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ARTICLES

Gas Chromatographic Identification of Low-Boiling Organic Solvents: Evaluation of the Information Content of Retention Indices

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Abstract—The special features of gas chromatographic identification of low-boiling organic solvents based on their retention index values on standard nonpolar polydimethylsiloxane stationary phases was considered with the use of 80 most common organic solvents as an example. It was shown that one-dimensional analytical parameters, such as retention indices, cannot provide unambiguous identification of all compounds of this group because their informative value R(RI) in this group is only about 29, which is lower than the number of objects in the group. To solve the problem, it is necessary to supplement the chromatographic data with independent characteristics, and refractive indices (n_D^{20}) can be recommended as these characteristics because their determination requires minimal time and sample quantities. Nevertheless, about 10% of the solvents under consideration cannot be distinguished even based on the combinations of RI + n_D^{20}. For comparison, the capabilities of using the dynamic viscosity of liquids as an additional analytical parameter were considered. The given table of retention indices for the most common organic solvents is of independent value for analytical practice.

Keywords: low-boiling organic solvents, gas chromatographic identification, insufficient information content, additional analytical parameters, refractive indices, dynamic viscosity

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Retention indices (RIs) are considered to be the most important chromatographic invariants (mainly in gas chromatography) for the identification of analytes, especially, in chromatography–mass spectrometry [1, 2]. A necessary condition for their use is the systematization of stationary phases, which are usually subdivided into standard nonpolar (polydimethylsiloxane elastomers), semistandard nonpolar (polydimethylsiloxane containing 5% phenyl groups), and standard polar (polyethylene glycols) phases; all other phases are classified as nonstandard [2].

In real analytical practice, identification based on retention indices alone is permissible only in special cases. Most often, it is feasible in the presence of a priori chemical or other information on the nature of the samples or their constituent components. For example, the products of free-radical chlorination of alkylaromatic hydrocarbons were unambiguously identified based on the RI values because the occurrence of components of any other chemical nature among them was almost excluded, or it could be easily detected [3]. In general, the most informative was a combination of chromatographic separation and mass spectrometric detection. Nevertheless, there are problems to solve which the use of mass spectrometry is not always reasonable, for example, the routine identification of low-boiling organic solvents or their components. Numerous examples illustrating the separation of representative sets of solvents with information mainly presented in the form of pictures (chromatograms) or, less often, absolute retention times and/or retention indices on different stationary phases or sorbents are well known (for example, see [4, 5]). The most representative data array (with the exception of the NIST database [2]) relates not only to solvents but also to volatile organic compounds in general [6].

The reason for the relatively low capabilities of chromatographic identification based on retention indices alone is that they relate to one-dimensional characteristics of organic compounds (A), the information content of which can be evaluated based on the value of $R(A)$, proposed back in 1993 [7]. If the interval of variations of the quantities A, which includes approximately 95% of their values, is denoted as ($A_{\max} - A_{\min}$) and their average standard deviation (a characteristic of interlaboratory variations) in this range is taken as s_A, the informative value of property A approximately corresponds to the following ratio:

$$R(A) \approx \frac{A_{\max} - A_{\min}}{2s_A}. \quad (1)$$

In other words, the informative value of property $R(A)$ is a hypothetical estimate of the maximum number of possible compounds that can be distinguished by the values of property A in the range of its variations.

For RI values on standard nonpolar polydimethylsiloxane stationary phases, the range of their variations (approximately 95% of the sample) is approximately $(3500 - 500) \approx 3000$ with standard deviations of 5–15 index units (on average, 8 index units) [7]. Then, we obtain $R(\mathrm{RI}) \approx 3000/16 \approx 200$. This means that a greater number of compounds cannot be identified unambiguously based on only retention indices on standard nonpolar polydimethylsiloxane stationary phases. It should be noted that the information content of retention indices on standard polar phases is lower due to both a smaller range of their variations and a larger interlaboratory error [7].

