1—112.5	108.8—109.0
Heptachloronaphthalenes	121.0—121.2	117.0—117.1
Octachloronaphthalene	132.0	124.5

adsorption. Comparison of the calculated and experimental results suggests that the experimental heats of adsorption are underestimated by 10—12 kJ mol^{-1}. The heats of adsorption for 1,8-dichloronaphthalene differ much less from the calculated values. Since the calculations using different AAP give close values of heats of adsorption, this is, most likely, an experimental error.

For other polychloronaphthalenes, differences in the heats of adsorption of isomers are also low. Therefore, only intervals of changing the values for each homologous group are presented in Table 7. It is seen that the difference in heats of adsorption calculated with and without corrections for *ortho*-effects increases regularly with increasing degree of substitution.

Thus, corrections in AAP taking into account differences in the position of the Cl atom in the naphthalene molecule were determined in this work. It was shown for mono- and dichloronaphthalenes that these corrections can be used to predict the order of elution of isomers from a column with GTC and to calculate Henry's constants and heats of adsorption of all isomeric polychloronaphthalenes. The data obtained can be used for calculations of the thermodynamic parameters of adsorption of molecules of other classes with a similar structural fragment and for estimation of the possibility of separating specific mixtures of chloronaphthalenes on columns with nonporous carbon sorbents of the GTC type.

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