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RETENTION INDICES IN GAS-SOLID CHROMATOGRAPHY

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SUMMARY

The retention volumes per unit surface area for the adsorbents graphitized thermal carbon black and hydrogen-treated graphitized thermal carbon black, which have very homogeneous surfaces, for different hydrocarbons up to C₁₁ and some halogenated and oxygenated derivatives have been determined. For convenience, the Kováts retention indices for these compounds have been calculated. The thermodynamic meaning of these indices and the possibility of their molecular-statistical estimation based on an approximate theory of intermolecular interaction is discussed.

INTRODUCTION

Retention indices have often been used for the identification of substances in gas-liquid chromatography. These indices make it possible to demonstrate the retention characteristics of different substances in comparison with a series of standard substances such as *n*-alkanes.

The most useful system in gas-liquid chromatography is the Kováts logarithmic system of retention indices¹. In gas-solid chromatography on non-porous and wide-pore adsorbents with a known specific surface area, this index is given by

$$I_x = 100 \left[\frac{\log V_{A,1(x)} - \log V_{A,1(n)}}{\log V_{A,1(n+1)} - \log V_{A,1(n)}} \right] + n \quad (1)$$

where $V_{A,1(n)} < V_{A,1(x)} < V_{A,1(n+1)}$ are the retention volumes per unit surface area of the adsorbent (subscript *A*) for zero sample size (subscript 1) of the substance in question (subscript *x*) and the nearest *n*-alkane, retained at the same temperature on the same adsorbent more strongly (subscript *n* + 1) or more weakly (subscript *n*) than the substance *x*, *n* being the number of carbon atoms in the molecule of this *n*-alkane.

Pilt *et al.*² demonstrated that, if the number of carbon atoms in unsaturated molecules remains constant and the double bond remains in the same position, the retention indices of *trans*-alkenes are higher than those of the corresponding *cis*-alkenes, while the retention indices of alkynes are lower than those of *cis*-alkenes. Engewald *et al.*³ determined the retention indices of cycloalkanes, cycloalkenes and

cycloalkadienes C_6-C_{13} on graphitized thermal carbon black (GTCB) and compared them with those on squalane. It was found that the difference in I values for most substances on GTCB is higher than on squalane. The I values on GTCB have been used successfully to identify the thermal decomposition products of 1,5,9-cyclododecatriene and its hydrogenation products⁴.

In this work we consider retention indices on GTCB and on hydrogen-treated graphitized thermal carbon black (HTGTCB)⁵⁻⁷ for numerous hydrocarbons of different structures and also for various halogenated and oxygenated derivatives. Different regularities were found that characterize the relationship between I and the molecular structures of these substances.

As the $V_{A,1}$ values are related to the Henry constants for adsorption, the retention index, I_x , is a definite thermodynamic constant which depends on the molecular structure of the substance x and of the corresponding n -alkanes and on the structure of the adsorbent as well as on the temperature. Eqn. 1 contains the differences $\log V_{A,1(x)} - \log V_{A,1(n)}$ and $\log V_{A,1(n+1)} - \log V_{A,1(n)}$, which are equal to the logarithms of relative retention volumes for zero sample size. Therefore, the relative retention volumes and the retention indices can be determined experimentally with a greater precision than the corresponding absolute retention volumes, $V_{A,1(x)}$, because the influence of the changes in separation parameters such as the flow-rate and the pressure drop in the column is eliminated. However, the dependence of I_x on the structure of the molecule x and on temperature is more complicated than for the Henry constant itself, $V_{A,1(x)}$, and for its relative value, $V_{A,1(x)}/V_{A,1(n)}$.

In this paper, we also consider the theoretical estimation of I_x based on molecular-statistical calculations of $V_{A,1(x)}$, $V_{A,1(n)}$ and $V_{A,1(n+1)}$.