The unambiguousness of identification (U) of compounds from certain groups can be evaluated on the basis of criterion (1). For this purpose, it is necessary to assume that the number of objects in such a group is N. Then,

$$U \approx N/R(A). \tag{2}$$

The peculiarity of such simple estimates of $R(A)$ is that they a priori correspond to a theoretically uniform distribution of RI values in the ranges of their variations, which is most often not the case in reality. The range of RI < 1000 contains a significantly larger number of known index values than, for example, the range of RI > 3000. On the other hand, compounds both with high RI reproducibility, $s_{\mathrm{RI}} < 8$ (isoalkanes, trimethylsilyl ethers, etc.), and with low reproducibility, $s_{\mathrm{RI}} \geqslant 8$ (polyols, amino alcohols, and polar polyfunctional compounds in general), are well known. As a result, the values of $R(A)$ for different groups of analytes may differ significantly. Consequently, when evaluating the capabilities of gas chromatographic identification of compounds from different groups, this feature forces one to obtain retention indices specifically for the characterized groups of analytes rather than to focus on average estimates of the information content of retention indices.

In this paper, the capabilities of gas chromatographic identification are considered based on the retention indices of 80 low-boiling organic solvents. The possibility of the combined use of retention indices with additional analytical parameters, namely, refractive indices, is also considered because unambiguous results with the use of retention indices alone can be obtained only as an exception. In addition, the use of dynamic viscosity values is discussed for comparison as an example of properties that are characterized by minimal correlation with gas chromatographic retention indices.

EXPERIMENTAL

Published data [6] or the NIST database [2] could be used as a source of reference values of the retention indices of low-boiling organic solvents on standard nonpolar polydimethylsiloxane stationary phases. However, preference was given to the information from the author's collection for the following reasons: In this collection, all compounds were characterized by the mean arithmetic values of RIs and the corresponding standard deviations, $\langle \mathrm{RI} \rangle \pm s_{\mathrm{RI}}$. In accordance with the laws of statistical data processing, about 68% of the samples of the initial RI values fall within the intervals of $\mathrm{RI} \pm s_{\mathrm{RI}}$, about 95% fall within the intervals of $\langle \mathrm{RI} \rangle \pm 2s_{\mathrm{RI}}$, and about 99.7% fall within the intervals of $\langle \mathrm{RI} \rangle \pm 3s_{\mathrm{RI}}$. This fact makes it relatively easy to evaluate the probability of overlapping signals of different compounds in chromatograms. Flanagen et al. [6] presented single RI values without statistical processing, which did not allow conclusions to be drawn about possible peak overlapping in chromatograms. In the NIST database [2], the spread of data has historically been characterized by medians of absolute deviations (MAD), so that only 50% of all values fall within the ranges of $\langle \mathrm{X} \rangle \pm \mathrm{MAD}$. In this case, the evaluation of ranges corresponding to a different confidence probability (for example, 90 or 95%) becomes a difficult task.

In addition, an attempt was made in the database [2] to separate the RIs into values obtained on standard nonpolar polydimethylsiloxane stationary phases and on (semistandard) stationary phases containing 5% phenyl groups. In the author's collection, statistical processing was carried out for the RI values determined on phases of both types without separating them because statistically reliable differences were not revealed in many cases.

The values of the refractive indices n_D^{20} of organic solvents were selected from handbooks [8, 9] and available Internet sources. Instead of averaging them (as is done for the retention indices), they were presented with three significant digits after the decimal point rather with four ones (as is usually accepted). The reason is that the presence of possible impurities, including water (especially in polar solvents), makes the fourth decimal place in the n_D^{20} values unreliable.

The values of dynamic viscosity (mPa·s, at 20 or 25°C) considered for comparison were taken from reference books and handbooks [9–15]. Limiting the sample to values measured only at one temperature is undesirable because it leads to gaps in the data array. Therefore, some of them were presented in the form of intervals with a lower value naturally corresponding to a higher temperature.

Processing of results. The Excel (Microsoft Office 2010) and Origin (versions 4.1 and 8.1) software were used for the statistical processing of results and the construction of histograms.

