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REVIEW

THIRTIETH ANNIVERSARY OF THE RETENTION INDEX ACCORDING TO KOVÁTS IN GAS–LIQUID CHROMATOGRAPHY

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1. INTRODUCTION

> *"Theory (when correct) and experiment (if carefully executed) describe the same truths".*
>
> *J. Calvin Giddings*[446]

As pointed out in our previous review dealing with the retention index system[47], the Kováts retention index[434], introduced in 1958, turned out to be perhaps the most significant contribution to the theory and practice of gas–liquid chromatography (GLC) since the pioneering discovery of the method by James and Martin in 1952[444].

Whereas the instrumental basis, technical level and capacity of GLC have reached the desired levels during about the last four decades, this is not so, unfortunately, with the retention index system. Although some researchers have obtained important results in this field, the badly needed decisive breakthrough has not yet occurred. In fact, only about one quarter of gas chromatographic workers are familiar with the retention index system and only about 10% of analytical chemists have adopted it for everyday use in research work, although current estimates show that about 10^5 gas chromatographs are being operated worldwide by nearly 250 000 experts.

The Kováts retention index is the only retention value in GLC in which the two fundamental quantities, *viz.*, the relative retention and the specific retention volume, are united[445]. Moreover, a series of explicit relationships between retention indices and the physico-chemical quantities related to GLC have been developed. Similarly, numerous linear relationships between the retention index and other fundamental quantities such as boiling point, carbon number, molecular weight and molar refraction have been derived.

Published retention data are given in many forms, and therefore their usefulness in different laboratories is limited. The Kováts retention index[434] solves the problem of the uniform expression of retention data.

Regarding the prevalence of the retention index concept, the first half of the 1980s were important years. The number of workers in gas chromatography interested in this topic grew over the years and important new research centres investigating the retention index system were set up[1–3,5,8,28,34,37,42,45,60,69,72,78,142,154,162,187,210,212,265,354].

An important year in the development and spreading of the retention index system was 1983, the Tenth Hungarian Chromatographic Symposium entitled the Twenty-Fifth Anniversary of the Retention Index System being held in Sárospatak (Hungary). Professor Kováts (Institute of Physical Chemistry, École Polytechnique, Lausanne, Switzerland) was the Chairman of the Retention Index Symposium. His opening lecture and further lectures dealt with the theoretical and practical questions of the retention index system[176,184,221,226,227,229,230,233,234]. These lectures and the subsequent discussions considerably promoted the further development of retention index system.

Numerous researchers in the second half of the 1980s have worked on various aspects of the retention index system, including the determination of the dead time, retention index determinations in temperature-programmed GC and the connection between retention index and molecular structure, and interesting results were published in nearly 200 papers[241–433]. This progress, although its rate was slower than in the past, is characteristic of the end 1980s.

Obviously, in this review we are unable to give a full account of the activities of the hundreds of researchers who have achieved important results in this field. Without aiming at completeness, the following and their co-workers have published numerous papers: Bata[1,41,97,147], Berezkin[2a,98,99,163,268], Bermejo[3,42,101,102,165–167,247,323–327], Boneva[5,43,44,249–253,259,329,330,407], Brooks[45,46,102a,331,402,403], Buryan[164,254,332,461], Calixto[8,9,51,51a,52,104,104a,138,170a], Castello[10,10a,10b,53,105,257,257a,404], Churácek[182,275,276,281,473], Cole[45,46,102a,331,402,403], Dimov[5,43,44,173,249,250,259–261,330,335,407], Fernandez[2,142,216–218,306,377–379], Franke[34,42a,168,265,266,328,344], García-Dominguez[2,142,216–218,306,377–379], García-Raso[8,9,51,51a,52,104,104a,138,170a,212a,212b,300,374,375], Golovnya[14,58,58a,58b,109a–d,174a,175a,175b,225a–c,267a,267b,268a,280a,290a,298a,305a,309a,347,347a,348,348a,411,460,470], Guillen[42,101,102,165–167,247,323–327], Haken[60–65,111–113,170b,177–180,269–271,469], Kersten[354,355,370,371,424], Korhonen[60–63,111,112,119–125,177–180,185–196,269,270,282–284],Lakszner[212,212a,227,298], Lamparczyk[72,73,126,200,287,287a,359a], Lind[187–190,193,194], Macák[164,254,332,461], Madden[60,64,113,180], Menendez[142,216,218,306,377–379],Molera[2,217,218,377,379,459], Munoz[2,217,218,377,379], Nabivach[69,164,254,322a,332,365,461,463], Osek[210,292,293,295,296], Oszczapowicz[210,292,293,295,296], Podmaniczky[212,212a,227,298], Pomaville[369–371,423], C. F. Poole[28,135,354,355,370,371,423,424,424a], S. K. Poole[370,371,424,424a], Radecki[72,73,126,287a], Rang[27,32,142b,268,373], Rimada[142,216,217,377–379], Soják[2a,35b,35c,142b,142c,142d,309,381,382,428,429,477], Szepesy[212,212a,226,227,298], Szymanowski[37,162,228,310,384], Vernon[64,88,89,271], Voelkel[162,228,310,387–389,432], Wainwright[90,222–224], T. Wang[235,392–395], F. Wang[154,234a,313,390,391], Wijsbeek[34,168,265,266,344] and De Zeeuw[168,265,266,328,344].

During research work carried out in the last 5 years, striking results have been obtained by individual researchers that have had a major influence on progress in studies of the retention index system. Without trying to be exhaustive, the research work of Albaiges, Berlizov, De Bertoli, Bonastre, Chien, Chretien, Cramers, Czerwiec, D'Agostino, D'Amato, Eglinton, Engewald, Eisen, Ellren, Ettre, Evans, García-Raso, Grenier, Guermouche, Hawkes, Janák, Jaworski, Kaliszan, Komarek, Kováts, Krupcik, Kuningas, Lee, Mihara, Orav, Pacákova, Papazova, Peetre, Rijks, Schomburg, Singliar, Tesarik, Torres, Tóth, Vigdergauz, Wu and Zhuravleva should be mentioned.

In the following, the main theoretical and practical questions concerning the retention index system will be summarized. First, the nomenclature and the most important definitions and relationships will be recapitulated.

2. NOMENCLATURE, SYMBOLS AND DEFINITIONS

During the last 5 years, about 500 papers have been published in this field of GLC and identical symbols were mostly used throughout. The uniform system of symbols of relating to retention indices was summarized in our previous review[47]. As pointed out by Ryba[435], the retention index is a dimensionless quantity. However, for the sake of a simpler discussion, "retention index units" (i.u.) were introduced. For similar reasons, retention index units are also considered to have "dimensions" in the case of structural index increments, ΔI values, etc.

The basic equation of the retention index elaborated by Kováts[434] and the various equations derived from this equation using equivalent mathematical transformations[a] are the most frequently discussed aspect of the retention index system and

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[a] The term "equivalent mathematical transformation" means that in the equation for the retention index (*e.g.*, eqn. 2 in ref. 47) the adjusted retention time (t'_R) is used rather than the specific retention volume (V_g).

have remained in the centre of interest of various investigators and research groups. Of the numerous outstanding results that have been published, those of Smith, Haken and Wainwright[223], Belyaev and Vigdergauz[245], Evans, Haken and Tóth[264], Heeg and Zinburg[274], Dose[338] and Gusev, Rang, Berezkin and Orav[268] should be mentioned.

Thermodynamic characteristics determined by Podmaniczky *et al.*[212a] from isothermal retention data were used for retention index calculations. The minimum retention index difference required for the identification of two adjacent compounds and the temperature dependence of retention index were discussed.

Several statistical and iterative methods for the calculations of the retention indices were compared by Smith *et al.*[222] using retention data obtained on a wide range of columns (SE-30, Apiezon-L, SF-96, OV-17, OV-25, etc.) at different column temperatures.

