



ELSEVIER

Journal of Chromatography A, 923 (2001) 127–136

JOURNAL OF
CHROMATOGRAPHY A

www.elsevier.com/locate/chroma

Partition coefficients of alkyl aromatic hydrocarbons and esters in a hexane–acetonitrile system

V.A. Isidorov^{a,*}, U. Krajewska^a, E.N. Dubis^b, M.A. Jdanova^c

^a*Institute of Chemistry, Białystok University, Al. Piłsudskiego 11/4, 15-443 Białystok, Poland*

^b*Urząd Celny w Białymstoku, Laboratorium Celne, ul. Octowa 2, 15-339 Białystok, Poland*

^c*Institute of Chemistry, St. Petersburg University, 198904 St. Petersburg, Russia*

Received 27 March 2001; accepted 1 May 2001

Abstract

Partition coefficients (K_p) in a heterogeneous system consisting of two immiscible organic solvents can be successfully used for a supplementary identification parameter in qualitative GC and GC–MS analysis of organic compounds. For rapid addition to database of K_p values, calculation methods based on the well-known ‘retention–structure relationships’ approach can be used. This paper reports the experimentally determined and calculated K_p values for 252 compounds including alkyl aromatic hydrocarbons and esters. It is shown that for group identification of components it is desirable to use not the K_p values themselves but the parameter j which is a combination of K_p and gas chromatographic retention indices: $j = kI - \log K_p$. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Partition coefficients; Solubility–structure relationships; Structure–solubility relationships; Hydrocarbons, aromatic; Alkylbenzenes; Esters

1. Introduction

To increase identification reliability for components in complex organic compound mixtures in gas chromatographic analysis, it has been proposed to use partition coefficients $K_p = C_1/C_2$, of the analytes between two immiscible liquids [1–3]. The efficiency of an approach based on simultaneous use of two parameters for identification: partition coefficient in a hexane–acetonitrile system and the retention index (I) was demonstrated in Refs. [4,5]. The analysis of essential oils from *Artemisia pallens*

(davana oil) and birch buds was taken as an example. It was shown that preliminary assignment of mixture components on the basis of K_p values to certain homologous series also greatly increases identification reliability in GC analysis with detection by low-resolution mass spectrometry. The main factor preventing wide application of this method in routine analytical practice is the absence of sufficiently detailed databases of partition coefficients in hexane–acetonitrile or an analogous heterogeneous system.

The results of experimental K_p determination in the hexane–acetonitrile system have been reported for 77 components often encountered in essential oil of plants [6]. For a further 25 monoterpenes the pure reference preparations of which are absent or dif-

*Corresponding author. Tel.: +48-85-457-580; fax: +48-85-457-581.

E-mail address: isidorov@noc.uwb.edu.pl (V.A. Isidorov).

difficult to obtain, these values were estimated on the basis of the structure–solubility relationship.

In this paper we report K_p for 252 organic compounds. For 177 of them, K_p was determined experimentally. These compounds belong to two classes: alkyl aromatic hydrocarbons and esters. The former are contained in motor fuels and various solvents and are the most common pollutants in natural and wastewaters. Esters of fatty and aromatic acids are also anthropogenic pollutants but they are often encountered in the vegetable kingdom as well: together with many compounds of other classes, they are contained in essential oils and lipids of cuticular wax. Therefore, in analytical practice it is often necessary to recognize these components in a background of representatives of other homologous series.

2. Experimental

2.1. Materials

Commercial C_7 – C_9 alkyl aromatic hydrocarbons, esters of C_1 – C_8 aliphatic alcohols and C_1 – C_6 carboxylic acids (Aldrich), as well as preparations of C_{10} – C_{17} aromatic hydrocarbons from the collection of the Institute of Chemistry of St. Petersburg University (Russia) were used. Esters of C_{10} – C_{20} carboxylic acids and acetate of C_{10} – C_{22} alcohols were synthesized by esterification method [7,8] in the Institute of Chemistry of Białystok University. Esters of aromatic, monoterpene and sesquiterpene alcohols, as well as lactones were obtained from a factory of aromatic substances (Firmenich, Grodzisk Mazowiecki, Poland).

Acetonitrile (Merck, HPLC grade), *n*-hexane (Baker, HPLC grade), chloroform and toluene were used without additional purification and drying.

2.2. Sample preparation and analysis

Samples were prepared for partition coefficient determination at room temperature ($20 \pm 2^\circ\text{C}$). A 2-ml flask was charged through a pipette with 0.5 ml of *n*-hexane and 0.5 ml of acetonitrile. In this flask were added 20–30 μl of hexane solution of 1–5 esters from the collection, 1 μl of toluene and 5 μl of C_7 – C_{14} or C_8 – C_{18} *n*-alkanes. Subsequently the

flask was closed and shaken for 30 s. After phase separation each of them was subjected to analysis. Gas chromatographic separation was carried out with a Hewlett–Packard HP-4890D GC system equipped with flame ionisation detector and fused-silica column (30 m \times 0.25 mm, film thickness, 0.25 μm) with HP-5 phase at a helium flow-rate of 1 ml/min (split 1:30). The analysis was carried out with temperature programming from 40 to 180 $^\circ\text{C}$ at a rate of 3 $^\circ\text{C}/\text{min}$.

The same procedure of sample preparation for analysis was used in K_p determination for esters of lower alcohols and carboxylic acids. Esters of C_{10} – C_{20} carboxylic acids and acetates of C_{10} – C_{22} alcohols as well as reference C_{10} – C_{25} *n*-alkanes were introduced into the hexane–acetonitrile system in the form of solutions diluted in chloroform. In this case *n*-pentylbenzene was used as internal standard. The total volume of esters, alkanes, and internal standard solutions did not exceed 3% of the volume of the hexane–acetonitrile heterogeneous system. In this case gas chromatographic separation was carried out in the splitless regime with temperature programming from 50 to 100 $^\circ\text{C}$ at a rate of 6 $^\circ\text{C}/\text{min}$ and from 100 to 280 $^\circ\text{C}$ at a rate of 4 $^\circ\text{C}/\text{min}$.

The values of retention time were used to calculate retention indices. Partition coefficients were calculated from the ratio of peak areas of the components by using Eq. (1):

$$K_p = (S_h^x/S_a^x)(S_a^t/S_h^t) \quad (1)$$

where S_h^x and S_a^x are the peak areas of the component *x* on the chromatograms of the hexane and the acetonitrile phases, respectively, and S_a^t and S_h^t are the peak areas of internal standard (toluene or *n*-pentylbenzene) on these chromatograms.

The prediction of partition coefficients and retention indices was made by the least-square method.