RETENTION VOLUMES OF C_3-C_8 HYDROCARBONS

Figs. 1-3 show examples of the dependences of $\log V_{A,1}$ on $1/T$ obtained from

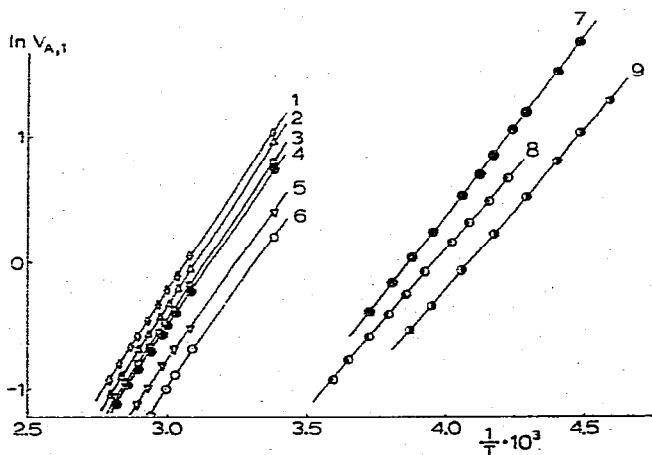


Fig. 1. Dependence of the logarithm of retention volume per unit surface area of GTCB ($\ln V_{A,1}$) on inverse temperature for C_5-C_4 hydrocarbons. 1 = *trans*-Butene-2; 2 = butadiene-1,3; 3 = *cis*-butene-2; 4 = *n*-butane; 5 = butene-1; 6 = isobutane; 7 = propane; 8 = propene; 9 = cyclopropane.

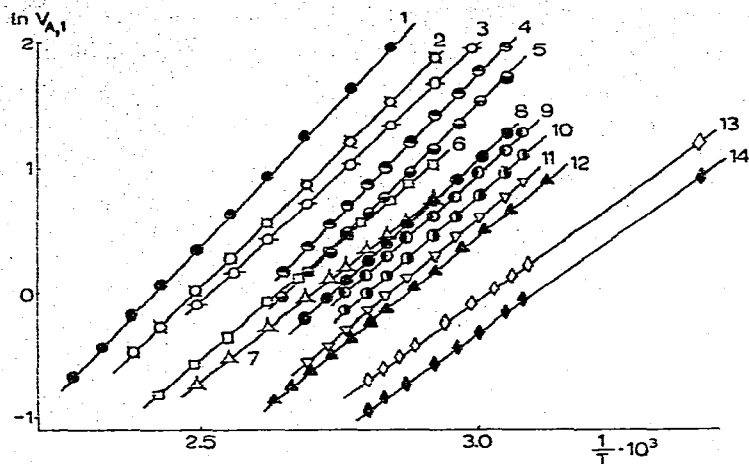


Fig. 2. Dependence of $\ln V_{A,1}$ for GTCB on inverse temperature for C_5 - C_6 hydrocarbons. 1 = *n*-Hexane; 2 = benzene; 3 = hexadiene-1,5 and hexyne-1; 4 = *trans*-pentadiene-1,3; 5 = *cis*-pentadiene-1,3; 6 = methylcyclopentane; 7 = cyclohexane; 8 = *n*-pentane; 9 = *trans*-pentene-2; 10 = *cis*-pentene-2; 11 = isopentane; 12 = pentadiene-1,4 and pentyne-1; 13 = cyclopentane; 14 = neopentane.

the experimental data⁸⁻¹⁰ for C_3 - C_4 (Fig. 1), C_5 - C_6 (Fig. 2) and C_7 - C_8 (Fig. 3) *n*-alkanes and for several different hydrocarbons with intermediate $V_{A,1}$ values. These dependences are almost linear, with the exception of those for butadiene-1,3 and other dienes with conjugated bonds, and also for butene-2 and methylated benzene derivatives. The lines for all hydrocarbons with equal *n* lie below the lines for *n*-alkanes with the same *n*. In some instances (e.g., for methylcyclopentane and *cis*-pentadiene-1,3) the lines cross, i.e., inversion of the sequence of retention volumes of the corresponding pair of hydrocarbons on GTCB occurs as the temperature changes¹¹. Care