Electric interaction indices for a series of twelve monomethylbenz[*a*]anthracenes were calculated by Lamparczyk and Ochocka[287] from GC relative retention times, using anthracene and benz[*a*]anthracene as reference compounds. Application of these electric interaction indices for structure–biological activity studies and the role of electric interactions in the retention index concept were discussed.

An interesting general model consisting of two terms was proposed by Dimov[335] for the calculation of the retention indices of isoalkanes on squalane as stationary phase. The first term (referred to as extensive) includes parameters that have the greatest correlation with the experimental value of the retention index. The second term (referred to as intensive) includes parameters that can modify the value of the roughly calculated retention index in the direction of the experimental value. The equations derived by Dimov[335] had correlation coefficients better then 0.99.

Some of the results relating to the above are given in Tables 1–6, without claiming to be comprehensive. For further details, see refs. 2a, 28a, 34a, 35a, 35b, 35c, 35d, 54, 55, 55a, 58a, 58b, 82, 90, 93a, 96, 105, 105b, 118a, 126a, 142a, 142b, 142c, 142d, 170b, 173, 198a, 200, 212b, 216, 217, 225b, 225c, 229, 233a, 251, 257a, 258a, 259, 267a, 267b, 268a, 274, 277, 287a, 290a, 298a, 305a, 307, 309a, 310, 311, 318a, 322a, 325, 341, 346a, 347a, 348a, 362, 379a, 386a, 401, 410a, 411a, 429b, 457 and 469.

TABLE 1

COMPARISON OF RETENTION INDICES CALCULATED BY BALLSCHMITER *ET AL.*[161] USING DIFFERENT CALCULATION METHODS

Carbon No.	*Calculated retention index (i.u.)*		
	Classical method	*x^3 polynomial method*	*x^4 polynomial method*
14	1399.04	1399.75	1399.96
15	1498.57	1500.02	1500.03
16	1598.63	1600.11	1600.05
17	1698.99	1700.00	1699.93
18	1800.00	1800.22	1800.18

TABLE 2

MOLECULAR STRUCTURAL COEFFICIENTS OF SELECTED COMPOUNDS ON APOLANE-87 STATIONARY PHASE AT 70°C

Compound	*Structural coefficient*	*Compound*	*Structural coefficient*
Cyclopentane	482.61	1-Chloroheptane	841.21
Cyclohexane	582.31	1-Bromopropane	416.31
Cycloheptane	718.31	1-Bromobutane	520.91
1-Pentyne	391.21	1-Bromopentane	623.51
1-Hexyne	494.01	1-Bromohexane	724.41
1-Heptyne	593.81	1-Bromoheptane	825.01
1-Octyne	692.51	Iodomethane	435.31
1-Nonyne	792.01	Iodoethane	524.31
Benzene	565.91	1-Iodopropane	627.01
Toluene	673.51	1-Iodobutane	726.01
Ethylbenzene	761.91	1-Iodopentane	824.51
n-Propylbenzene	849.71	1-Butanol	508.91
1-Chloropropane	433.61	1-Pentanol	607.01
1-Chlorobutane	537.11	1-Hexanol	704.71
1-Chloropentane	638.91	1-Heptanol	805.01
1-Chlorohexane	740.01		

TABLE 3

MOLECULAR STRUCTURAL COEFFICIENT OF SELECTED HYDROCARBONS MEASURED BY CHIEN *ET AL.*[54] ON OV-101 STATIONARY PHASE AT DIFFERENT COLUMN TEMPERATURES

Compound	*Structural coefficient*[a]			
	30°C	*50°C*	*70°C*	*90°C*
n-Pentane	421.79	402.70	381.28	357.15
n-Hexane	521.87	502.73	481.25	457.07
n-Heptane	621.82	602.70	581.23	557.04
n-Octane	721.76	702.72	681.22	656.87
n-Nonane	821.83	802.71	781.21	756.97
n-Decane	921.84	902.68	881.17	856.92
cis-2-Pentene	437.06	417.60	395.73	371.05
2,2-Dimethylbutane	455.81	438.12	418.32	396.08
Benzene	569.02	553.85	536.81	517.61

[a] Value calculated by Antoine equation:

$$S^{\text{OV-101}}_{c\ \text{substance}}(T) = a^* + \frac{b^*}{T + c^*} \qquad b^* \tag{1}$$

where S_c is the molecular structural coefficient, T is the column temperature (K) and a^*, b^* and c^* are constants in eqn. 1. For example, for benzene $a^* = -2.8458$, $b^* = 1603.8490$ and $c^* = -0.8747$.

TABLE 4

KOVÁTS COEFFICIENTS ON SQUALANE STATIONARY PHASE AT DIFFERENT COLUMN TEMPERATURES

Carrier gas, nitrogen.

Column temperature (°C)	*Kováts coefficient*	*Column temperature (°C)*	*Kováts coefficient*
30	71.43	80	108.70
40	78.19	90	117.32
50	85.28	100	126.40
60	92.71	110	135.98
70	100.51	120	146.10

TABLE 5

KOVÁTS COEFFICIENTS ON SE-30 AND APOLANE-87 STATIONARY PHASES AT DIFFERENT COLUMN TEMPERATURES

Carrier gas, helium.

Column temperature (°C)	*Kováts coefficient*	
	SE-30	*Apolane-87*
30	66.36	73.71
40	75.96	80.39
50	86.00	86.92
60	97.10	93.29
70	108.30	99.52
80	120.30	105.60

TABLE 6

KOVÁTS COEFFICIENTS ON SOME OV STATIONARY PHASES AT 80°C

Carrier gas, helium. Retention data used for calculations are from Chien *et al.*[54,55].

Stationary phase	*Phenyl (%)*	*Kováts coefficient*
OV-1	0	117.49
OV-101	0	130.18
OV-3	10	149.10
OV-7	20	166.47
OV-61	33	187.04
OV-11	35	190.02
OV-17	50	211.00
OV-22	65	229.81
OV-25	75	241.30

3. RETENTION INDICES IN PROGRAMMED TECHNIQUES IN GLC

In order to facilitate the analytical application of GLC to the investigation of samples with wide boiling point ranges (most natural samples belong to this group), programmed techniques were developed, involving temperature, flow and double temperature and flow programming[448–450].

Under the conditions of pressure- and/or flow-programmed GLC, the retention index will remain constant and identical with the value measured without programming, as the carrier gas influences only the calculation of the net retention volumes and not the retention indices[47].

The widespread use of personal and home computers in the laboratory has provided the possibility of calculating double programmed retention indices, but the progress is far from satisfactory. The problem is not connected with the computer software, but with a lack of reliable GC data to be used in calculations.

Temperature-programmed GLC is one of the most important techniques and about 75% of GLC analyses are carried out under these conditions. The main problem is connected with the reproducibility of the retention indices under different laboratory conditions. Only part of the difficulties can be attributed to a lack of reliable data or to the discrepancy between the various methods for retention index calculations. The basic problem is due to the wide variety of carrier gas systems, column temperature control units and other regulation systems used in gas chromatographs of different types. In addition, column used influences the elution temperature. Although in this review we cannot discuss all these problems in detail, relevant publications are cited.

Consider the use of a linear temperature programme with a constant heating rate during the whole analysis, starting at the instant of sample introduction, so that all components are eluted during this programme. Under such conditions (classical temperature programming), the temperature-programmed retention index (I_{TPGC} or I_{TP}) can be calculated from the equation of Van den Dool and Kratz[47]. The calculation of the temperature-programmed retention index when temperature programming is combined with isothermal periods or where the programming rate is changed during the analysis (I_{cTPGC} or I_{cTP}) is more complicated[436].

In order to study elution temperatures, the interactions on Apolane-87 and OV-101 at different column temperatures were investigated by Borwitzky and Schomburg[6]. A method based on polynomial interpolation for calculating linear temperature-programmed retention indices was described by Knoeppel *et al.*[20,21]. The determination of linear temperature-programmed retention indices and the identification of phenols were discussed by White and Li[39a].