3. Results and discussion

In this work K_p values of 34 alkyl aromatic hydrocarbons were determined experimentally (Table 1). However, this is only a small fraction of known individual compounds of this class present in various industrial mixtures and environmental samples. Pure preparations of most of them are difficult to obtain. Hence, the experimental determination of

Table 1
Retention indices and K_p values of alkyl aromatic hydrocarbons

| Hydrocarbon | Boiling point (K) | n_C | I^{exp} | K_p^{exp} | K_p^{calc} (2a) | K_p^{calc} (2b) |
|--|-------------------|-------|------------------|--------------------|--------------------------|--------------------------|
| Toluene | 383.78 | 1 | 760 | 1.07±0.15 | 1.09 | 1.09 |
| Ethyl benzene | 409.3 | 2 | 857 | 1.39±0.18 | 1.40 | 1.41 |
| <i>p</i> -Xylene | 411.5 | 2 | 866 | 1.42±0.32 | 1.42 | 1.43 |
| <i>m</i> -Xylene | 412.25 | 2 | 868 | 1.44±0.20 | 1.43 | 1.43 |
| <i>o</i> -Xylene | 417.56 | 2 | 888 | 1.49±0.18 | 1.48 | 1.48 |
| Isopropylbenzene (cumene) | 425.54 | 3 | 926 | 1.70±0.22 | 1.71 | 1.72 |
| <i>n</i> -Propylbenzene | 432.15 | 3 | 950 | 1.81±0.21 | 1.79 | 1.78 |
| 1,3,5-Trimethylbenzene | 437.85 | 3 | 994 | 1.88±0.31 | 1.85 | 1.89 |
| 1,2,4-Trimethylbenzene | 442.5 | 3 | 1004 | 1.92±0.29 | 1.90 | 1.92 |
| Isobutylbenzene | 445.15 | 4 | 1009 | 2.15±0.32 | 2.13 | 2.13 |
| 1,2,3-Trimethylbenzene | 449.23 | 3 | 1018 | 1.96±0.29 | 1.98 | 1.95 |
| <i>p</i> -Cymene | 450.40 | 4 | 1022 | 2.23±0.21 | 2.20 | 2.17 |
| 1,3-Diethylbenzene | 454.25 | 4 | 1045 | 2.23±0.24 | 2.26 | 2.23 |
| <i>n</i> -Butylbenzene | 456.42 | 4 | 1054 | 2.35±0.23 | 2.28 | 2.26 |
| 1,2-Diethylbenzene | 456.6 | 4 | 1055 | 2.27±0.30 | 2.29 | 2.26 |
| 1,4-Diethylbenzene | 456.9 | 4 | 1056 | 2.28±0.25 | 2.29 | 2.26 |
| 2,4-Dimethyl-1-ethylbenzene | 461.56 | 4 | 1075 | 2.33±0.28 | 2.35 | 2.32 |
| <i>tert.</i> -Pentylbenzene | 463.15 | 5 | 1090 | 2.63±0.30 | 2.62 | 2.61 |
| <i>sec.</i> -Pentylbenzene | 465.15 | 5 | 1098 | 2.65±0.31 | 2.65 | 2.63 |
| 1-Methyl-4- <i>tert.</i> -butylbenzene | 468.95 | 5 | 1101 | 2.71±0.30 | 2.71 | 2.64 |
| 1,2-Dimethyl-4-isopropylbenzene | 474.95 | 5 | 1139 | 2.78±0.28 | 2.81 | 2.76 |
| 1-Methyl-3,5-diethylbenzene | 475.6 | 5 | 1143 | 2.79±0.11 | 2.82 | 2.78 |
| 1,2-Di-isopropylbenzene | 477.15 | 6 | 1156 | 3.14±0.32 | 3.13 | 3.11 |
| <i>n</i> -Pentylbenzene | 478.55 | 5 | 1154 | 2.89±0.39 | 2.86 | 2.81 |
| 1,2-Dimethyl-4-propylbenzene | 482.05 | 5 | 1169 | 2.87±0.21 | 2.92 | 2.86 |
| 1,2-Dimethyl-4- <i>tert.</i> -butylbenzene | – | 6 | 1205 | 3.14±0.30 | – | 3.28 |
| 1,2-Dimethyl-4- <i>sec.</i> -butylbenzene | – | 6 | 1222 | 3.21±0.31 | – | 3.35 |
| 1,2-Dimethyl-4-isobutylbenzene | – | 6 | 1241 | 3.25±0.32 | – | 3.41 |
| Isopropylmesitylene | – | 6 | 1250 | 3.31±0.31 | – | 3.45 |
| <i>sec.</i> -Butylmesitylene | – | 7 | 1258 | 3.62±0.35 | – | 3.84 |
| 1,4-Dimethyl-4-butylbenzene | – | 6 | 1321 | 3.91±0.26 | – | 3.71 |
| <i>n</i> -Butylmesitylene | – | 7 | 1368 | 4.20±0.35 | – | 4.29 |
| 1,4-Di-isopentylbenzene | – | 10 | 1491 | 7.00±0.68 | – | 6.64 |
| 1,4-Di-isobutylmesitylene | – | 11 | 1640 | 7.88±0.78 | – | 8.09 |

Coefficients of (2a): $\log K_p = a \log T + bn_C + c$; $a=2.7413$; $b=0.0424$; $c=-7.0270$; $N=25$; $R=0.999$; $R^2=0.998$; $F=5489$.
Coefficients of (2b): $\log K_p = a \log I + bn_C + c$; $a=1.3186$; $b=0.0430$; $c=-3.8039$; $N=34$; $R=0.998$; $R^2=0.996$; $F=3860$.

K_p is virtually impossible. Therefore, for a rapid increase in databases, it is necessary to apply calculation methods analogous to those based on the known ‘retention–structure relationships’ approach [9].

For the calculation of K_p values we used the three-parameter correlation equation:

$$\log K_p = a \log X + bY + c \quad (2)$$

in which descriptors X and Y are weakly inter-correlated physicochemical or structural characteris-

tics of the representatives of this homologous series [6,10].

The last two columns in Table 1 contain K_p values calculated from Eq. (2). In the first case (2a) reference book [11,12] data on boiling temperatures at atmospheric pressure were used as descriptor X (nine out of the hydrocarbons listed in Table 1 are not present in these reference books). In the second case (2b), the retention indices of hydrocarbons measured on the HP-5 column served as descriptor X . The independent variable Y in Eq. (2) was the total number of carbon atoms in alkyl groups (n_C) of

the corresponding hydrocarbons. The lower lines in Table 1 contain the values of the coefficients a , b , and c in the equation for both calculation variants and those determination coefficients R^2 and the F -tests. It can be seen that in both cases there is good agreement between measured and calculated K_p values. Consequently, there is no fundamental difference between the results of calculation according to Eq. (2) when boiling temperatures or carefully determined retention indices are used as one of the variables. In practice, the choice between them may be determined by the degree of presentation of these characteristics in the available databases. For example, boiling temperatures at atmospheric pressure are extensively presented in various reference books. Hence, the K_p values and retention indices can be calculated by using this parameter. Table 2 gives K_p and I calculated in this way from Eq. (2) for 48 alkyl aromatic hydrocarbons.

Unlike hydrocarbons, many esters are not represented in databases on boiling temperatures at atmospheric pressure. This is especially true for high boiling and relatively labile esters of terpene alcohols. On the other hand, these compounds are often encountered in essential oils of plants and are rather well characterized by retention indices. For example, in Ref. [13] the values of I are given for many tens of compounds of this class. Therefore, to predict the K_p values for esters, it is reasonable to use the retention index as the independent variable X in Eq. (2).