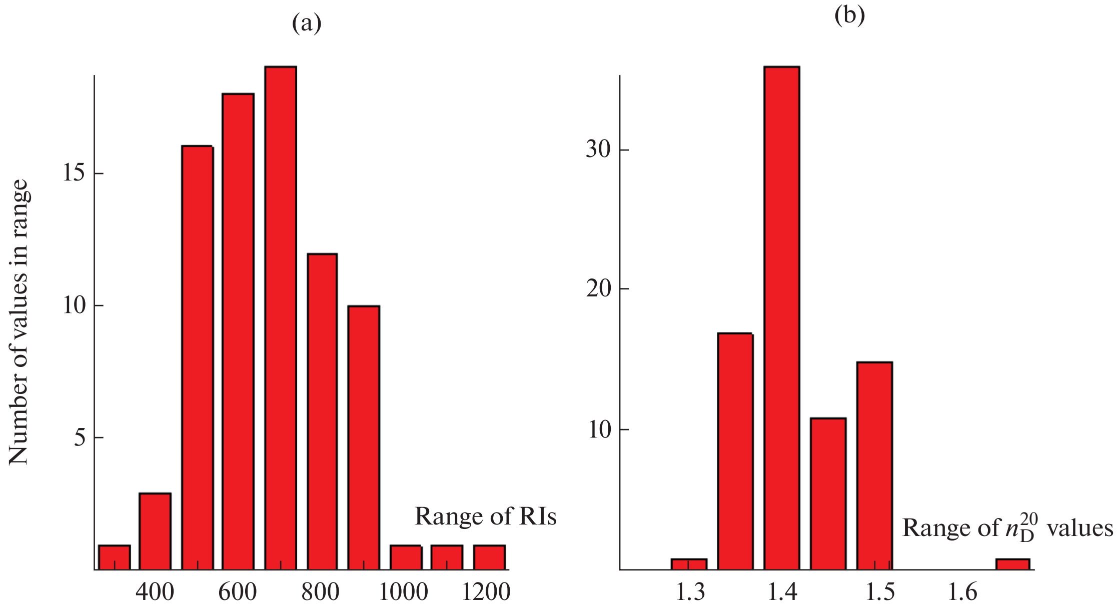

Fig. 1. (a) Histogram of the distribution of retention index values of organic solvents in the range 300–1200 (95% of the values fall in the range 400–900). The histogram step is 100 index units. (b) A distribution histogram for the refractive indices of organic solvents in the range 1.23–1.68 (95% of the values fall in the range 1.33–1.52). The histogram step is 0.05.

RESULTS AND DISCUSSION

Possibilities of Identification of Low-Boiling Organic Solvents by Gas Chromatographic Retention Indices

Table 1 presents the characteristics of $N = 80$ low-boiling organic solvents (water was additionally included in the list) in the range of their gas chromatographic retention indices on standard nonpolar polydimethylsiloxane stationary phases from 380 to 960 (excluding data for butyl cellosolve acetate and glycerol). These data include molecular weights (Da), the RI values and their standard deviations s_{RI}, refractive indices n_D^{20} rounded to three significant digits, and dynamic viscosity values (or ranges) corresponding to temperatures of 20–25°C (see discussion below). All compounds are listed in order of increasing retention indices from 380 for methanol (for water, RI is 319 ± 7) to glycerol (RI of ~1200 ± 30). The average value of standard deviations of RIs is 10 index units, which is consistent with early estimates [7] and fits well with the MAD values (confidence probability, 50%) in the NIST database [2].

From the histogram of the distribution of RI values in a range of 300–1200 index units shown in Fig. 1a, it follows that they form a compact group; 95% of all values fall within a range of 380–960. If we estimate the informative value $R(A)$ for retention indices within this local group, we obtain $(960 - 380)/(2 \times 10) \approx 29$. This means that unambiguous identification of all 80 low-boiling organic solvents listed in Table 1 using only chromatographic data is fundamentally impossible. Checking the possible overlap of “neighboring” values in Table 1 using the criterion $|\mathrm{RI}_1 - \mathrm{RI}_2| < \max[s_{\mathrm{RI},1}; s_{\mathrm{RI},2}]$ (in other words, when the differences in retention indices of closely eluted compounds are lower than the largest of their standard deviations) showed that such uncertainties are probable for 68 pairs of solvents from Table 1; of course, this is unacceptable. By the way (although this is just an assumption), the difference between the number of objects in the group (80) and the informative value (29) is 51, which corresponds to the number of identified index overlaps in terms of the order of magnitude.

For the sake of correct presentation, it should be noted here that the expression *most common solvents,* frequently used both in literature and on the Internet, is subjective and vague; as a result, the lists of these solvents may differ significantly. For this reason, Table 2 additionally summarizes the analytical parameters of 12 less commonly used organic solvents as a kind of supplement to Table 1. It is clear that their list can be supplemented and expanded if necessary. The data in Table 2 can be used for independent confirmation of the regularities formulated above. Thus, according to Table 2, the range of RI variations is 620–1260 (excluding tributyl phosphate), and the average value of the standard deviation s_{RI} is 10, which leads to almost the same informative value $R(A) = (1260 - 620)/20 \approx 31$ as before. This corresponds to the possibility of their unambiguous chromatographic identification because the number of compounds in Table 2 is only 12.