More than 180 peaks were identified and their corresponding temperature-programmed retention indices determined by Wu and Lu[93a]. The retention indices obtained varied with the GC conditions such as column length, film thickness and heating rate. A short overview of some of the most important papers dealing with the determination of temperature-programmed retention indices was given by Szepesy *et al.*[227].

Akporhonor *et al.*[241] dealt with the conversion of retention indices into those under temperature-programmed conditions. A method was presented by Podmaniczky *et al.*[298] for the calculation of retention indices in linear temperature-programmed GLC on the basis of isothermal retention data and the operating conditions (initial temperature, heating rate, etc.) of the run.

Interesting mathematical procedures were described by Akporhonor *et al.*[318a] for the calculation of temperature-programmed retention indices. A new method was presented by Chen *et al.*[319] for the calculation of the retention indices under linear temperature programming conditions with or without an initial isothermal period.

A simple procedure was demonstrated by Krupčik *et al.*[358] for the prediction of temperature-programmed retention indices from isothermal retention indices. The effect of the solute sample size on the measurement of temperature-programmed retention indices was studied by Wang and Sun[392]. Temperature-programmed retention indices calculated according to three different definitions were compared by Wang and Sun[394]. The advantages and shortcomings of these definitions were discussed in terms of their theoretical background, accuracy, ease of calculation and applicability. A broad research programme was carried out by the same group[395] using various compounds as model substances.

Summarizing this theme, some interesting results are presented in Tables 7–25. For further information about temperature-programmed retention indices, see also refs. 16, 20, 21, 24, 38, 132, 142a, 157, 171, 172, 235, 239, 240, 262, 302, 305, 380 and 393.

4. RETENTION INDEX AND GAS CHROMATOGRAPHIC PARAMETERS

The retention index depends on the chemical nature of the substance examined, on the chemical nature of the stationary phase and on the column temperature[47,434]. The most important requirement is to know the exact quality and amount (retention index calculation without specific retention volume) of the stationary phase used and their effects on the value of the retention index. Whereas it is true that the effect of the amount of the stationary phase can be eliminated by using the specific retention volume (V_g) in the retention index calculations, the quality differences between

TABLE 7

COMPARISON OF RETENTION INDICES (i.u.) MEASURED BY KRUPČIK *ET AL.*[358] UNDER CONDITIONS OF TPGC WITH DIFFERENT HEATING RATES

Initial temperature, 50°C; stationary phase, squalane.

Compound[a]	*Heating rate (°C/min)*			
	1	*2*	*3*	*5*
2,3,5-M_3C_6	812.0	813.1	813.6	814.7
2,3-M_2C_7	848.6	850.2	851.2	852.4
3,3-E_2C_5	867.0	869.5	871.2	873.7
Isopropylbenzene	906.3	907.7	908.6	910.2
4,4-M_2C_8	916.6	918.0	918.8	919.9
1,3,5-M_3-benzene	945.8	948.5	950.4	952.7
sec.-Butylcyclo-C_6	1012.8	1015.3	1017.2	1020.0
n-Butylcyclo-C_6	1020.4	1023.0	1024.8	1027.3
1,2-E_2-benzene	1036.1	1039.3	1041.4	1044.5
1,3-M_2-4-E-benzene	1054.2	1057.7	1059.6	1062.7

[a] M = methyl; E = ethyl; C_5 = pentane; C_6 = hexane; C_7 = heptane.

TABLE 8

RETENTION INDEX REPRODUCIBILITY (n = 5) AFTER WATTS AND SIMONICK[396]

Drugs were analysed under TPGC conditions using 5% phenyl- and 50% phenylmethylsilicone fused-silica capillary columns

Drug	*Retention index (i.u.)*			
	Ultra-2 (5% phenyl)		*HP-17 (50% phenyl)*	
	Mean	*S.D.*	*Mean*	*S.D.*
Amphetamine	368	0.55	436	0.55
Meperidine	615	0.55	712	0.00
Diazepam	878	0.00	1085	0.55
Cocaine	786	0.00	949	0.55
Phencyclidine	668	0.00	755	0.45
Morphine	873	0.00	1080	0.45
Lidocaine	663	0.55	776	0.89
Methaqualone	769	0.55	954	0.45
Methadone	764	0.00	882	0.45
Codeine	855	0.00	1048	0.45

stationary phases supplied commercially under the same trade name lead to unpredictable errors that are difficult to detect (Table 26).

After having studied the latter problem for several years, we have recently found[429b] a very simple and easy-to-use practical method for the characterization of stationary phases by introducing the so-called Kováts coefficient (eqn. 17a). In classical GLC, when the column temperature, inlet pressure and/or flow-rate of carrier gas are constant, the Kováts coefficient is constant. As can be deduced from eqn. 17a, the Kováts coefficient depends on the quality of both the stationary phase and the

TABLE 9

COMPARISON OF RETENTION INDICES MEASURED AND CALCULATED BY CHEN *ET AL.*[319] AND CALCULATED BY THE METHOD OF VAN DEN DOOL AND KRATZ[437] UNDER CONDITIONS OF TPGC ON CROSS-LINKED METHYLSILICONE

Compound	*Retention index (i.u.)*		
	Van den Dool and Kratz method	*Chen et al. method*	*Difference*
2-Methyl-2-butene	512.9	519.5	−6.6
2,3-Dimethylbutane	553.8	564.7	−0.9
2-Methylpentane	559.1	569.4	−10.3
3-Methylpentane	576.3	583.4	−7.1
2-Methyl-2-pentene	604.2	606.3	−2.1
2,2,5-Trimethylhexane	779.3	783.3	−4.0
n-Propylbenzene	933.3	935.6	−2.3
1-Methyl-4-ethylbenzene	944.8	946.3	−1.5

TABLE 10

COMPARISON OF RETENTION INDICES MEASURED AND CACULATED BY DONNELLY *ET AL.*[337] ON 5% PHENYLMETHYLSILICONE (DB-5) UNDER CONDITIONS OF TPGC

Compound[a]	*Retention index (i.u.)*		
	Measured	*Calculated*	*Difference*
2,7-PCDD	1985	1976	9
2,8-PCDD	1985	1976	9
1,2,4-PCDD	2152	2143	9
1,3,6,8-PCDD	2290	2290	0
1,3,7,9-PCDD	2304	2304	0
1,3,6,9-PCDD	2315	2319	−4
1,3,7,8-PCDD	2340	2338	2
1,2,7,9-PCDD	2364	2363	1
1,2,3,4,7-PCDD	2573	2576	−3

[a] PCDD = *p*-chlorodibenzodioxin.

carrier gas used, in addition to the column temperature. However, it is independent of all other GC parameters, including the type of *n*-alkanes applied for the determination of the b value (eqn. 17b), if $z \geqslant 8$. Similarly the Kováts coefficient is independent of the type of *n*-alkane applied for determination of the specific rention volume if $z \geqslant 8$. Some Kováts coefficients and retention polarities[429b] on various stationary phases are given in Table 27.

The dependence of the retention index on the column temperature can be described, in theory, by an Antoine-type equation[47]:

$$I = A + \frac{B}{T + C} \tag{1}$$

TABLE 11

COMPARISON OF RETENTION INDICES MEASURED AND CALCULATED BY WANG *ET AL.*[395] UNDER DIFFERENT TPGC CONDITIONS ON OV-101

Compound	*Retention index (i.u.)*		
	Constant inlet pressure	*Constant mass flow-rate*	*Difference*
Isobutyl acetate	754.5	755.6	−1.1
p-Xylene	867.0	867.8	−0.8
n-Heptanol	953.3	952.8	+0.5
Limonene	1030.9	1031.9	−1.0
Camphor	1134.9	1136.4	−1.5
Eugenol	1336.0	1336.7	−0.7
Diphenyl ether	1384.7	1385.2	−0.5
Caryophyllene	1435.2	1435.8	−0.6
β-Ionone	1472.8	1473.2	−0.4
n-Hexyl benzoate	1559.4	1559.9	−0.5

TABLE 12

COMPARISON OF RETENTION INDICES (i.u.) BY CHEN *ET AL.*[319] UNDER DIFFERENT TPGC CONDITIONS ON CROSS-LINKED METHYLSILICONE.