Table 3 lists experimental and calculated (marked by an asterisk) K_p values for 170 compounds. In the case of esters of aliphatic C_1 – C_{22} alcohols, the number of carbon atoms in the molecule of the corresponding alcohol was used as the second descriptor Y in Eq. (2). In the case of esters of C_{10} – C_{20} fatty acids, it was the number of carbon atoms in the molecule of the corresponding acid. Most acetates of terpene alcohols are represented by isomers differing in the degree of formal unsaturation. Hence, to predict K_p values for 44 esters, the number of rings in the molecule was used in Eq. (2) as the parameter Y .

Table 4 gives the coefficients of regression in Eq. (2) calculated by the least-squares method using only experimentally determined K_p values. It can be seen that in all cases they are characterized by high

coefficients of determination R^2 and by the data of the F -test indicating the equation is significant at least at the 95% significance level. The least reliable values of coefficients were obtained for acetates of terpene alcohols. This is due to the fact that up to the present, K_p values were determined experimentally with sufficient accuracy only for a few representatives of this series of compounds.

The data of Tables 1–3 show that in different homologous series the values of K_p increase monotonically on passing from lower to higher homologues. For instance, for C_7 – C_{11} aromatic hydrocarbons, they range from 1 to 8, whereas for acetates of C_4 – C_{20} aliphatic alcohols they range from 0.5 to 25. In other words, the K_p values for members of these series partially overlap. This feature decreases the value of K_p as an identification characteristic. However, in Ref. [3] a close relationship between retention indices and partition coefficients was pointed out. This relationship is described by a linear equation of the form:

$$\log K_p = kI + j. \quad (3)$$

Fig. 1 shows that straight lines of the plot in a system of coordinates $\log K_p$ – I referring to different

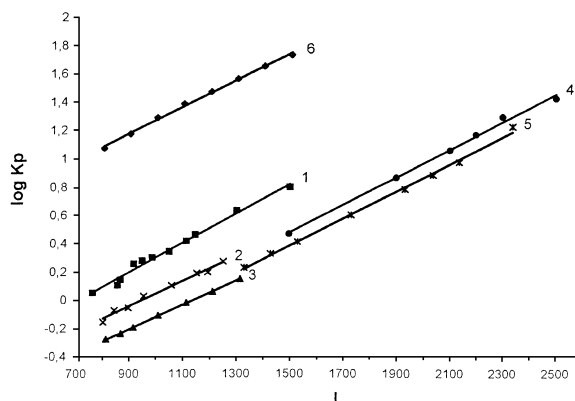


Fig. 1. Plots of $\log K_p$ against retention indices: (1) aromatic hydrocarbons ($y = 0.001x - 0.7318$; $R^2 = 0.987$, $F = 683$); (2) butanoate of aliphatic C_1 – C_6 alcohols ($y = 0.0009x - 0.84319$; $R^2 = 0.986$, $F = 423$); (3) acetates of aliphatic C_1 – C_6 alcohols ($y = 0.0009x - 0.9763$; $R^2 = 0.999$, $F = 4995$); (4) propyl esters of C_{10} – C_{20} carboxylic acids ($y = 0.001x - 0.9937$; $R^2 = 0.996$, $F = 996$); (5) methyl esters of C_{10} – C_{20} carboxylic acids ($y = 0.001x - 1.0625$; $R^2 = 0.997$, $F = 1994$); (6) n -alkanes C_8 – C_{15} ($y = 0.0009x + 0.3439$; $R^2 = 0.997$, $F = 1994$).

Table 2

Calculation of K_p and I values for alkyl aromatic hydrocarbons according to Eq. (2) (variable parameters X and Y are the boiling point and the number of carbon atoms in the side chain in the molecule, respectively)

| Hydrocarbon | Boiling point (K) | n_c | K_p^{calc} | I^{calc} |
|--|-------------------|-------|---------------------|-------------------|
| 1-Methyl-3-ethylbenzene | 434.45 | 3 | 1.81 | 960 |
| 1-Methyl-4-ethylbenzene | 435.14 | 3 | 1.82 | 963 |
| 1-Methyl-2-ethylbenzene | 438.30 | 3 | 1.86 | 976 |
| <i>tert.</i> -Butylbenzene | 442.27 | 4 | 2.10 | 993 |
| <i>sec.</i> -Butylbenzene | 446.45 | 4 | 2.15 | 1012 |
| <i>o</i> -Cymene | 451.50 | 4 | 2.22 | 1034 |
| 1-Methyl-3-propylbenzene | 454.90 | 4 | 2.26 | 1049 |
| 1,3-Dimethyl-5-ethylbenzene | 456.15 | 4 | 2.28 | 1055 |
| 1-Methyl-2-propylbenzene | 457.90 | 4 | 2.30 | 1063 |
| 1,4-Dimethyl-2-ethylbenzene | 460.06 | 4 | 2.33 | 1072 |
| 1,2-Dimethyl-4-ethylbenzene | 462.15 | 4 | 2.36 | 1082 |
| 1-Methyl-3- <i>tert.</i> -butylbenzene | 462.41 | 5 | 2.61 | 1083 |
| 1,2,3,4-Tetramethylbenzene | 463.05 | 4 | 2.38 | 1086 |
| 1,3-Dimethyl-2-ethylbenzene | 463.25 | 4 | 2.38 | 1087 |
| 1-Isopropyl-3-ethylbenzene | 465.15 | 5 | 2.65 | 1095 |
| 1-Methyl-4- <i>tert.</i> -butylbenzene | 465.91 | 5 | 2.66 | 1099 |
| 1,2-Dimethyl-3-ethylbenzene | 467.06 | 4 | 2.43 | 1104 |
| 1-Methyl-3-isobutylbenzene | 467.15 | 5 | 2.68 | 1104 |
| 1-Methyl-3- <i>sec.</i> -butylbenzene | 467.15 | 5 | 2.68 | 1104 |
| 1,3-Dimethyl-5-isopropylbenzene | 467.65 | 5 | 2.69 | 1107 |
| 1-Propyl-4-ethylbenzene | 467.65 | 5 | 2.69 | 1107 |
| 2-Methyl-4-phenylbutane | 468.45 | 5 | 2.70 | 1110 |
| 1-Methyl-4-isobutylbenzene | 469.15 | 5 | 2.71 | 1114 |
| 1-Methyl-4- <i>sec.</i> -butylbenzene | 469.15 | 5 | 2.71 | 1114 |
| 1,4-Dimethyl-2-isopropylbenzene | 469.35 | 5 | 2.72 | 1114 |
| 1-Isopropyl-4-ethylbenzene | 469.75 | 5 | 2.72 | 1116 |
| 1-Methyl-2- <i>sec.</i> -butylbenzene | 470.15 | 5 | 2.73 | 1118 |
| 1-Methyl-3-butylbenzene | 470.65 | 5 | 2.74 | 1120 |
| 1,2,4,5-Tetramethylbenzene | 471.15 | 4 | 2.49 | 1123 |
| Isopentylbenzene | 471.65 | 5 | 2.75 | 1125 |
| 1-Methyl-4-butylbenzene | 471.65 | 5 | 2.75 | 1125 |
| 1,3-Diethyl-5-methylbenzene | 472.15 | 5 | 2.76 | 1127 |
| 2,4-Dimethyl-1-isopropylbenzene | 472.25 | 5 | 2.76 | 1128 |
| 1-Methyl-2- <i>tert.</i> -butylbenzene | 473.60 | 5 | 2.78 | 1134 |
| 1-Methyl-2-butylbenzene | 473.65 | 5 | 2.78 | 1134 |
| 1,3-Dimethyl-5-propylbenzene | 475.45 | 5 | 2.81 | 1143 |
| 1,3-Di-isopropylbenzene | 476.35 | 6 | 3.12 | 1146 |
| 1,4-Dimethyl-2-propylbenzene | 477.45 | 5 | 2.39 | 1152 |
| 1,2,3,5-Tetramethylbenzene | 478.15 | 4 | 2.59 | 1156 |
| 2,4-Dimethyl-1-propylbenzene | 479.75 | 5 | 2.88 | 1163 |
| 1,4-Di-isopropylbenzene | 483.15 | 6 | 3.24 | 1178 |
| 1-Isobutyl-4-ethylbenzene | 484.15 | 6 | 3.26 | 1183 |
| Isohexylbenzene | 487.65 | 6 | 3.32 | 1200 |
| 1,4-Di- <i>tert.</i> -butylbenzene | 509.65 | 8 | 4.56 | 1306 |
| Hexamethylbenzene | 538.15 | 6 | 4.34 | 1454 |
| 1,2,3,5-Tetraethylbenzene | 523.15 | 8 | 4.89 | 1374 |
| 1,2,3,4-Tetraethylbenzene | 524.15 | 8 | 4.92 | 1380 |
| Hexaethylbenzene | 571.15 | 12 | 9.17 | 1627 |