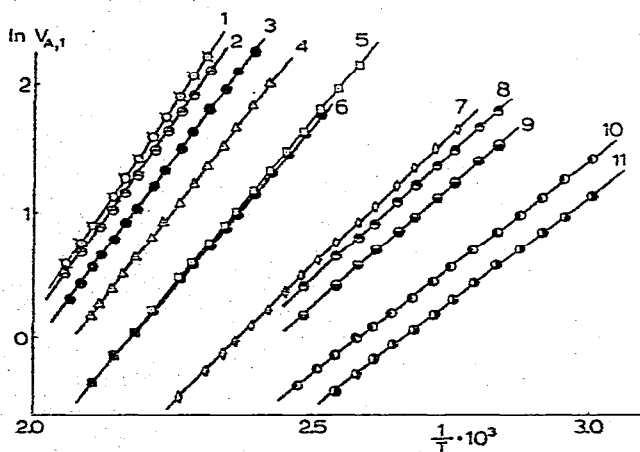


Fig. 3. Dependence of $\ln V_{A,1}$ for GTCB on inverse temperature for C_7 - C_8 hydrocarbons. 1 = *o* + *p*-Xylene; 2 = *m*-xylene; 3 = *n*-octane; 4 = ethylbenzene; 5 = toluene; 6 = *n*-heptane; 7 = methylcyclohexane; 8 = *exo*-5-methylnorbornene; 9 = *endo*-5-methylnorbornene; 10 = norbornane; 11 = norbornene.

TABLE I
KOVÁTS RETENTION INDICES FOR C₄ HYDROCARBONS ON GTCB

Hydrocarbon	$I_{22.5^{\circ}\text{C}}^{\text{GTCB}}$	ΔI per 10°C
Isobutane	374	0.2
Butene-1	384	0.3
<i>cis</i> -Butene-2	402	0.1
<i>trans</i> -Butene-2	415	0.4
Butadiene-1,3	410	0.2

is therefore essential when investigating the dependence of either $V_{A,1}$ or I on temperature.

RETENTION INDICES OF C₄-C₆ HYDROCARBONS

The I values for a series of hydrocarbons of different classes are given in Tables I-III. Many C₄-C₆ hydrocarbons have a lower retention index on GTCB compared with those for n -alkanes with the same n value. As for $V_{A,1}$, the only exceptions are diene hydrocarbons with conjugated bonds and *trans*-isomers of alkenes-2. For these hydrocarbons, the retention indices are higher than those for the corresponding n -alkanes. The retention indices of alkynes are lower than those of the corresponding alkenes. For diene hydrocarbons with unconjugated double bonds, the difference in retention indices between alkenes and diene hydrocarbons is closer to the difference in values between the corresponding n -alkanes and alkenes. Hydrocarbon chain branching in alkanes sharply reduces the retention indices. It can be seen particularly for isopentane ($I_{75^{\circ}\text{C}}^{\text{GTCB}} = 468$) and neopentane ($I_{75^{\circ}\text{C}}^{\text{GTCB}} = 410$). This effect is due to the decrease in the number of atoms or groups of atoms of the adsorbed molecule that can be in contact with the plane surface of GTCB. Cyclization of the hydrocarbon chain also decreases the I value because the carbon atoms of cyclanes do not lie in one plane. If the I values for isomeric molecules of methylcyclopentane and cyclohexane are compared, it can be seen that the molecule of methylcyclopentane (which is flatter) has a higher I value.

Hence the dependence of I on the geometrical structure of molecules is much greater in gas-solid chromatography on GTCB than in gas-liquid chromatography.

TABLE II
KOVÁTS RETENTION INDICES FOR C₅ HYDROCARBONS ON GTCB

Hydrocarbon	$I_{26^{\circ}\text{C}}^{\text{GTCB}}$	ΔI per 10°C
Isopentane	468	0.6
Neopentane	410	1.2
Cyclopentane	426	1.2
Pentane-1	479	0.3
<i>cis</i> -Pentene-2	481	0.8
<i>trans</i> -Pentene-2	493	0.4
Pentadiene-1,4	462	1.8
Pentyne-1	463	1.0
<i>cis</i> -Pentadiene-1,3	526	0.2
<i>trans</i> -Pentadiene-1,3	539	0.2

TABLE III

KOVÁTS RETENTION INDICES FOR C₆ HYDROCARBONS ON GTCB

Hydrocarbon	I_{100}^{GTCB}	ΔI per 10°C
Hexene-1	577	0.7
Hexyne-1	560	1.3
Hexadiene-1,5	560	1.4
Methylcyclopentane	524	2.6
Cyclohexane	508	4.1
Cyclohexene	535	1.7
Cyclohexadiene	539	1.5
Benzene	572	0.4