Initial temperature: 30°C.

Compound	*Heating rate (°C/min)*		
	2[a]	*5*[b]	*10*[a]
2-Methyl-2-butene	512.9	520.4	514.6
2-Methylpentane	559.1	569.5	561.5
3-Methylpentane	576.3	583.1	578.5
Benzene	639.3	648.0	645.6
Cyclohexane	647.7	656.4	655.3
cis-2-Heptene	706.3	712.1	709.4
Toluene	746.4	752.8	754.4
p-Xylene	852.0	854.3	860.6

[a] Calculation method of Van den Dool and Kratz (classical method)[437].
[b] Special calculation method of the authors.

where: I is the isothermal retention index (i.u.), T is the column temperature (K) and A, B and C are constants. Nevertheless, we emphasize again that in practical applications one is allowed to make use of the fact that on apolar stationary phases the Antoine equation can possess a wide linear range, within which the linear approximation can provide excellent results even without using the Antoine equation (Table 28).

TABLE 13

COMPARISON OF RETENTION INDICES MEASURED AND CALCULATED BY KRUPČIK *ET AL.*[358] UNDER TPGC CONDITIONS ON SQUALANE

Compound[a]	*Retention index (i.u.)*		
	Measured	*Calculated*	*Difference*
1,1,3-M_3-cyclo-C_5	722.2	721.8	0.4
1,*trans*-2,*cis*-4-M_3-cyclo-C_5	739.4	738.8	0.6
1,*trans*-2,*cis*-3-M_3-cyclo-C_5	746.1	746.7	−0.6
1,*cis*-2,*cis*-4-M_3-cyclo-C_5	775.6	777.7	−2.1
1,*cis*-2,*trans*-3-M_3-cyclo-C_5	780.0	781.1	−1.1
1,*cis*-3-M_2-cyclo-C_6	787.8	787.3	0.5
1,*trans*-4-M_2-cyclo-C_6	787.8	787.3	0.5
1,1-M_2-cyclo-C_6	790.6	792.4	−1.8
1-M-*trans*-3-E-cyclo-C_5	789.4	789.0	0.4
1-M-*cis*-3-E-cyclo-C_5	792.8	791.8	1.0
1-M-*trans*-2-E-cyclo-C_5	793.3	791.8	1.5
1-M-1-E-cyclo-C_5	797.2	796.9	0.3

[a] M = methyl; E = ethyl; C_5 = pentane; C_6 = hexane.

TABLE 14

COMPARISON OF RETENTION INDICES MEASURED AND CALCULATED BY BUCHMAN *ET AL.*[103] UNDER TPGC CONDITIONS ON SE-30 AND ON PEG-20M

Compound	*Retention index (i.u.)*			
	SE-30		*PEG-20M*	
	Measured	*Calculated*	*Measured*	*Calculated*
3-Iodotoluene	1148	1143	1674	1665
3-Bromotoluene	1033	1040	1498	1487
2-Cyclohexene-1-ol	880	890	1481	1499
3-Methylcyclohexanone	945	946	1376	1369
3-Methylcyclohexylamine	926	927	1231	1218
1,3-Dimethylcyclohexane	782	792	814	795
3-Methylcyclohexanol	947	950	1463	1450
1,3-Cyclohexanediol	1089	1108	2070	2105
4-Bromocyclohex-1-ene	969	974	1370	1388
3-Methyl-2-cyclohexen-1-one	1039	1026	1644	1587

TABLE 15

COMPARISON OF RETENTION INDICES MEASURED AND CALCULATED BY RAYMER *ET AL.*[213] ON SE-30 UNDER TPGC CONDITIONS.

Compound	*Retention index (i.u.)*		
	Measured	*Calculated*	*Difference*
2-Hexanone	600.0	588.3	11.7
4-Heptanone	681.5	686.6	−5.1
5-Nonanone	882.5	883.5	−1.0
6-Undecanone	1080.1	1080.4	−0.3
7-Tridecanone	1277.9	1277.2	0.7
8-Pentadecanone	1476.5	1474.1	2.4
9-Heptadecanone	1675.2	1671.0	4.2
10-Nonadecanone	1873.7	1867.8	5.9

TABLE 16

RETENTION INDICES OF SOME SUBSTITUTED PYRIDINES MEASURED BY PREMECZ AND FORD[372] UNDER TPGC CONDITIONS ON 5% PHENYLMETHYLSILICONE (DB-5) AND ON PEG-20M

Compound	*Retention index (i.u.)*	
	DB-5	*PEG-20M*
Pyridine	736.3	1182.7
2-Methylpyridine	813.5	1215.7
3-Methylpyridine	861.0	1283.5
4-Methylpyridine	861.9	1289.3
2,6-Dimethylpyridine	884.2	1243.1
2,4-Dimethylpyridine	931.8	1325.3
3,5-Dimethylpyridine	979.9	1390.8
3,4-Dimethylpyridine	1003.4	1444.9

TABLE 17

RETENTION INDICES OF SOME SULPHUR VESICANT AND RELATED COMPOUNDS ON DB-1 (100% DIMETHYLPOLYSILOXANE), DB-5 (95% METHYL-, 5% DIPHENYLPOLYSILOXANE) AND DB-1701 (86% DIMETHYL-, 14% CYANOPROPYLPHENYLPOLYSILOXANE), AFTER D'AGOSTINO AND PROVOST[398]

Column temperature, 2 min at 50°C, then programmed at 10°C/min to 300°C, maintained at 300°C for 5 min. Carrier gas, helium.

Compound	*Retention index (i.u.)*		
	DB-1	*DB-5*	*DB-1701*
1,4-Thioxane	850.7	880.0	964.1
2-Chloroethyl vinyl sulphide	873.7	903.0	992.1
(2-Vinylthio)ethanol	889.6	923.2	1089.2
Bis(2-chloroethyl) ether	948.3	984.0	1107.5
1,4-Dithiane	1018.7	1060.2	1156.7
1,4,5-Oxadithiapane	1117.8	1162.7	1289.9
Mustard	1123.8	1172.7	1325.8
Thiodiglycol	1130.9	1181.5	1458.2
Hemisulphur mustard	1132.3	1177.5	1400.0
1,2,5-Trithiapane	1300.0	1361.7	1513.3
Sesquimustard	1622.7	1688.8	1922.7

TABLE 18

RETENTION INDICES OF SOME AMINO ACID DERIVATIVES IN URINE MEASURED BY SCHNEIDER *ET AL.*[219] ON OV-101 UNDER TPGC CONDITIONS

Compound	*Retention index (i.u.)*	*Compound*	*Retention index (i.u.)*
Alanine	1159	Ornithine	1690
Glycine	1173	N(O)-TFA-tyrosine[a]	1769
α-Aminoisobutyric acid	1235	Glutamic acid	1807
Threonine	1246	Glutamine	1807
Serine	1257	Lysine	1811
Valine	1280	N-α-Methyllysine	1851
β-Aminoisobutyric acid	1282	2-Aminoadipic acid	1868
N-Methylproline	1328	1-Methylhistidine	1888
Leucine	1349	3-Methylhistidine	1888
Isoleucine	1358	Glycylproline	1931
Nicotinic acid	1384	N-TFA-Tyrosine[a]	1976
Creatinine	1440	Monoacylhistidine	1983
Aspartic acid	1676	N-α-Acetyllysine	2019
Asparagine	1676	Propylhydroxyproline	2058
Phenylalanine	1678		

[a] TFA = trifluoroacetyl.

TABLE 19

COMPARISON OF RETENTION INDICES (i.u.) MEASURED BY GNAUCK[109] WITH DIFFERENT HEATING RATES ON SE-30 UNDER TPGC CONDITIONS

Initial temperature, 363.16 K.