Table 3
Retention indices and K_p values of esters

| No. | Compound | Formula | I^{lit} [13] | $I^{exp} \pm \sigma$ | $K_p \pm \sigma$ |
|------------------|------------------------------------|--|----------------|----------------------|------------------|
| Aliphatic esters | | | | | |
| 1 | Butyl formate | C ₅ H ₁₀ O ₂ | – | 737±2 | 0.33±0.04 |
| 2 | Isopentyl formate | C ₆ H ₁₂ O ₂ | 792 | 792±2 | 0.39±0.04 |
| 3 | <i>n</i> -Pentyl formate | C ₆ H ₁₂ O ₂ | – | 825±2 | 0.39±0.04 |
| 4 | <i>n</i> -Hexyl formate | C ₇ H ₁₄ O ₂ | – | 927±3 | 0.46±0.08 |
| 5 | Ethyl acetate | C ₄ H ₈ O ₂ | 630 | – | 0.50* |
| 6 | <i>n</i> -Propyl acetate | C ₅ H ₁₀ O ₂ | 719 | – | 0.58* |
| 7 | <i>n</i> -Butyl acetate | C ₆ H ₁₂ O ₂ | 812 | 812±1 | 0.53±0.05 |
| 8 | Isopentyl acetate | C ₇ H ₁₄ O ₂ | 876 | 867±2 | 0.58±0.02 |
| 9 | <i>n</i> -Pentyl acetate | C ₇ H ₁₄ O ₂ | 915 | 916±2 | 0.64±0.03 |
| 10 | <i>n</i> -Hexyl acetate | C ₈ H ₁₆ O ₂ | 1008 | 1008±2 | 0.78±0.04 |
| 11 | <i>n</i> -Heptyl acetate | C ₉ H ₁₈ O ₂ | 1113 | 1112±2 | 0.96±0.04 |
| 12 | <i>n</i> -Octyl acetate | C ₁₀ H ₂₀ O ₂ | 1211 | 1210±2 | 1.15±0.04 |
| 13 | <i>n</i> -Nonyl acetate | C ₁₁ H ₂₂ O ₂ | 1312 | – | 1.41* |
| 14 | <i>n</i> -Decyl acetate | C ₁₂ H ₂₄ O ₂ | 1409 | – | 1.74* |
| 15 | <i>n</i> -Dodecanol acetate | C ₁₄ H ₂₈ O ₂ | – | 1610±2 | 2.65±0.36 |
| 16 | <i>n</i> -Tridecanol acetate | C ₁₅ H ₃₀ O ₂ | – | 1710±2 | 3.14±0.40 |
| 17 | <i>n</i> -Tetradecanol acetate | C ₁₆ H ₃₂ O ₂ | – | 1810±2 | 4.24±0.72 |
| 18 | <i>n</i> -Pentadecanol acetate | C ₁₇ H ₃₄ O ₂ | – | 1911±2 | 5.05±0.63 |
| 19 | <i>n</i> -Hexadecanol acetate | C ₁₈ H ₃₆ O ₂ | – | 2009±2 | 6.22±0.59 |
| 20 | <i>n</i> -Octadecanol acetate | C ₂₀ H ₄₀ O ₂ | 2210 | 2211±2 | 9.26±0.87 |
| 21 | <i>n</i> -Eicosanol acetate | C ₂₂ H ₄₄ O ₂ | – | 2413±2 | 14.33±0.92 |
| 22 | <i>n</i> -Docosanol acetate | C ₂₄ H ₄₈ O ₂ | – | 2613±2 | 24.42±2.82 |
| 23 | Ethyl propanoate | C ₅ H ₁₀ O ₂ | 714 | 714±2 | 0.45±0.05 |
| 24 | Propyl propanoate | C ₆ H ₁₂ O ₂ | 806 | – | 0.59* |
| 25 | <i>sec</i> -Butyl propanoate | C ₇ H ₁₄ O ₂ | – | 889±2 | 0.74±0.02 |
| 26 | <i>n</i> -Butyl propanoate | C ₇ H ₁₄ O ₂ | – | 908±3 | 0.75±0.04 |
| 27 | Isopentyl propanoate | C ₈ H ₁₆ O ₂ | – | 969±3 | 0.94±0.03 |
| 28 | <i>n</i> -Pentyl propanoate | C ₈ H ₁₆ O ₂ | 972 | – | 0.94* |
| 29 | Methyl butanoate | C ₄ H ₈ O ₂ | 724 | 724±1 | 0.64±0.08 |
| 30 | Ethyl butanoate | C ₆ H ₁₂ O ₂ | 800 | 800±2 | 0.70±0.08 |
| 31 | Isopropyl butanoate | C ₇ H ₁₄ O ₂ | 842 | 843±2 | 0.85±0.03 |
| 32 | <i>n</i> -Propyl butanoate | C ₇ H ₁₄ O ₂ | 896 | 896±2 | 0.88±0.04 |
| 33 | <i>sec</i> -Butyl butanoate | C ₈ H ₁₆ O ₂ | – | 953±3 | 1.07±0.04 |
| 34 | <i>n</i> -Butyl butanoate | C ₈ H ₁₆ O ₂ | 993 | – | 1.04* |
| 35 | <i>n</i> -Pentyl isobutanoate | C ₉ H ₁₈ O ₂ | 1057 | – | 1.27* |
| 36 | Isopentyl butanoate | C ₉ H ₁₈ O ₂ | 1060 | 1060±3 | 1.26±0.02 |
| 37 | <i>n</i> -Pentyl butanoate | C ₉ H ₁₈ O ₂ | 1093 | 1094±2 | 1.23±0.04 |
| 38 | <i>n</i> -Hexyl isobutanoate | C ₁₀ H ₂₀ O ₂ | 1150 | – | 1.55* |
| 39 | Hexyl butanoate | C ₁₀ H ₂₀ O ₂ | 1191 | 1190±3 | 1.57±0.05 |
| 40 | <i>n</i> -Heptyl isobutanoate | C ₁₁ H ₂₂ O ₂ | 1248 | – | 1.88* |
| 41 | Isopropyl 3-methyl butanoate | C ₈ H ₁₆ O ₂ | – | 904±4 | 1.02±0.04 |
| 42 | Isobutyl 3-methyl butanoate | C ₉ H ₁₈ O ₂ | – | 1006±3 | 1.35±0.08 |
| 43 | Methyl pentanoate | C ₆ H ₁₂ O ₂ | 825 | 825±3 | 0.89±0.03 |
| 44 | Ethyl pentanoate | C ₇ H ₁₄ O ₂ | 898 | 898±3 | 1.07±0.02 |
| 45 | Isopentyl 2-methyl butanoate | C ₁₀ H ₂₀ O ₂ | 1099 | – | 1.63* |
| 46 | Isopentyl 3-methyl butanoate | C ₁₀ H ₂₀ O ₂ | 1103 | – | 1.64* |
| 47 | <i>n</i> -Hexyl 2-methyl butanoate | C ₁₁ H ₂₂ O ₂ | 1234 | – | 2.09* |
| 48 | <i>n</i> -Hexyl 3-methyl butanoate | C ₁₁ H ₂₂ O ₂ | 1243 | – | 2.12* |
| 49 | Ethyl hexanoate | C ₈ H ₁₆ O ₂ | 996 | 998±2 | 1.61±0.03 |