Nevertheless, it is unreasonable to abandon gas chromatographic analysis of solvents as the first stage

Table 1. Analytical characteristics of the most common organic solvents

Solvent	Molecular weight, Da	RI	n_D^{20}	Dynamic viscosity, mPa s
Water	18	319 ± 7	1.333	0.89–1.0
Methanol	32	381 ± 15	1.327	0.55–0.60
Freon 114	171	406 ± 4	1.369	0.38–0.40
2,2,2-Trifluoroethanol	100	441 ± 7	1.291	1.8–2.0
Ethanol	46	452 ± 18	1.360	1.1–1.2
Freon 11	137.5	457 ± 13	1.386	0.43–0.46
Acetonitrile	41	460 ± 13	1.344	**0.34–0.37***
Acetone*	**58**	**472 ± 12**	**1.358**	**0.31–0.34***
Diethyl ether*	**74**	**485 ± 10**	**1.352**	0.22–0.24
Isopropanol	**60**	**486 ± 9**	**1.377**	2.1–2.4
Isopropyl chloride	**78.5**	**496 ± 5**	**1.378**	0.32
***n*-Pentane**	**72**	**500**	**1.357**	0.24
Methyl acetate	**74**	**510 ± 5**	**1.361**	0.36–0.38
Methylal	76	518 ± 9	1.354	0.33
tert-Butanol	74	518 ± 9	1.387	3.4
Freon 114B2	260	520	1.369	0.78
Carbon disulfide	76	530 ± 9	1.628	0.36
Nitromethane	**61**	**531 ± 6**	**1.382**	0.63–0.66
***n*-Propyl chloride**	**78.5**	**531 ± 5**	**1.389**	**0.35**
Diethylamine	**73**	**538 ± 8**	**1.386**	**0.35**
Allyl alcohol	58	550 ± 10	1.413	1.4
n-Propanol	60	552 ± 13	1.384	1.9–2.2
Dimethyl carbonate	**90**	**556**	**1.369**	1.46
Methyl *tert*-butyl ether	**88**	**567 ± 12**	**1.371**	0.35
Cyclopentane	70	570 ± 8	1.406	**0.44**
Methyl ethyl ketone	72	578 ± 12	1.379	**0.41–0.43**
Diisopropyl ether	**102**	**598 ± 5**	**1.368**	**0.30–0.37**
***n*-Hexane**	**86**	**600**	**1.375**	**0.29–0.32**
sec-Butanol	74	600 ± 13	1.397	3.1–3.9
Ethyl acetate	88	602 ± 9	1.372	**0.43–0.45**
Tetrahydrofuran	72	619 ± 11	1.409	**0.46–0.52**
Isobutanol	74	625 ± 10	1.396	4.0
Dichloroethane	**99**	**632 ± 9**	**1.445**	**0.78–0.83**
Methyl chloroform	**132**	**636 ± 11**	**1.438**	**0.79–0.85**
Acetic acid	60	638 ± 10	1.372	**1.1–1.3**
Methyl isopropyl ketone	**86**	**641 ± 11**	**1.388**	0.41–0.58
Glyme	**90**	**642 ± 8**	**1.380**	**1.1**
Isopropyl acetate	**102**	**642 ± 7**	**1.378**	0.52–0.56
Benzene	78	657 ± 9	1.501	0.60–0.65
n-Butanol	74	658 ± 12	1.398	2.6–3.0
Tetrachloromethane	154	658 ± 14	1.506	**0.91–0.97**
Cyclohexane	84	666 ± 8	1.426	**0.90–0.98**

Table 1. (Contd.)