Compound[a]	*Heating rate (°C/min)*				*Standard deviation*
	4	*6*	*8*	*10*	*(i.u.) (n = 4)*
Allyl alcohol mono-EO-adduct acetate	981	980	981	983	2.26
Di-EO-adduct	1253	1253	1258	1252	2.41
3-EO-adduct	1526	1526	1522	1524	2.81
4-EO-adduct	1800	1799	1800	1800	2.30
5-EO-adduct	2080	2075	2075	2071	2.63

[a] EO = ethylene oxide.

TABLE 20

COMPARISON OF RETENTION INDICES (i.u.) MEASURED BY GNAUCK[109] WITH DIFFERENT INITIAL TEMPERATURES ON SE-30 UNDER TPGC CONDITIONS

Heating rate, 4°C/min.

Compound[a]	*Initial temperature (°C)*		
	50	*70*	*90*
Allyl alcohol mono-EO-adduct acetate	982	984	981
Di-EO-adduct	1258	1252	1253
3-EO-adduct	1524	1529	1526
4-EO-adduct	1803	1804	1800
5-EO-adduct	2080	2077	2080
6-EO-adduct	2349	2343	2344

[a] See Table 19.

TABLE 21

INFLUENCE OF THE SOLUTE SAMPLE SIZE ON RETENTION INDICES MEASURED BY WANG AND SUN[392] UNDER TPGC CONDITIONS ON OV-101

Compound	*Retention index (i.u.)*				
	OV-101				
	Sample size (ng)				
	0.1	*1.0*	*10*	*100*	*1500*
Isobutyl acetate	749.9	750.2	749.7	750.0	753.3
p-Xylene	859.6	859.9	859.8	860.5	864.7
Limonene	1026.2	1026.3	1026.3	1027.0	1031.8
Camphor	1129.5	1129.9	1129.7	1130.5	1136.4
n-Hexyl benzoate	1557.3	1557.2	1557.4	1559.8	1567.0

TABLE 22

RETENTION INDICES OF SOME MYCOTOXINS ON SE-52 DETERMINED BY BATA *ET AL.*[97] UNDER TPGC CONDITIONS

Toxin	*Retention index (i.u.)*	*Toxin*	*Retention index (i.u.)*
T-2 toxin	2822	Monoacetoxyscirpenol	2317
HT-2 toxin	2809	Scirpentriol	2260
Neosolaniol	2652	Fusarone-X	2485
T-2 tetraol toxin	2547	Deoxynivalenol	2323
Diacetoxyscirpenol	2421	Zearalenone	2867

TABLE 23

REPRODUCIBILITY OF RETENTION INDEX ON METHYLSILICONE (DB-1) UNDER TPGC CONDITIONS MEASURED BY NEWTON AND FOERY[134]

Compound	*Mean retention index (i.u.)*	*Standard deviation (i.u.)*	*Coefficient of variation (%)*	
			Within-run	*Day-to-day*
Barbital	1462.2	0.21	0.014	0.008
Butabarbital	1629.9	0.26	0.016	0.012
Pentobarbital	1711.2	0.27	0.016	0.010
Lidocaine	1853.0	0.28	0.015	0.004
Diazepam	2456.8	0.33	0.013	0.006

TABLE 24

COLUMN-TO-COLUMN REPRODUCIBILITY OF RETENTION INDEX ON 5% PHENYLMETHYLSILICONE (DB-5) UNDER TPGC CONDITIONS MEASURED BY NEWTON AND FOERY[134]

Compound	*Retention index (i.u.)*			
	Column 1	*Column 2*	*Column 3*	*Maximum range*
Barbital	1509.5	1511.6	1510.0	2.1
Lidocaine	1906.1	1905.4	1905.4	0.7
Propoxyphene	2232.9	2231.3	2229.3	3.6
Oxazepam	2386.9	2388.3	2387.0	1.4
Nordiazepam	2569.8	2566.3	2567.0	3.5

For example, the retention indices of 2,2,3-trimethylpentane on OV-101 at 40, 50 and 60°C are as follows:

$$I^{\text{OV-101}}_{2,2,3\text{-M3C5}}(40^\circ\text{C}) = 733.4 \text{ i.u.} \tag{2}$$

$$I^{\text{OV-101}}_{2,2,3\text{-M3C5}}(50^\circ\text{C}) = 734.3 \text{ i.u.} \tag{3}$$

$$I^{\text{OV-101}}_{2,2,3\text{-M3C5}}(60^\circ\text{C}) = 735.1 \text{ i.u.} \tag{4}$$

TABLE 25

RETENTION INDEX SHIFTS AS A FUNCTION OF DRUG CONCENTRATION ON 5% PHENYLMETHYLSILICONE (DB-5) UNDER TPGC CONDITIONS MEASURED BY NEWTON AND FOERY[134]

Drug	*Retention index (i.u.)*		
	Concentration (ng/µl)		*Shift*
	5	*50*	
Ethchlorvynol	1024.0	1024.4	0.4
Nicotine	1342.7	1343.0	0.3
Barbital	1510.8	1514.5	3.7
Methylprylon	1553.8	1559.2	5.4
Propoxyphene	2225.1	2225.9	0.8
Lidocaine	1905.7	1904.7	−1.0
Morphine	2476.0	2481.3	5.3
Chlordiazepam	2575.3	2576.4	1.1

The Antoine equation of 2,2,3-trimethylpentane is

$$I^{\text{OV-101}}_{2,2,3\text{-M3C5}}(T) = 748.7 - \frac{2448.0}{T - 153.2} \tag{5}$$

The linear equation is

$$I^{\text{OV-101}}_{2,2,3\text{-M3C5}}(T) = -\frac{8870.8}{T} + 761.73 \tag{6}$$

The retention index differences were not significant. For example:

$$\text{at } 80°\text{C: } I(\text{Antoine}) - I(\text{linear}) = -0.1 \text{ i.u.} \tag{7}$$

$$\text{at } 100°\text{C: } I(\text{Antoine}) - I(\text{linear}) = -0.4 \text{ i.u.} \tag{8}$$

TABLE 26

INFLUENCE OF THE ORIGIN OF THE STATIONARY PHASE ON McREYNOLDS CONSTANTS DETERMINED ON DEGS AT 120°C, AFTER ETTRE[438]

Supplier	*McReynolds constant*				
	Benzene	*n-Butanol*	*2-Pentanone*	*Nitropropane*	*Pyridine*
Supelco (No. 1045)	1123	1295	1185	1440	1478
Chemical Research Services	1145	1323	1208	1485	1490
Supelco (No. 1303)	1149	1336	1217	1489	1534
PolyScience	1152	1341	1220	1492	1559

TABLE 27

KOVÁTS COEFFICIENTS ON SELECTED STATIONARY PHASES AT 120°C; FUNDAMENTAL DATA MEASURED BY McREYNOLDS[439]

Carrier gas, helium.