Table 3. Continued

| No. | Compound | Formula | I^{lit} [13] | $I^{\text{exp}} \pm \sigma$ | $K_p \pm \sigma$ |
|-----------------------------|---|--|-----------------------|-----------------------------|------------------|
| 50 | Propyl hexanoate | C ₉ H ₁₈ O ₂ | 1092 | 1089±3 | 2.00±0.03 |
| 51 | Butyl hexanoate | C ₁₀ H ₂₀ O ₂ | 1188 | 1188±3 | 2.50±0.03 |
| 52 | Pentyl hexanoate | C ₁₁ H ₂₂ O ₂ | – | 1287±3 | 3.14±0.03 |
| 53 | Hexyl hexanoate | C ₁₂ H ₂₄ O ₂ | 1383 | 1382±2 | 4.01±0.03 |
| 54 | Methyl decanoate | C ₁₁ H ₂₂ O ₂ | 1326 | 1326±2 | 1.70±0.80 |
| 55 | Methyl undecanoate | C ₁₂ H ₂₄ O ₂ | 1425 | – | 2.12* |
| 56 | Methyl dodecanoate | C ₁₃ H ₂₆ O ₂ | 1525 | 1527±2 | 2.58±0.17 |
| 57 | Methyl tridecanoate | C ₁₄ H ₂₈ O ₂ | 1626 | – | 3.12* |
| 58 | Methyl tetradecanoate | C ₁₅ H ₃₀ O ₂ | 1726 | 1728±2 | 4.00±0.34 |
| 59 | Methyl pentadecanoate | C ₁₆ H ₃₂ O ₂ | 1827 | – | 4.86* |
| 60 | Methyl hexadecanoate | C ₁₇ H ₃₄ O ₂ | 1927 | 1929±2 | 6.09±0.45 |
| 61 | Methyl heptadecanoate | C ₁₈ H ₃₆ O ₂ | – | 2030±2 | 7.69±0.64 |
| 62 | Methyl octadecanoate | C ₁₉ H ₃₈ O ₂ | 2128 | 2130±2 | 9.50±0.15 |
| 63 | Methyl nonadecanoate | C ₂₀ H ₄₀ O ₂ | 2228 | – | 12.80* |
| 64 | Methyl eicosanoate | C ₂₁ H ₄₂ O ₂ | – | 2332±2 | 17.02±3.32 |
| 65 | Ethyl decanoate | C ₁₂ H ₂₄ O ₂ | 1394 | 1399±2 | 2.27 |
| 66 | Ethyl undecanoate | C ₁₃ H ₂₆ O ₂ | 1493 | – | 2.85* |
| 67 | Ethyl dodecanoate | C ₁₄ H ₂₈ O ₂ | 1593 | – | 3.60* |
| 68 | Ethyl tridecanoate | C ₁₅ H ₃₀ O ₂ | 1693 | – | 4.52* |
| 69 | Ethyl tetradecanoate | C ₁₆ H ₃₂ O ₂ | 1793 | 1798±2 | 5.60 |
| 70 | Ethyl hexadecanoate | C ₁₈ H ₃₆ O ₂ | 1993 | 1999±2 | 8.87 |
| 71 | Ethyl heptadecanoate | C ₁₉ H ₃₈ O ₂ | – | 2098±2 | 11.08 |
| 72 | Ethyl octadecanoate | C ₂₀ H ₄₀ O ₂ | 2194 | 2199±2 | 13.77 |
| 73 | Ethyl nonadecanoate | C ₂₁ H ₄₂ O ₂ | 2294 | – | 16.88* |
| 74 | Ethyl eicosanoate | C ₂₂ H ₄₄ O ₂ | – | 2400±2 | 20.74±1.06 |
| 75 | Propyl decanoate | C ₁₃ H ₂₆ O ₂ | – | 1493±2 | 2.93 |
| 76 | Propyl undecanoate | C ₁₄ H ₂₈ O ₂ | 1592 | – | 3.72* |
| 77 | Propyl dodecanoate | C ₁₅ H ₃₀ O ₂ | 1692 | – | 4.73* |
| 78 | Propyl tridecanoate | C ₁₆ H ₃₂ O ₂ | 1792 | – | 5.99* |
| 79 | Propyl tetradecanoate | C ₁₇ H ₃₄ O ₂ | – | 1893±2 | 7.39 |
| 80 | Propyl pentadecanoate | C ₁₈ H ₃₆ O ₂ | 1992 | – | 9.47* |
| 81 | Propyl hexadecanoate | C ₁₉ H ₃₈ O ₂ | – | 2094±2 | 11.51 |
| 82 | Propyl heptadecanoate | C ₂₀ H ₄₀ O ₂ | – | 2193±2 | 14.81 |
| 83 | Propyl octadecanoate | C ₂₁ H ₄₂ O ₂ | – | 2294±2 | 19.81 |
| 84 | Propyl nonadecanoate | C ₂₂ H ₄₄ O ₂ | 2392 | – | 22.64* |
| 85 | Propyl eicosanoate | C ₂₃ H ₄₆ O ₂ | – | 2495±2 | 26.93 |
| Esters of aromatic alcohols | | | | | |
| 86 | Benzyl acetate | C ₉ H ₁₀ O ₂ | 1163 | 1163±1 | 0.13±0.01 |
| 87 | 1-Phenyl ethyl acetate (stralyl acetate) | C ₁₀ H ₁₂ O ₂ | 1192 | 1194±1 | 0.18±0.01 |
| 88 | Phenyl propyl acetate | C ₁₁ H ₁₄ O ₂ | – | 1370±1 | 0.19±0.01 |
| 89 | 4-Phenyl 2-butyl acetate | C ₁₂ H ₁₆ O ₂ | – | 1423±1 | 0.26±0.02 |
| 90 | Phenyl pentyl acetate | C ₁₃ H ₁₈ O ₂ | – | 1492±1 | 0.40±0.01 |
| 91 | Carvacrol acetate | C ₁₂ H ₁₆ O ₂ | 1371 | 1369±1 | 0.09±0.01 |
| 92 | <i>p</i> -Anisyl acetate | C ₁₀ H ₁₂ O ₂ | 1416 | 1419±1 | 0.06±0.01 |
| 93 | Cinnamyl acetate (<i>E</i>) | C ₁₁ H ₁₂ O ₂ | 1443 | 1444±1 | 0.10±0.01 |
| 94 | Allyl phenoxy acetate | C ₈ H ₈ O ₃ | – | 1452±1 | 0.04±0.01 |
| 95 | Phenyl ethyl 3-methyl butanoate | C ₁₃ H ₁₈ O ₂ | 1489 | 1490±1 | 0.35±0.01 |
| 96 | Isoeugenol acetate (<i>E</i>) | C ₁₂ H ₁₄ O ₂ | 1611 | 1617±7 | 0.06±0.01 |
| 97 | Cinnamyl pentyl acetate (<i>Z</i>) | C ₁₆ H ₂₂ O ₂ | – | 1761±1 | 0.68±0.01 |
| 98 | Cinnamyl pentyl acetate (<i>E</i>) | C ₁₆ H ₂₂ O ₂ | – | 1781±1 | 0.54±0.01 |