Solvent	Molecular weight, Da	RI	n_D^{20}	Dynamic viscosity, mPa s
Methyl propyl ketone	86	670 ± 8	1.391	0.50
1-Methoxy-2-propanol	90	680 ± 18	1.404	1.7
Isooctane	114	691 ± 3	1.391	0.50
Propyl acetate	102	692 ± 10	1.384	**0.54–0.58**
Trichloroethylene	131.5	693 ± 6	1.477	**0.55–0.58**
n-Heptane	100	700	1.388	0.39–0.42
1,4-Dioxane	88	702 ± 13	1.422	1.2–1.3
Ethyl cellosolve	90	710 ± 15	1.488	2.1
Ethylene glycol	62	726 ± 28	1.432	16–20
2-Methoxy-1-propanol	**90**	**729**	**1.403**	1.7
Isoamyl alcohol	**88**	**730 ± 12**	**1.407**	3.7
Pyridine	79	731 ± 20	1.510	0.88–0.97
Methyl isobutyl ketone	100	733 ± 11	1.396	0.57
Dimethylformamide	73	738 ± 9	1.429	0.80–0.92
1,1,2-Trichloroethane	133.5	748 ± 9	1.471	1.16
n-Pentanol	88	759 ± 11	1.408	3.5–4.1
Toluene	92	760 ± 9	1.497	0.56–0.59
Propylene glycol	76	783 ± 34	1.432	40–60
Morpholine	87	788 ± 15	1.454	**2.0**
Dimethyl sulfoxide	78	790 ± 18	1.478	**2.0**
Butyl acetate	**116**	**794 ± 8**	**1.394**	0.69–0.73
***n*-Octane**	**114**	**800**	**1.397**	0.44
Tetrachloroethylene	166	803 ± 10	1.506	0.78 –0.88
Methyl cellosolve acetate	118	823 ± 13	1.402	1.1
Dimethylacetamide	87	833 ± 9	1.438	0.92–1.0
Chlorobenzene	112.5	839 ± 13	1.525	0.80
Ethylbenzene	106	854 ± 9	1.496	0.65–0.78
Isoamyl acetate	130	860 ± 4	1.403	0.87
***p*-Xylene**	**106**	**863 ± 8**	**1.496**	0.60–0.65
***m*-Xylene**	**106**	**865 ± 8**	**1.497**	**0.82**
o-Xylene	106	885 ± 9	1.505	0.76–0.80
Ethyl cellosolve acetate	132	887 ± 11	1.405	1.20
Amyl acetate	130	895 ± 6	1.402	1.6
sym-Tetrachloroethane	166	895 ± 18	1.479	1.7–1.8
Butyl cellosolve	118	900 ± 14	1.420	3.3–3.6
Anisole	108	902 ± 7	1.517	1.3
Chlorex	142	954 ± 7	1.458	2.4
Butyl cellosolve acetate	160	1073 ± 8	1.413	2.4
Glycerol	92	1196 ± 28	1.474	940–1400
Number of indistinguishable combinations of the specified parameter with retention indices:			9 + 2**	9

* Here and below, hard-to-distinguish property values and names of solvents are highlighted in bold. ** Number of triple matches.

Table 2. Analytical characteristics of less commonly used organic solvents

Solvent	Molecular weight, Da	RI	n_D^{20}	Dynamic viscosity, mPa s
Formamide	45	637 ± 20	1.448	3.3–3.8
Tetrahydropyran	86	689 ± 6	1.419	0.80
Trifluoroacetic acid	114	744 ± 6	1.284	0.81–0.93
Diethyl carbonate	118	761 ± 4	1.384	0.81
Cyclohexanone	98	873 ± 14	1.450	2.0
Diglyme	134	929 ± 6	1.409	1.9
Diethylene glycol	106	941 ± 14	1.447	30
Benzonitrile	103	953 ± 10	1.528	1.2–1.3
Nitrobenzene	123	1062 ± 11	1.556	1.8–2.0
Sulfolane	120	1134 ± 16	1.482	10
Hexamethapol	179	1262 ± 9	1.459	3.3
Tributyl phosphate	266	1617 ± 6	1.423	3.4–3.9

Table 3. Typical results of gas chromatographic analysis of a commercial multicomponent solvent

Entry	S_{rel}, %	RI_{expt}	RI_{ref}	Possible results of identification
1	5	<500	11 values from Table 1	–
2	2	<500	The same	–
3	17	661	658 ± 12	Benzene, **1-butanol***, carbon tetrachloride, and cyclohexane
4	8	708	710 ± 15	1,4-Dioxane and **ethyl cellosolve**
5	12	792	794 ± 8	Dimethyl sulfoxide, **butyl acetate**, and *n*-octane
6	56	765	760 ± 9	1-Pentanol and **toluene**

* The components of solvent 646 are shown in bold.

of a possible sequence of subsequent operations. The fact is that a conclusion on the identity of samples (or its absence) follows from the chromatographic data. When several components are detected, the probability of identifying such composite solvents increases multiplicatively, but this same fact indicates the inappropriateness of their characterization by other parameters that are informative only for individual substances (including n_D^{20}). As an example, the typical results of monitoring the composition of a commercial multicomponent solvent given in Table 3 can be cited.