Stationary phase	*Kováts coefficient [dim]*	*Retention polarity (p.u.)*
Apiezon J	178.55	6.38
Apiezon L	166.87	4.39
Apiezon M	167.02	4.24
Apiezon N	175.95	6.67
Dioctyl sebacate	139.42	20.39
DC-550	193.94	19.25
Diisodecyl phthalate	194.59	23.93
Dioctyl phthalate	199.15	25.93
Tricresyl phosphate	262.54	44.34
UCON 50-HB-2000	253.93	49.39
NPGA	294.45	56.63
Pluronic-F88	288.60	58.70
Triton X-305	368.34	61.14
NPGS	336.72	65.23
PEG-20M	332.72	71.91
PEG-6000	330.20	71.95
XF-1150	370.55	75.43
PEG-1000	342.34	79.84
PEG-600	358.74	81.90
EGA	453.01	82.61
DEGA	455.52	85.61
PEG-1540	321.36	86.24
DEGS	614.53	106.63
PEG-4000	338.05	73.32

TABLE 28

COMPARISON OF MEASURED AND CALCULATED RETENTION INDICES OF 2,2,3-TRIMETHYLBUTANE ON APOLANE-87 STATIONARY PHASE AT DIFFERENT COLUMN TEMPERATURES

Column temperature (°C)	*Retention index (i.u.)*				
	Measured	*Calculated by linear equation*	*Difference*	*Calculated by Antoine equation*	*Difference*
50	639.2	638.9	0.3	639.2	0
70	642.1	642.3	−0.2	642.4	−0.3
90	645.5	645.6	−0.1	645.6	−0.1
110	648.9	649.0	−0.1	648.9	0
130	652.5	652.4	0.1	652.2	0.3
150	655.8	655.8	0	655.6	0.2
170	659.2	659.2	0	659.0	0.2

TABLE 29

RETENTION INDICES OF DIASTEREOMERS OF PRISTANE AND PHYTANE MEASURED BY BORWITZKY AND SHOMBURG[6] ON DIFFERENT STATIONARY PHASES AT DIFFERENT COLUMN TEMPERATURES

Stationary phase	*Retention index (i.u.)*							
	Pristane				*Phytane*			
	120°C	*130°C*	*150°C*	*180°C*	*120°C*	*130°C*	*150°C*	*180°C*
Apolane-87	–	–	1688.8	1689.2	–	–	1791.7	1792.6
	–	–	1690.2	1690.2	–	–	1793.3	1793.9
OV-101	1707.7	1708.4	–	–	1809.5	1810.6	–	–
	1709.4	1710.0	–	–	1811.6	1812.4	–	–

Sixty-seven I *versus* $1/T$ equations were presented by Rang *et al.*[373] for alkenes on OV-101 stationary phase.

Castello and Gerbino[404] studied the effect of column temperature on OV-1 and on SP-1000 stationary phase. An Antoine-type equation, the constants A, B and C of which can be calculated starting from experimental values, was found to be useful for the calculation of retention indices at any temperature on both polar and non-polar stationary phases. Their tables listed the constants of the Antoine equations which describe the dependence of the retention indices of 34 halogenated compounds on column temperature on OV-1 and SP-1000 stationary phases.

Ge *et al.*[108] used liquid crystal stationary phases to study the temperature dependence of the retention index. Chien *et al.*[54,55] studied the temperature dependence of the retention indices of selected compounds on OV stationary phases at different column temperatures.

Although many researchers have realized the necessity to carry out measurements at at least three different isothermal column temperatures for the given isothermal GC system being used[6,7,64,75,89,147,179,204,236,249,270,330,364], this prac-

TABLE 30

RETENTION INDICES OF SOME ALKYLNAPHTHALENES MEASURED BY BREDAEL[7] ON SE-30 AT DIFFERENT COLUMN TEMPERATURES

Compound	*Retention index (i.u.)*			
	80°C	*100°C*	*130°C*	*150°C*
2-Methylnaphthalene	1252	1265	1286	1300
1-Methylnaphthalene	1268	1281	1303	1318
2-Ethylnaphthalene	1328	1340	1358	1370
1-Ethylnaphthalene	1343	1357	1379	1393
2,3-Dimethylnaphthalene	1381	1395	1419	1433

TABLE 31

PRECISION OF RETENTION INDEX DETERMINATION OF TOLUENE MEASURED BY HAKEN *ET AL.*[64] ON A 10% SQUALANE COLUMN AT 100°C

Run No.	*Retention index (i.u.)*	*Run No.*	*Retention index (i.u.)*
1	760.3	7	760.6
2	760.4	8	760.7
3	760.5	9	760.6
4	760.4	10	760.6
5	760.4	11	760.4
6	760.4	12	760.6

Average 760.5
Standard deviation 0.14

TABLE 32

EFFECT OF VARYING THE SAMPLE TO *n*-ALKANE RATIO ON THE RETENTION INDEX OF *n*-HEPTANE MEASURED BY HAKEN *ET AL.*[64] ON SQUALANE AT 100°C

n-C$_6$:n-C$_7$:n-C$_8$ ratio	*Mean retention index (i.u.) (n = 10)*	*Standard deviation (i.u.)*
1:2:1	701.9	0.1
1:3:1	701.3	0.1
2:2:2	700.4	0.1

TABLE 33

COMPARISON OF RETENTION INDICES OF SOME AROMATICS MEASURED BY LUBECK AND SUTTON[75] ON 5% PHENYLMETHYLSILICONE (DB-5) WITH DIFFERENT FILM THICKNESSES AT 60°C

Compound	*Retention index (i.u.)*		
	Column 1 (0.25 μm)	*Column 2 (1.00 μm)*	*Difference*
Benzene	670.6	670.4	0.2
Toluene	772.7	772.8	−0.1
Ethylbenzene	865.0	865.1	−0.1
m-Xylene	872.4	872.4	0
p-Xylene	873.0	873.0	0
o-Xylene	895.7	895.8	−0.1
1,3,5-Trimethylbenzene	968.8	968.8	0
1,2,4-Trimethylbenzene	992.6	992.7	−0.1

TABLE 34

RETENTION INDICES OF *n*-ALKYLBENZENES MEASURED BY VERNON AND SURATMAN[89] ON APIEZON-L AND ON PEG-20M AT DIFFERENT COLUMN TEMPERATURES

Compound	*Retention index (i.u.)*					
	110°C		*130°C*		*150°C*	
	APL	*PEG-20M*	*APL*	*PEG-20M*	*APL*	*PEG-20M*
Benzene	687.2	974.2	693.7	983.4	700.2	992.6
Toluene	795.6	1073.3	802.3	1083.4	809.0	1093.5
Ethylbenzene	885.4	1158.9	892.6	1169.8	899.8	1180.7
n-Propylbenzene	–	–	981.5	1250.7	988.8	1261.6

tical solution has not found general application, mostly owing to the time shortage involved. Some interesting results are summarized in Tables 29–43. See also refs. 147, 266, 275, 276, 321, 353, 404 and 462.

5. ERRORS IN RETENTION INDEX DETERMINATION

As in our previous review[47], this is still one of the most frequently discussed aspects of retention index systems. In the last 5 years many researchers have dealt with the accuracy and reproducibility of retention index determinations and the following

TABLE 35

EFFECT OF SAMPLE PROPORTIONS MEASURED BY VERNON AND SURATMAN[89] ON SQUALANE AT 100°C

Components	*Proportions*	*Retention index (i.u.)*	*Standard deviation (i.u.) (n = 12)*
C_7:benzene:C_8	1:1:1	706.1	0.2
	1:1:2	705.2	0.4
	1:1:3	704.5	0.5
	1:2:1	704.2	0.4
	1:3:1	703.0	0.6
	2:2:1	707.1	0.4
	2:1:1	709.4	0.2
	3:1:1	711.1	0.1
C_7:1-propanol:C_8	1:1:1	694.8	0.1
	1:2:1	694.4	0.2
	2:2:1	696.9	0.4
	3:1:1	697.6	0.2
C_7:2-pentanone:C_8	1:1:1	768.3	0.2
	1:1:3	764.1	0.4
	2:1:1	768.1	0.5

TABLE 36

RETENTION INDICES OF SOME MYCOTOXINS ON SE-52 STATIONARY PHASE AT DIFFERENT COLUMN TEMPERATURES MEASURED BY TAKÁCS *ET AL.*[147]

Toxin[a]	*Retention index (i.u.)*			
	190°C	*210°C*	*230°C*	*250°C*
Deoxynivalenol-TMS	2317.3	2330.0	2346.2	2367.8
Diacetoxycirpenol-TMS	2421.9	2430.0	2437.1	2444.0
Fusarenone-X-TMS	2439.5	2456.9	2475.0	2493.9
HT-2-TMS	2800.3	2817.5	2836.4	2858.3
T-2-TMS	2803.6	2815.9	2832.0	2853.8

[a] TMS = Trimethylsilyl derivative.