Table 3. Continued

| No. | Compound | Formula | I^{lit} [13] | $I^{\text{exp}} \pm \sigma$ | $K_p \pm \sigma$ |
|------------------------------|--|--|-----------------------|-----------------------------|------------------|
| Acetates of terpene alcohols | | | | | |
| 99 | Linalool | C ₁₂ H ₂₀ O ₂ | 1257 | 1257±2 | 0.93±0.04 |
| 100 | Chrysanthenyl, <i>cis</i> - | C ₁₂ H ₁₈ O ₂ | 1262 | 1261±1 | 1.12±0.03 |
| 101 | Isobornyl | C ₁₂ H ₂₀ O ₂ | 1285 | 1289±2 | 1.14±0.04 |
| 102 | Bornyl | C ₁₂ H ₂₀ O ₂ | 1285 | 1291±2 | 1.28±0.04 |
| 103 | Sabiny, <i>trans</i> - | C ₁₂ H ₁₈ O ₂ | 1291 | 1291±2 | 1.17±0.03 |
| 104 | Verbenyl, <i>trans</i> - | C ₁₂ H ₁₈ O ₂ | 1292 | 1294±3 | 1.24±0.04 |
| 105 | α-Terpenyl | C ₁₂ H ₂₀ O ₂ | 1350 | 1351±1 | 1.26±0.06 |
| 106 | Citronellyl | C ₁₂ H ₂₂ O ₂ | 1354 | 1355±1 | 1.18±0.04 |
| 107 | Santolyl | C ₁₂ H ₂₀ O ₂ | 1171 | – | 0.75* |
| 108 | Artemisyl | C ₁₂ H ₂₀ O ₂ | 1173 | – | 0.75* |
| 109 | Myrcenol, dihydro- | C ₁₂ H ₂₂ O ₂ | 1215 | – | 0.84* |
| 110 | Sabinene hydrate, <i>cis</i> - | C ₁₂ H ₂₀ O ₂ | 1219 | – | 1.01* |
| 111 | Fenchyl, <i>endo</i> - | C ₁₂ H ₂₀ O ₂ | 1220 | – | 1.02* |
| 112 | Fenchyl, <i>exo</i> - | C ₁₂ H ₂₀ O ₂ | 1234 | – | 1.05* |
| 113 | Myrtenyl | C ₁₂ H ₁₈ O ₂ | 1235 | – | 1.06* |
| 114 | Sabinenehydrate, <i>trans</i> - | C ₁₂ H ₂₀ O ₂ | 1253 | – | 1.10* |
| 115 | Lavandulol, tetrahydro- | C ₁₂ H ₂₄ O ₂ | 1270 | – | 0.96* |
| 116 | 3-Thujyl, <i>neo</i> - | C ₁₂ H ₂₀ O ₂ | 1271 | – | 1.15* |
| 117 | Isopulegol | C ₁₂ H ₂₀ O ₂ | 1273 | – | 1.06* |
| 118 | Isopulegol, <i>neo</i> - | C ₁₂ H ₂₀ O ₂ | 1273 | – | 1.06* |
| 119 | Menthyl, <i>neo</i> - | C ₁₂ H ₂₂ O ₂ | 1275 | – | 1.06* |
| 120 | 3-Thujyl, <i>neo</i> -, <i>iso</i> - | C ₁₂ H ₂₀ O ₂ | 1278 | – | 1.17* |
| 121 | Isopulegol, <i>iso</i> - | C ₁₂ H ₂₀ O ₂ | 1281 | – | 1.08* |
| 122 | Verbenyl, <i>cis</i> - | C ₁₂ H ₁₈ O ₂ | 1282 | – | 1.18* |
| 123 | Lavandulil | C ₁₂ H ₂₀ O ₂ | 1289 | – | 1.01* |
| 124 | 3-Thujyl, <i>trans</i> - | C ₁₂ H ₂₀ O ₂ | 1291 | – | 1.21* |
| 125 | Menthyl | C ₁₂ H ₂₂ O ₂ | 1294 | – | 1.11* |
| 126 | Pinocarvyl, <i>trans</i> - | C ₁₂ H ₁₈ O ₂ | 1297 | – | 1.23* |
| 127 | α-Terpenyl, dihydro-, <i>cis</i> - | C ₁₂ H ₂₂ O ₂ | 1298 | – | 1.13* |
| 128 | 3-Thujyl, <i>iso</i> - | C ₁₂ H ₂₀ O ₂ | 1301 | – | 1.24* |
| 129 | Dihydrocarveol, <i>neo</i> - | C ₁₂ H ₂₀ O ₂ | 1303 | – | 1.14* |
| 130 | Dihydrocarveol | C ₁₂ H ₂₀ O ₂ | 1305 | – | 1.14* |
| 131 | Verbanol, <i>iso</i> - | C ₁₂ H ₂₀ O ₂ | 1306 | – | 1.25* |
| 132 | Isomenthyl | C ₁₂ H ₂₂ O ₂ | 1306 | – | 1.15* |
| 133 | Isopulegol, <i>neo</i> -, <i>iso</i> - | C ₁₂ H ₂₀ O ₂ | 1308 | – | 1.15* |
| 134 | Pinocarvyl, <i>cis</i> - | C ₁₂ H ₁₈ O ₂ | 1309 | – | 1.26* |
| 135 | α-Terpenyl, dihydro-, <i>trans</i> - | C ₁₂ H ₂₂ O ₂ | 1315 | – | 1.17* |
| 136 | Verbanol, <i>neo</i> - | C ₁₂ H ₂₀ O ₂ | 1318 | – | 1.29* |
| 137 | Dihydro citronellol | C ₁₂ H ₂₄ O ₂ | 1320 | – | 1.08* |
| 138 | Dihydrocarveol, <i>iso</i> - | C ₁₂ H ₂₀ O ₂ | 1325 | – | 1.20* |
| 139 | Verbanol, <i>neo</i> -, <i>iso</i> - | C ₁₂ H ₂₀ O ₂ | 1328 | – | 1.32* |
| 140 | Piperitol, <i>cis</i> - | C ₁₂ H ₂₀ O ₂ | 1330 | – | 1.21* |
| 141 | Carvyl, <i>trans</i> - | C ₁₂ H ₁₈ O ₂ | 1337 | – | 1.23* |
| 142 | Piperitol, <i>trans</i> - | C ₁₂ H ₂₀ O ₂ | 1340 | – | 1.24* |
| 143 | Verbanol | C ₁₂ H ₂₀ O ₂ | 1340 | – | 1.35* |
| 144 | Terpin-4-ol | C ₁₂ H ₂₀ O ₂ | 1340 | – | 1.24* |
| 145 | Dihydrocarveol, <i>neo</i> - | C ₁₂ H ₂₀ O ₂ | 1356 | – | 1.29* |
| 146 | Neryl | C ₁₂ H ₂₀ O ₂ | 1365 | – | 1.20* |
| 147 | Carvyl, <i>cis</i> - | C ₁₂ H ₁₈ O ₂ | 1362 | – | 1.31* |
| 148 | Myrtanol, <i>trans</i> - | C ₁₂ H ₂₀ O ₂ | 1381 | – | 1.49* |
| 149 | Geranyl | C ₁₂ H ₂₀ O ₂ | 1383 | – | 1.25* |
| 150 | 1- <i>p</i> -Menthen-9-yl | C ₁₂ H ₂₀ O ₂ | 1420 | – | 1.49* |