RETENTION INDICES OF BRIDGED BICYCLO(2,2,1)HEPTANES

The C₇-C₁₀ bridged hydrocarbons considered (Table IV) have *I* values between those of *n*-pentane and *n*-octane. With bicycloheptane hydrocarbons (norbornane series), some atoms or groups of atoms of the molecule at any orientation remain raised over the flat surface of GTCB, and some of them are a considerable distance from the surface. As a result, the energy of intermolecular interaction of these molecules with the adsorbent is much lower than that for *n*-alkanes with the same number of carbon atoms in the molecule.

TABLE IV

KOVÁTS RETENTION INDICES FOR NORBORNANE DERIVATIVES ON GTCB

Hydrocarbon	I_{100}^{GTCB}	ΔI per 10°C
Norbornane [bicyclo(2,2,1)heptane]	534	2.5
Norbornene [bicyclo(2,2,1)heptene-2]	517	2.8
<i>endo</i> -5-Methylbicyclo(2,2,1)heptene-2	578	2.6
<i>exo</i> -5-Methylbicyclo(2,2,1)heptene-2	597	2.2
1-Methylbicyclo(2,2,1)heptane	586	3.0
<i>endo</i> -2-Methylbicyclo(2,2,1)heptane	592	3.2
<i>exo</i> -2-Methylbicyclo(2,2,1)heptane	606	2.5
2-Methylenebicyclo(2,2,1)heptane	594	2.6
7,7-Dimethylbicyclo(2,2,1)heptane	643	3.6
<i>endo</i> -5-Vinylbicyclo(2,2,1)heptene-2	648	2.8
<i>exo</i> -5-Vinylbicyclo(2,2,1)heptene-2	669	2.8
<i>endo</i> -1,2-Dimethylbicyclo(2,2,1)heptane	649	3.5
<i>exo</i> -1,2-Dimethylbicyclo(2,2,1)heptane	668	3.1
<i>trans</i> -5-Ethylidenebicyclo(2,2,1)heptene-2	666	3.3
<i>cis</i> -5-Ethylidenebicyclo(2,2,1)heptene-2	689	2.3
1,4-Dimethylbicyclo(2,2,1)heptane	666	3.6
<i>endo-endo</i> -2,3-Dimethylbicyclo(2,2,1)heptane	667	2.6
<i>trans</i> -2,3-Dimethylbicyclo(2,2,1)heptane	675	3.2
<i>exo-exo</i> -2,3-Dimethylbicyclo(2,2,1)heptane	694	2.7
<i>exo</i> -2,2,3-Trimethylbicyclo(2,2,1)heptane	678	3.5
<i>endo</i> -2,2,3-Trimethylbicyclo(2,2,1)heptane	697	2.7
2,2-Dimethyl-3-methylenebicyclo(2,2,1)heptane	694	4.7
<i>endo</i> -2-Ethylbicyclo(2,2,1)heptane	689	4.1
<i>exo</i> -2-Ethylbicyclo(2,2,1)heptane	703	2.7
<i>endo</i> -Trimethylenebicyclo(2,2,1)heptane	717	3.5

Norbornene and its methyl-substituted derivatives have lower I values than the corresponding derivatives of norbornane. Dimethylnorbornane with two methyl groups on one carbon atom is characterized by lower I values than those for derivatives that have the methyl substituents on two different carbon atoms. Of the dimethyl derivatives of norbornane, 7,7-dimethylbicyclo(2,2,1)heptane has the lowest I value.

All *endo*-isomers of mono- and disubstituted derivatives of norbornane and norbornene have lower I values than the *exo*-isomers, the difference being 14–20 units. The regularity of the values obtained allows one to determine the structures of the isomers and to determine the ratio of the contents of *endo*- and *exo*-isomers in the mixtures under investigation.

The changes in the I values obtained in this instance are also connected with the geometrical structure of the adsorbate molecules and their optimal orientation on a flat surface. Actually, in all instances the geometry of the *endo*-isomers is such that they can be arranged on the surface of GTCB less efficiently and parts of their molecules are further from the basal face of graphite than with the *exo*-isomers.