TABLE 37

RETENTION INDICES OF SATURATED C_3–C_5 BRANCHED-CHAIN ALCOHOLS ON SE-30 AT DIFFERENT COLUMN TEMPERATURES, AFTER HAKEN AND KORHONEN[179]

Alcohol	*Retention index (i.u.)*					
	60°C	*80°C*	*100°C*	*120°C*	*140°C*	*160°C*
2-Propanol	491	453	508			
2-Methyl-2-propanol	531	500	548			
2-Butanol	605	577	615	622		
2-Methyl-2-butanol	644	628	652	662	642	
2-Methyl-1-propanol	629	609	629	641	620	
3-Methyl-2-butanol	683	668	683	690	699	
2-Pentanol	697	683	692	701	704	
3-Methyl-1-butanol	733	721	723	727	738	

TABLE 38

PRECISION OF RETENTION INDEX DETERMINATION AS THE STANDARD DEVIATION (n = 5) ON OV-101 AND OV-17 STATIONARY PHASES AT 200°C MEASURED BY MACEK AND SMOLKOVÁ-KEULEMANSOVÁ[204]

Compound	*Retention index (i.u.)*		*Standard deviation (i.u.)*	
	OV-101	*OV-17*	*OV-101*	*OV-17*
2-Phenylpropionic acid	1299.7	1453.0	±1.2	±0.9
2-(4-Methylphenyl)propionic acid	1385.6	1547.8	±0.7	±0.9
2-(4-Ethylphenyl)propionic acid	1473.1	1634.2	±0.8	±0.4
2-(4-Isobutylphenyl)propionic acid	1614.3	1751.9	±0.3	±0.8
2-(4-Methoxyphenyl)propionic acid	1528.6	1735.2	±0.2	±0.3

TABLE 39

RETENTION INDICES OF SOME α-HALOGENOCARBOXYLIC ACIDS MEASURED BY WATABE AND GIL-AV[236] ON (*R*)-N-LAUROYL-α-(1-NAPHTHYL)ETHYLAMINE AT DIFFERENT COLUMN TEMPERATURES

tert.-Butylamide	*Retention index (i.u.)*		
	110°C	*130°C*	*150°C*
(*S*)-α-Chloropropanoic acid	1264	1263	1268
(*R*)-α-Chloropropanoic acid	1275	1271	1277
(*S*)-α-Chloro-*n*-butanoic acid	1353	1353	1355
(*R*)-α-Chloro-*n*-butanoic acid	1365	1363	1364
(*S*)-α-Chloroisopentanoic acid	1394	1399	1403
(*R*)-α-Chloroisopentanoic acid	1405	1409	1411
(*S*)-α-Chloro-*n*-pentanoic acid	1441	1444	1444
(*R*)-α-Chloro-*n*-pentanoic acid	1451	1453	1454

TABLE 40

RETENTION INDICES OF SOME ALKENES ON OV-101 AND SQUALANE STATIONARY PHASES AT 50 AND 70°C, AFTER BONEVA AND DIMOV[249]

Compound	*Retention index (i.u.)*			
	OV-101		*Squalane*	
	50°C	*70°C*	*50°C*	*70°C*
trans-2-Pentene	507.0	506.8	500.2	500.0
cis-2-Pentene	512.0	512.4	505.0	505.2
4-Methyl-*cis*-2-pentene	565.6	566.1	556.2	556.6
4-Methyl-*trans*-2-pentene	569.1	568.8	562.1	561.9
cis-3-Hexene	602.4	602.7	592.8	593.1
trans-3-Hexene	602.8	602.4	592.5	591.9
cis-2-Hexene	613.6	614.3	604.0	614.6
3-Methyl-*trans*-2-pentene	620.6	620.9	613.1	613.3
4,4-Dimethyl-*trans*-2-pentene	621.3	621.2	614.7	614.7
4,4-Dimethyl-*cis*-2-pentene	645.1	646.9	635.8	637.8
4-Methyl-*trans*-2-hexene	665.0	665.6	657.0	657.6
4-Methyl-*cis*-2-hexene	660.0	661.2	655.1	656.1
3,4-Dimethyl-*trans*-2-pentene	685.1	685.8	678.0	678.7
3,4-Dimethyl-*cis*-2-pentene	676.7	677.7	670.9	671.7
3-Methyl-*cis*-3-hexene	691.0	691.3	684.8	685.1
3-Methyl-*cis*-2-hexene	701.0	701.7	693.8	694.4
2,2-Dimethyl-*cis*-3-hexene	723.2	724.7	717.0	718.7
2,5-Dimethyl-*trans*-3-hexene	703.7	703.2	695.0	694.5
trans-2-Heptene	709.0	709.2	698.6	698.7
cis-3-Heptene	696.1	696.9	690.5	691.1
trans-3-Heptene	694.0	694.2	687.5	687.5
trans-4-Octene	792.8	793.1	783.9	784.1

can be mentioned: Huizing[18], Bogusz *et al.*[42a], Enqvist *et al.*[56], Hangac *et al.*[66], Knoeppel *et al.*[70], Vernon and Suratman[89], Svetlova *et al.*[145], Bermejo and Guillen[165], Asselin[244], Smith *et al.*[308] and Wang and Sun[392].

Additional interesting data were published by Larson *et al.*[474], Enqvist and

TABLE 41

RETENTION INDICES OF SOME C_1–C_8 MONOCHLORINATED *n*-ALKYL ACETATES ON SE-30 AND OV-351 AT DIFFERENT COLUMN TEMPERATURES, AFTER HAKEN AND KORHONEN[270]

Isomeric acetate	*Retention index (i.u.)*					
	SE-30			*OV-351*		
	60°C	*80°C*	*100°C*	*60°C*	*80°C*	*100°C*
Methyl	508	505	505	823	839	844
Chloro	691	680	674	1181	1180	1164
Ethyl	613	577	607	881	880	875
1-Chloro	744	724	726	1150	1153	1123
2-Chloro	817	801	796	1315	1319	1297
Propyl	711	685	676	981	978	943
1-Chloro	838	821	806	1217	1222	1198
2-Chloro	864	848	835	1296	1304	1283
3-Chloro	924	916	902	1418	1425	1414

	SE-30				*OV-351*			
	80°C	*100°C*	*120°C*	*140°C*	*80°C*	*100°C*	*120°C*	*140°C*
Butyl	810	786	774	781	1079	1053	1064	1154
1-Chloro	930	906	895	912	1298	1278	1279	1342
2-Chloro	964	944	930	951	1384	1370	1375	1425
3-Chloro	981	961	949	972	1432	1422	1427	1478
4-Chloro	1038	1021	1008	1033	1539	1533	1540	1585
Pentyl	912	885	867	879	–	1195	1182	1212
1-Chloro	1026	1006	990	1011	–	1401	1387	1419
2-Chloro	1051	1033	1017	1041	–	1469	1460	1492
3-Chloro	1078	1062	1048	1072	–	1528	1525	1558
4-Chloro	1089	1073	1058	1084	–	1563	1564	1594
5-Chloro	1143	1129	1116	1142	–	1652	1657	1687

	SE-30				*OV-351*			
	100°C	*120°C*	*140°C*	*160°C*	*100°C*	*120°C*	*140°C*	*160°C*
Hexyl	1008	972	993	1000	1277	1255	1286	1295
1-Chloro	1117	1086	1108	1114	1472	1457	1492	1500
2-Chloro	1147	1121	1143	1151	1540	1532	1576	1574
3-Chloro	1166	1143	1166	1173	1581	1578	1627	1629
4-Chloro	1186	1163	1187	1194	1626	1627	1679	1679
5-Chloro	1194	1171	1194	1202	1647	1650	1700	1703
6-Chloro	1247	1227	1249	1257	1747	1737	1789	1796

(*Continued on p. 24*)

TABLE 41 (*continued*)