Table 3. Continued

| No. | Compound | Formula | I^{lit} [13] | $I^{\text{exp}} \pm \sigma$ | $K_p \pm \sigma$ |
|------------------------------------|--|-------------------|-----------------------|-----------------------------|------------------|
| Acetates of sesquiterpene alcohols | | | | | |
| 151 | Caryophyllene | $C_{17}H_{28}O_2$ | 1700 | 1704 ± 1 | 2.90 ± 0.10 |
| 152 | Nerolidol (<i>E</i>) | $C_{17}H_{28}O_2$ | 1714 | 1715 ± 2 | 2.60 ± 0.25 |
| 153 | Guaiol | $C_{17}H_{28}O_2$ | 1724 | 1727 ± 1 | 2.84 ± 0.10 |
| 154 | γ -Eudesmol | $C_{17}H_{28}O_2$ | 1778 | 1778 ± 1 | 3.37 |
| 155 | Amboryl (acetoxymethyl-isolongifolene) | $C_{18}H_{28}O_2$ | – | 1782 ± 1 | 2.24 ± 0.10 |
| 156 | α -Bisabolol | $C_{17}H_{28}O_2$ | 1796 | 1797 ± 1 | 3.13 ± 0.10 |
| 157 | Farnesyl | $C_{17}H_{28}O_2$ | 1818 | 1820 ± 2 | 4.99 ± 0.18 |
| Other esters | | | | | |
| 158 | 3-Hexenol acetate (<i>Z</i>) | $C_8H_{14}O_2$ | 1007 | 1007 ± 1 | 0.45 ± 0.01 |
| 159 | Citronellyl formate | $C_{11}H_{20}O_2$ | 1275 | 1271 ± 1 | 0.70 ± 0.04 |
| 160 | Linalool propanoate | $C_{13}H_{22}O_2$ | – | 1340 ± 1 | 1.33 ± 0.09 |
| 161 | Nopyl acetate | $C_{13}H_{20}O_2$ | 1424 | 1327 ± 1 | 1.23 ± 0.06 |
| 162 | Citryl acetate | $C_{13}H_{20}O_2$ | – | 1517 ± 2 | 0.84 ± 0.02 |
| 163 | Geranyl butanoate | $C_{14}H_{24}O_2$ | 1562 | 1564 | 1.73 ± 0.05 |
| Lactones | | | | | |
| 164 | γ -Octalactone | $C_8H_{14}O_2$ | – | 1256 ± 1 | 0.07 ± 0.01 |
| 165 | Octalactone, β -methyl | $C_9H_{16}O_2$ | – | 1290 ± 2 | 0.10 ± 0.01 |
| 166 | γ -Nonalactone | $C_9H_{16}O_2$ | 1360 | 1362 ± 1 | 0.08 ± 0.01 |
| 167 | γ -Decalactone | $C_{10}H_{18}O_2$ | 1463 | 1467 ± 1 | 0.10 ± 0.02 |
| 168 | δ -Decalactone | $C_{10}H_{18}O_2$ | 1493 | 1500 ± 1 | 0.31 ± 0.02 |
| 169 | γ -Undecalactone | $C_{11}H_{20}O_2$ | – | 1574 ± 1 | 0.13 ± 0.01 |
| 170 | δ -Dodecalactone | $C_{12}H_{22}O_2$ | – | 1711 ± 1 | 0.34 ± 0.02 |

groups of homologues have approximately the same slope. This fact implies that the coefficient k in Eq. (3) characterizes the given heterogeneous system: for the hexane–acetonitrile system $k = (1.1 \pm 0.2) \times 10^{-3}$ whereas for the hexane–nitromethane system it is $(1.33 \pm 0.30) \times 10^{-3}$. At the same time the coefficient j in this equation is the characteristic of members of

a certain homologous series. Hence, it can be used as a group identification parameter. Table 5 gives the values of the parameter j obtained in this work and calculated from data obtained in Ref. [6] for representatives of some classes of organic compounds. This table shows that although the K_p values for the representatives of a certain homologous series can