RETENTION INDICES OF C_7 - C_{11} AROMATIC HYDROCARBONS

The $V_{A,1}$ value^{10,12} for benzene on GTCB at 100°C (Table III) is lower than that for *n*-hexane, and the I value for benzene is 28 units lower than that for *n*-hexane. In isomeric alkylbenzenes, the I value depends on the structure of the alkyl group and on the number of these groups attached to the aromatic nucleus (Table V).

For mono-*n*-alkylbenzenes the increment of I per methylene group is 87 units and mono-*n*-alkylbenzenes are retained on GTCB less than *n*-alkanes with the same number of carbon atoms. It is important to note that the series of mono-*n*-alkylbenzenes with a linear dependence of I on the number of carbon atoms in the side *n*-alkyl chain begins with ethylbenzene, toluene, which has only one methyl group, behaving as the first representative of a polymethylbenzene series. In the series of polymethylbenzenes, the replacement of each hydrogen atom of the ring by a methyl

TABLE V

KOVÁTS RETENTION INDICES FOR C_7 - C_{11} AROMATIC HYDROCARBONS ON GTCB

Hydrocarbon	$I_{200^\circ C}^{GTCB}$	ΔI per $10^\circ C$
Toluene	704	0.1
Ethylbenzene	761	0.3
<i>m</i> -Xylene	828	0.2
<i>p</i> -Xylene	838	0.2
<i>o</i> -Xylene	838	0.2
<i>n</i> -Propylbenzene	849	0.5
Isopropylbenzene	793	0.3
1,3,5-Trimethylbenzene	949	0.2
1,2,4-Trimethylbenzene	966	0.7
1,2,3-Trimethylbenzene	973	0.8
<i>n</i> -Butylbenzene	936	0.8
1,2,4,5-Tetramethylbenzene	1097	0.1
1,2,3,5-Tetramethylbenzene	1101	0.1
<i>n</i> -Amylbenzene	1018	0.2

group does not lead to a constant increment in the retention index. It increases by 128 units per methyl group on average and, beginning with toluene, the retention indices of polymethylbenzenes are higher than those of the corresponding *n*-alkanes.

THEORETICAL ESTIMATION OF RETENTION INDICES ON GTCB

The molecular-statistical calculations of $V_{A,1}$ and other thermodynamic retention characteristics of many hydrocarbons on GTCB have been made on the basis of the approximate theory of the intermolecular interaction¹²⁻¹⁵. By comparison with the experimental $V_{A,1}$ values for a few hydrocarbons of different classes, these calculations enabled us to establish the influence of the valence of carbon atoms in hydrocarbon molecules on the intermolecular interaction with GTCB and to find semi-empirical expressions for the following atom-atom potential functions of this interaction: $\varphi_{C(\text{graphite})...C(\text{alkane})}$, $\varphi_{C(\text{graphite})...C(\text{alkene, aromatic hydrocarbon})}$, $\varphi_{C(\text{graphite})...C(\text{alkyne})}$ and $\varphi_{C(\text{graphite})...H(\text{hydrocarbon})}$. The results of molecular-statistical calculations based on these atom-atom potential functions were in good agreement with the experimental values of $V_{A,1}$ for many different hydrocarbons within the limits of error of the experimental determination of $V_{A,1}$. Fig. 4 for example, illustrates the agreement between the calculated and experimental $\log V_{A,1}$ values for C_5 hydrocarbons. These calculations enabled us to predict the separation, *i.e.*, the sequence of $V_{A,1}$ values, in the cases when these values differ greatly. However, when the $V_{A,1}$ values of the hydrocarbons compared are similar, the calculated sequence of $V_{A,1}$ values do not agree with the experimental values in some instances. These discrepancies are the result of errors in the calculation which are due to some uncertainties in the geometry of the molecules, as well as to the approximations of the method used for the calculation of the potential function Φ of the intermolecular interaction of the molecule with the adsorbent^{12,15}. For example, the calculated values of $\log V_{A,1}$ for neopentane are higher than those for cyclopentane, but the experimental values are lower for neopentane than those for cyclopentane.