Despite the impossibility of determining the retention indices of the first two components of the solvent (short retention times) and the usual ambiguity of identification of the remaining four components, the identification of consistent combinations of responses (highlighted in bold in Table 3) made it possible to conclude the following: The sample was commercial solvent 646 with a composition somewhat distorted in comparison with the reference data, which was most likely due to evaporation of the most volatile components in the course of storage and the unequal sensitivity of a chromatographic detector to different compounds.

Use of Additional Analytical Parameters: Combinations of Retention Indices with Refractive Indices

Thus, the information content of gas chromatographic retention indices as one-dimensional analytical parameters is insufficient for unambiguous identification of low-boiling organic solvents. To solve this problem, it is necessary to involve additional characteristics that do not correlate with retention indices and whose determination does not require significantly larger quantities of samples and time expenditures.

If two (or more) analytical parameters are theoretically not correlated with each other, the informative value of their combination is multiplicative [7]:

$$R(AB) \approx R(A) \times R(B). \qquad (3)$$

If properties A and B correlate with each other, expression (3) is transformed into the inequality $R(AB) < R(A) \times R(B)$. In other words, the smaller the correlation coefficients of variables A and B, the more informative their combination is for identification purposes.

According to the above criteria of minimal required sample quantities and time expenditures, preference

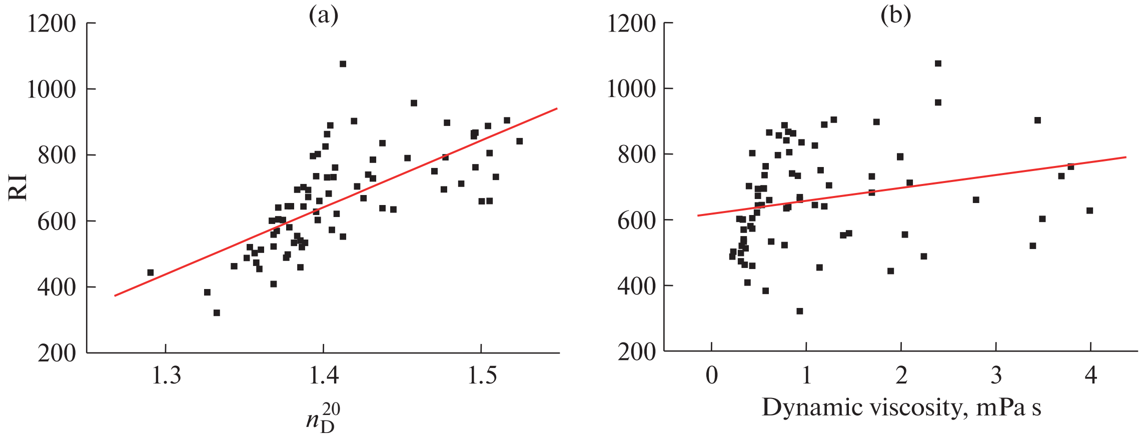

Fig. 2. Graphs illustrating the relationships between two one-dimensional analytical parameters: (a) the dependence of retention indices on refractive indices, RI(n_D^{20}); correlation coefficient $R = 0.70$ (excluding the data for carbon disulfide: RI = 530 ± 9, n_D^{20} = 1.628); (b) the relationship between retention indices and dynamic viscosity values, RI(η); correlation coefficient $R = 0.25$.

should be given to refractive indices (n_D^{20}), although their correlation with retention indices seems quite expected. According to the data in Table 1, the correlation coefficient (R) of the RI and n_D^{20} values is 0.70, but it decreased to $R = 0.29$ according to the data in Table 2, which includes more "exotic" compounds. Figure 2a illustrates the correlation between RI and n_D^{20} values. Note that the possibility of calculating gas chromatographic retention indices based on the linear regression RI = $an_D^{20} + b$ should not be considered even with a correlation coefficient of $R = 0.70$ because the average accuracy of RI estimates (the value of the general dispersion S_0) is 109, which is unacceptable for practical purposes.