Table 4

Regression coefficients of the equation $\log K_p = a \log I + bn_C + c$

| Esters | N | a | b | c | R^2 | F |
|--|-----|---------|---------|---------|-------|------|
| Formate | 4 | 1.2520 | 0.0098 | –4.1100 | 0.999 | 499 |
| Acetate C_4 – C_{22} | 14 | –0.2796 | 0.0997 | 0.1248 | 0.999 | 5494 |
| Propanoate | 4 | 0.3147 | 0.08943 | –1.4144 | 0.998 | 245 |
| Butanoate | 7 | –0.0156 | 0.08552 | –0.2762 | 0.994 | 331 |
| Pentanoate | 4 | 3.2430 | –0.0325 | –9.4790 | 0.999 | 499 |
| Hexanoate | 5 | –1.2599 | 0.14369 | 3.6973 | 0.999 | 999 |
| Methyl esters of C_{10} – C_{20} acids | 7 | –2.7716 | 0.1650 | 7.2451 | 0.997 | 665 |
| Ethyl esters of C_{10} – C_{20} acids | 6 | 0.8691 | 0.0762 | –3.1416 | 0.999 | 1498 |
| Propyl esters of C_{10} – C_{20} acids | 6 | 1.5442 | 0.0639 | –5.0775 | 0.997 | 498 |
| Aryl acetate | 5 | –4.7470 | 0.2474 | 11.4390 | 0.993 | 142 |
| Acetate of terpene alcohols | 8 | 3.1006 | 0.0390 | –9.6406 | 0.876 | 17.7 |
| γ -Lactone | 5 | –3.6681 | 0.2097 | 8.5237 | 0.986 | 70.4 |

Table 5
Limits of K_p and average $j \pm \sigma$ values of several group of organic compounds

| Compounds | <i>N</i> | Range of <i>I</i> values | Range of K_p values | $j \pm \sigma$ |
|--|----------|--------------------------|-----------------------|----------------|
| <i>n</i> -Alkane C ₈ –C ₁₅ | 8 | 800–1500 | 11.9–53.6 | –0.27±0.03 |
| Monoterpene C ₁₀ H ₁₆ hydrocarbons | 12 | 896–1088 | 3.99–7.99 | 0.28±0.19 |
| Sesquiterpene C ₁₅ H ₂₄ Hydrocarbons | 10 | 1428–1528 | 6.0–11.0 | 0.55±0.09 |
| Alkyl aromatic C ₇ –C ₁₈ hydrocarbons | 34 | 760–1640 | 1.07–7.88 | 0.70±0.02 |
| Hexanoate of aliphatic C ₂ –C ₆ alcohols | 5 | 996–1382 | 1.61–4.01 | 0.79±0.01 |
| Pentanoate of aliphatic C ₃ –C ₅ alcohols | 8 | 825–1243 | 0.89–1.35 | 0.88±0.01 |
| Butanoate of aliphatic C ₁ –C ₆ alcohols | 9 | 800–1190 | 0.64–1.00 | 0.96±0.04 |
| Propyl esters of C ₁₀ –C ₂₀ carboxylic acids | 6 | 1493–2495 | 2.93–26.9 | 1.01±0.02 |
| Propanoate of aliphatic C ₂ –C ₅ alcohols | 5 | 714–969 | 0.46–0.94 | 1.02±0.02 |
| Ethyl esters of C ₁₀ –C ₂₀ carboxylic acids | 6 | 1394–2400 | 2.27–20.7 | 1.04±0.01 |
| Methyl esters of C ₁₀ –C ₂₀ carboxylic acids | 7 | 1326–2332 | 1.7–17.0 | 1.12±0.02 |
| Acetate of aliphatic C ₄ –C ₂₂ alcohols | 14 | 812–2613 | 0.53–22.4 | 1.17±0.05 |
| Terpene epoxide | 9 | 1072–1585 | 0.38–4.3 | 1.22±0.20 |
| Formate of aliphatic C ₄ –C ₆ alcohols | 4 | 737–927 | 0.33–0.46 | 1.23±0.03 |
| Acetate of monoterpene alcohols | 8 | 1171–1420 | 0.93–1.28 | 1.24±0.04 |
| Acetate of sesquiterpene alcohols | 7 | 1700–1782 | 2.24–4.99 | 1.32±0.09 |
| Monoterpene carbonyls | 6 | 1087–1271 | 0.38–0.60 | 1.48±0.15 |
| Monoterpene alcohols | 7 | 1100–1227 | 0.25–0.50 | 1.62±0.09 |
| Sesquiterpene alcohols | 16 | 1537–1759 | 0.52–1.10 | 1.71±0.09 |
| Acetate of phenyl alkyl alcohols | 5 | 1192–1781 | 0.13–0.40 | 2.00±0.08 |
| Lactones | 7 | 1256–1711 | 0.08–0.34 | 2.32±0.17 |

vary 5–10-fold, the average value of the parameter *j* falls in a narrow range, which usually is in the limits of ±5% rel.

Consequently, the joint use of partition coefficients and retention indices makes it possible to carry out a two-stage identification algorithm. In the first stage, the component is assigned to a certain homologous series (or to a limited number of these series) from the calculated *j* value. Then it is identified from the retention index within the chosen series. The *m/z* value of the maximum peak in the compound's mass spectrum can be used as an additional identification characteristic if the GC analysis proceeds in combination with low-resolution mass spectrometry. This approach makes it possible to exclude identification errors based on the comparison of mass spectra recorded during analyses and those contained in the computer memory [4,5].

References

- [1] M. Beroza, M.C. Bowman, *Anal. Chem.* 37 (1965) 291.
- [2] V.G. Berezkin, V.D. Loshilova, A.G. Pankov, V.D. Yagodovskii, *Khromato-Raspredelitelnyi Metod*, Nauka, Moscow, 1976, in Russian.
- [3] I.G. Zenkevich, A.V. Vasil'ev, *Russ. J. Anal. Chem.* 48 (1993) 473, in Russian.
- [4] V.A. Isidorov, U. Krajewska, J. Jaroszynska, K. Bal, A. Niesluchowska, L. Vetchinnikova, I. Fuksman, *Chem. Anal. (Warsaw)* 45 (2000) 513.
- [5] V.A. Isidorov, I.G. Zenkevich, U. Krajewska, E.N. Dubis, J. Jaroszynska, K. Bal, *Phytochem. Anal.* 12 (2001) 87.
- [6] V.A. Isidorov, I.G. Zenkevich, E.N. Dubis, A. Slowikowski, E. Wojciuk, *J. Chromatogr. A* 814 (1998) 253.
- [7] R.J. Hamilton, S. Hamilton, *Lipid Analysis. A Practical Approach*, Oxford University Press, New York, 1992.
- [8] K. Blau, J. Hockett, *Handbook of Derivatives for Chromatography*, J. Wiley, Chichester, 1993.
- [9] R. Kaliszan, *Quantitative Structure–Chromatographic Retention Relationships*, Wiley, New York, 1987.
- [10] V. Isidorov, I. Zenkevich, T. Sacharewicz, *Chem. Anal. (Warsaw)* 42 (1997) 627.
- [11] *Reference Book of Chemist*, Vol. 2, Khimiya, Moscow, 1965.
- [12] *Propriety of Organic Compounds. Reference Book*, Khimiya, Leningrad, 1984.
- [13] R.P. Adams, *Identification of Essential Oil Components by GC–MS*, Allurd, Carol Stream, IL, 1995.