In the determination of the retention indices from eqn. 1, the errors in the calculation of $\ln V_{A,1}$, $\ln V_{A,1(n)}$ and $V_{A,1(n+1)}$ can add together, which can lead to considerable errors in calculated *I* values. A comparison of theoretically calculated

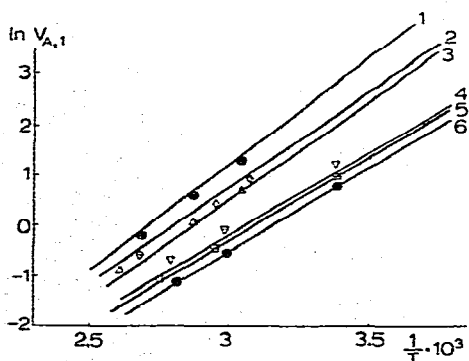


Fig. 4. Dependence of $\ln V_{A,1}$ for GTCB on inverse temperature for *n*-butane and some C_5 hydrocarbons. Lines, theoretically calculated; symbols, experimental data. 1 = *n*-Pentane; 2 = isopentane; 3 = pentyne-1; 4 = neopentane; 5 = cyclopentane; 6 = *n*-butane.

TABLE VI

COMPARISON OF RELATIVE RETENTION VOLUMES (RELATIVE TO THE *n*-ALKANE WITH THE SAME CARBON NUMBER) AND RETENTION INDICES FOR SOME HYDROCARBONS ON GTCB, OBTAINED FROM MEASUREMENTS AND CALCULATED ON THE BASIS OF AN APPROXIMATE THEORY OF INTERMOLECULAR INTERACTION

Hydrocarbon	T (°K)	Relative retention volume		Retention index	
		Experimental	Calculated	Experimental	Calculated
Neopentane	329	0.24	0.24	410	422
Cyclopentane	329	0.31	0.22	426	412
Isopentane	329	0.60	0.63	468	473
Pentyne-1	329	0.56	0.51	463	458
<i>cis</i> -Pentadiene-1,3	329	1.55	1.10	526	505
<i>trans</i> -Pentadiene-1,3	329	2.01	1.26	539	516
Benzene	373	0.66	0.50	572	550
Cyclohexane	373	0.26	0.28	508	515

I values with experimentally determined values for some hydrocarbons on GTCB is shown in Table VI. Because of this effect, the determination of I_x from the absolute values of $V_{A,1(x)}$, $V_{A,1(n)}$ and $V_{A,1(n+1)}$ calculated theoretically often does not yield precise values for analytical purposes.

Two methods are possible for obtaining better results in the theoretical calculation of I_x . The first method is to make the calculation of the potential function Φ more precise, and the second is to use the molecular-statistical method in the calculation of not the absolute values of $V_{A,1(x)}$, $V_{A,1(n)}$ and $V_{A,1(n+1)}$ but the relative values $V_{A,1(x)}/V_{A,1(n)}$ and $V_{A,1(n)}/V_{A,1(n+1)}$, which are present in eqn. 1. Some errors in the calculated $\ln V_{A,1}$ values can be thus expected to be eliminated. Both methods are of theoretical interest and will enable one to clarify the dependence of I not only on the structures of molecules but also on the temperature, which is of practical importance.

RETENTION INDICES OF HALOGENATED DERIVATIVES OF HYDROCARBONS

For primary monohalogenated C_1 - C_6 *n*-alkanes, equations have been obtained^{13,16} that connect the retention indices with the number of carbon atoms, n , in their molecules:

Fluoroalkanes:

$$I_{100^\circ\text{C}}^{\text{GTCB}} = 100n + 20 \quad (2)$$

Chloroalkanes:

$$I_{100^\circ\text{C}}^{\text{GTCB}} = 100n + 130 \quad (3)$$

Bromoalkanes:

$$I_{100^\circ\text{C}}^{\text{GTCB}} = 100n + 178 \quad (4)$$

Iodoalkanes:

$$I_{100^\circ\text{C}}^{\text{GTCB}} = 100n + 249 \quad (5)$$

It can be seen from the above equations that the retention indices of primary monohalogenated *n*-alkanes are higher than those for the corresponding *n*-alkanes, for fluoralkanes by 20, for chloroalkanes by 130, for bromoalkanes by 178 and for iodoalkanes by 249 units.