It is advisable to measure the refractive indices of analytes only if the samples are single-component ones and this can be established based on the results of gas chromatographic analysis. Table 1 gives the values of n_D^{20} for all solvents. Figure 1b shows the histogram corresponding to this data set, from which it follows that about 95% of the values fall in the range 1.33–1.52. Since the average interlaboratory reproducibility of the refractive indices is approximately 0.001, according to the data in Table 1, their estimated informative value $R(n_D^{20})$ is about 95, which is somewhat lower than that for more representative data sets [7]. The value $R = 95$ exceeds the number of compounds in the sample ($N = 80$); however, the data in Table 1 should be ranked in ascending order of n_D^{20} in order to check the possibility of differentiating compounds with close refractive index values. It was found that the number of pairs of compounds that are difficult to distinguish by this criterion is only slightly lower than that by retention indices alone; for 50 pairs, differences between adjacent values of n_D^{20} are ≤0.002. This means that unambiguous identification based only on refractive indices is also impossible, and the possibility of identification by combinations of RI + n_D^{20} should be checked.

All problematic cases of small differences between both RI and n_D^{20} values are highlighted in bold in Table 1. There are nine of them; in addition, two more triple matches were found for closely eluted compounds, namely: nitromethane–1-chloropropane–diethylamine and methyl isopropyl ketone–glyme–isopropyl acetate. The occurrence of such matches means that the combination of analytical parameters RI + n_D^{20} is certainly more informative than each of them separately, but it also does not guarantee unambiguous identification of the compounds listed in Table 1. Such identification is possible for a smaller number of solvents (see data in Table 2).

Thus, the combination of two one-dimensional analytical parameters—gas chromatographic retention indices and refractive indices—cannot provide unambiguous identification of low-boiling organic solvents in all cases. It can be assumed that combinations of retention indices with other one-dimensional analytical characteristics will also prove to be insufficiently informative. Among them, it seems interesting to test the combination of retention indices with the values of dynamic viscosity of organic solvents as quantities whose correlation with retention indices appears to be very weak.

Combinations of Retention Indices with Dynamic Viscosity Values of Organic Solvents

In general, the information content of such a characteristic of organic liquids as their dynamic viscosity (η) is noticeably lower than that of the RI or n_D^{20} values. An approximately estimated informative value for the range of variations in dynamic viscosity of 0.2–4.1 (except for anomalous values for glycols and glycerol) and with an average standard deviation value of 0.12 is $R(\eta) \approx 16$, which is lower than that for retention indices or refractive indices. In addition, it should be noted that viscosity measurements require significantly more time and higher quantities of samples (tens of milliliters); because of this, the use of them is not always reasonable in analytical practice. However, this characteristic is of particular interest since, according to the data in Table 1, the correlation coefficient of the viscosity values and retention indices is only 0.25, that is, significantly lower than that for the refractive indices. Figure 2b illustrates the correlation of the RI and η values. It can be seen even visually that, in this case, it was worse than that for the RI and n_D^{20} variables (Fig. 2a).

Close values of dynamic viscosity for compounds with close RI values are highlighted in bold in Table 1. There are nine of them, which is comparable with the number of identification ambiguities based on the combinations RI + n_D^{20} (9 + 2). An interesting conclusion follows from the above: dynamic viscosity is a less informative characteristic of organic compounds according to the *R* value; nevertheless, it provided almost the same number of unambiguous identification results as the more informative refractive indices. The reason is precisely the worse correlation of viscosity values with gas chromatographic retention indices than that for refractive indices.

It seems likely that the simultaneous measurement of all three characteristics of organic solvents (RI + n_D^{20} + η) is of purely speculative interest. Nevertheless, from the standpoint of assessing the information content, it can be noted that only one example of a coincidence of the values of all three properties was found among the solvents listed in Table 1.

CONCLUSIONS

Thus, one of the objectives of this work was to specify concepts of the information content of gas chromatographic retention indices on standard nonpolar polydimethylsiloxane stationary phases using the example of a group of 80 most common low-boiling organic solvents. It was shown that retention indices as one-dimensional analytical parameters, either by themselves or in combination with other one-dimensional analytical parameters, refractive indices (n_D^{20}), cannot provide unambiguous identification of all representatives of this group. Among the solvents considered, about 10% of pairs indistinguishable based on the combinations of RI + n_D^{20} were found. The replacement of the refractive indices with dynamic viscosity values did not significantly increase the number of unambiguous results, which was apparently close to the limiting value obtained with the use of one-dimensional analytical characteristics.

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CONFLICT OF INTEREST

As author of this work, I declare that I have no conflicts of interest.

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