When the halogen atom is transferred from position 1 to position 2, the *I* values decrease. For example, for 2-bromoalkanes the difference in the retention indices compared with the corresponding *n*-alkanes is 160 units instead of 178 for 1-bromoalkanes.

For the polyhalogenated derivatives of methane and ethane investigated, the retention indices increased proportionally to the number of halogen atoms until all of the halogen atoms in the molecule were able to touch the flat surface. For dihalogenated derivatives, each halogen atom introduces the same number of retention index units as for 1-halogenated *n*-alkanes. For example, for CH_2Cl_2 $I_{100^\circ\text{C}}^{\text{GTCB}} = 363$, for CH_2Br_2 $I_{100^\circ\text{C}}^{\text{GTCB}} = 469$ and for CH_2I_2 $I_{100^\circ\text{C}}^{\text{GTCB}} = 604$.

However, the retention indices of chloroform and carbon tetrachloride differ by only 50 units (for CHCl_3 $I_{100^\circ\text{C}}^{\text{GTCB}} = 448$ and for CCl_4 $I_{100^\circ\text{C}}^{\text{GTCB}} = 499$). This result is connected with the geometry of the molecules: in the most favourable orientation, one chlorine atom of the adsorbed CCl_4 molecule is removed from the flat surface of graphite and the contribution of this atom to the total energy of intermolecular interaction of the molecule with GTCB is much less than for the other three atoms.

RETENTION INDICES OF OXYGENATED DERIVATIVES OF HYDROCARBONS

In order to eliminate the additional specific interaction of carbonyl and hydroxyl groups of oxygenated compounds with trace amounts of chemisorbed oxygen complexes on the GTCB surface, the retention indices of oxygenated compounds were determined on GTCB that had previously been treated with hydrogen at 1000°C (HTGTCB)^{5-8,12}.

The following linear dependences of retention indices of oxygenated derivatives of different classes on the number of carbon atoms in their molecules, *n*, were found^{7,13}:

Ethers:

$$I_{150^\circ\text{C}}^{\text{HTGTCB}} = 100n + 37 \quad (6)$$

Aldehydes:

$$I_{150^\circ\text{C}}^{\text{HTGTCB}} = 100n + 61 \quad (7)$$

Methyl ketones:

$$I_{150^\circ\text{C}}^{\text{HTGTCB}} = 100n + 66 \quad (8)$$

Symmetrical ketones:

$$I_{150^\circ\text{C}}^{\text{HTGTCB}} = 100n + 41 \quad (9)$$

Primary alcohols:

$$I_{150^\circ\text{C}}^{\text{HTGTCB}} = 100n + 87 \quad (10)$$

Acetates:

$$I_{150^\circ\text{C}}^{\text{HTGTCB}} = 93n + 127 \quad (11)$$

Propionates:

$$I_{150^{\circ}\text{C}}^{\text{HTGT CB}} = 95n + 117 \quad (12)$$

Butyrates:

$$I_{150^{\circ}\text{C}}^{\text{HTGT CB}} = 92n + 125 \quad (13)$$

For molecules of mono-oxygenated derivatives that contain the same number of carbon atoms, ethers have the lowest retention indices, being only 37 units higher than those of the corresponding *n*-alkanes.

This effect is connected with the elevated position of the oxygen atom situated between the methyl or methylene groups of greater Van der Waals radii. The retention indices of aldehydes and methyl ketones with the same number of carbon atoms are very similar. Primary alcohols have the highest retention indices of the mono-oxygenated compounds. The retention index of each homologue of the first five series of oxygenated substances considered changes by 100 units, as for *n*-alkanes, which shows that the contribution of one methylene group in both *n*-alkanes and the oxygenated derivatives is the same.

The retention indices of esters change from one homologue to another by 92–95 units. However, eqns. 11–13 must be regarded as approximate, because only esters with not more than 10 carbon atoms have been investigated.

Simple correlations can connect the retention indices of oxygenated compounds with their boiling temperatures, which enable one to calculate the boiling temperature of an unidentified substance from its retention index. Equations connecting the boiling temperatures with the retention indices of the members of each homologous series of oxygenated compounds have been published⁷, as well as examples of the identification of oxygenated compounds using retention indices on HTGT CB.

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