Isomeric acetate	*Retention index (i.u.)*									
	SE-30					*OV-351*				
	100°C	*120°C*	*140°C*	*160°C*	*180°C*	*100°C*	*120°C*	*140°C*	*160°C*	*180°C*
Heptyl	1095	1070	1086	1090	1093	1385	1372	1401	1400	1385
1-Chloro	1211	1191	1211	1215	1212	1582	1578	1602	1607	1615
2-Chloro	1235	1217	1239	1244	1242	1647	1647	1673	1673	1675
3-Chloro	1254	1238	1260	1266	1262	1686	1691	1718	1720	1725
4-Chloro	1266	1251	1273	1278	1276	1717	1723	1753	1757	1759
5-Chloro	1284	1269	1292	1297	1295	1749	1756	1787	1791	1797
6-Chloro	1291	1276	1298	1303	1299	1767	1775	1806	1809	1818
7-Chloro	1342	1329	1350	1354	1354	1846	1857	1889	1894	1904
Octyl	1194	1165	1188	1189	1190	1468	1454	1490	1486	1485
1-Chloro	1306	1287	1312	1314	1315	1659	1658	1702	1704	1711
2-Chloro	1328	1312	1338	1343	1344	1722	1724	1771	1771	1775
3-Chloro	1345	1331	1358	1362	1364	1758	1764	1814	1819	1824
4-Chloro	1355	1342	1369	1373	1373	1787	1794	1845	1850	1856
5-Chloro	1365	1352	1379	1384	1385	1802	1811	1862	1867	1874
6-Chloro	1382	1370	1396	1402	1405	1830	1840	1893	1899	1909
7-Chloro	1385	1372	1399	1403	1405	1842	1852	1905	1912	1922
8-Chloro	1435	1452	1451	1456	1458	1918	1932	1987	1994	2006

TABLE 42

RETENTION INDICES OF C_4–C_5 EPOXIDES ON OV-101 STATIONARY PHASE AT DIFFERENT COLUMN TEMPERATURES MEASURED BY BONEVA AND DIMOV[330]

Compound	*Retention index (i.u.)*		
	70°C	*80°C*	*90°C*
2-Methyl-1,2-epoxypropane	534.4	534.7	535.0
trans-2,3-Epoxybutane	543.5	543.6	543.7
1,2-Epoxybutane	587.0	587.4	587.8
cis-2,3-Epoxybutane	572.6	573.1	573.6
3-Methyl-1,2-epoxybutane	612.0	613.3	613.8
1,2-Epoxypentane	624.5	624.7	624.9
2-Methyl-1,2-epoxybutane	633.3	633.7	634.0
trans-2,3-Epoxypentane	654.9	655.0	655.1
cis-2,3-Epoxypentane	658.4	659.4	660.4
2-Methyl-2,3-epoxybutane	668.0	668.1	668.2

TABLE 43

RETENTION INDICES OF SOME DRUGS ON SE-30 AT DIFFERENT COLUMN TEMPERATURES MEASURED BY MUSUMARRA *ET AL.*[364]

Drug	*Retention index (i.u.)*		
	140°C	*160°C*	*180°C*
Amantadine	1272	–	–
Amphetamine	1115	–	–
Beclamide	–	–	1697
Caffeine	–	–	1809
Clobutinol	–	–	1758
Cropropamide	–	–	1706
Crotethamide	–	–	1661
Cyclopentamine	1100	–	–
Ephedrine	1388	–	–
Ethosuximide	1250	–	–
Fenfluramine	–	1240	–
Heptaminol	1188	–	–
Hordenine	–	1495	–
Ketamine	–	–	1820
Lefetamine	–	1670	–
Lidocaine	–	–	1875
Meperidine	–	–	1741
Mephentermine	–	1305	–
Methamphetamine	1188	–	–
Methoxyphenamine	–	1390	–
Metronidazole	–	–	1618
Mexiletine	1408	–	–
Nicametate	–	1648	–
Nicotine	–	1360	–
Nikethamide	1520	–	–
Oxyfedrine	1380	–	–
Phenacetin	–	–	1695
Phendimetrazine	–	1450	–

Hesso[12], Enqvist *et al.*[174], Haken *et al.*[64], Hangac *et al.*[66], Pacholec and Poole[135], Ballschmiter *et al.*[161] and Dimov[261].

6. DETERMINATION AND/OR CALCULATION OF THE GAS HOLDUP (DEAD) TIME

Determination and/or calculation of the gas holdup (dead) time (t_M) is still a particularly widely discussed problem[149,150,222,224,230,312], as reported in the previous review also[47]. Computer-assisted studies are of special importance.

Tóth and Zala[149,150] dealt with the calculation of the constants of the *n*-alkane retention time curve and the gas holdup time in GLC. The numerical results obtained with their calculation method were compared with those obtained by Gröbler and Bálizs' iterative method[440] and the results agreed well.

Smith *et al.*[222] compared some mathematical methods for the calculation of dead time and Kováts retention indices[224]. They also dealt with the linearity of the plot of log(adjusted retention time) *versus* carbon number for *n*-alkanes. Seven methods, together with two modified approaches allowing the optimization of t_M while simultaneously fitting a cubic or fifth-degree polynomial to the data, were compared[222]. Their studies and results are of great interest and their review is the most important paper in this field.

Summarizing the results on gas holdup times, it can be stated that if correct retention time data are available, the simple mathematical method applying three consecutive *n*-alkanes is equivalent to the more complicated computer methods. With incorrect retention time data, even a skilful computer operator is unable to produce correct retention index values. Therefore, it is essential to select correct, calculated or determined gas holdup times for the calculations of exact retention indices.

7. SLOPE OF THE *n*-ALKANE PLOT. THE *b* VALUE. TEMPERATURE DEPENDENCE OF THE *b* VALUE ON DIFFERENT STATIONARY PHASES

By the *n*-alkane plot we mean the plot of $\log X(z)$ *versus* carbon number (z) relationship for *n*-alkanes, where X is the retention value used in the calculation. In the most frequent treatment, values of the adjusted retention times (t'_R) or net retention times (t_N), and also values of specific (V_g) or net retention volumes (V_N) should be substituted for X.

The *n*-alkane plots are generally linear except for the first seven members of the homologous series[47]. The reason is that for the *n*-alkanes of low carbon number, owing to the individual bonds in their molecules, the deviation from linearity decreases from methane to *n*-hexane. Previously, we described the structure of the first eight *n*-alkanes[451] and their bond codes[385]. It can be seen that the first six members of the homologous series (up to *n*-hexane) contain different types of individual bonds. Thus, they will interact differently with the stationary phase, and therefore, the relationship cannot be linear. Linear relationships start with *n*-heptane; from here on, each *n*-alkane molecule contains the same types of bonds and they differ from each other only in the number of these bonds.

The dependence of the *b* value on the column temperature can be described, in theory, by an Antoine-type equation, similarly to the retention index and Kováts coefficient[47]. Nevertheless, the temperature dependence of the *b* value can be approximately described with the following equation:

$$b_T^{\text{st.ph.}} = \frac{D}{T} + E \tag{9}$$

where D and E are constants and T is the column temperature (K). Eqn. 9 is a practical possibility for checking the effective column temperature, as

$$T = \frac{D}{b_T^{\text{st.ph.}} - E} \tag{10}$$

The equations used for temperature control of columns with some OV stationary phases are as follows:

$$\text{OV-1: } T = \frac{215.97}{b + 0.2898} \tag{11}$$

$$\text{OV-3: } T = \frac{238.40}{b + 0.3452} \tag{12}$$

$$\text{OV-7: } T = \frac{225.62}{b + 0.3037} \tag{13}$$

$$\text{OV-11: } T = \frac{234.12}{b + 0.3293} \tag{14}$$

$$\text{OV-22: } T = \frac{245.44}{b + 0.3769} \tag{15}$$

$$\text{OV-25: } T = \frac{277.26}{b + 0.4732} \tag{16}$$

We compared the calculated data obtained by using different equations and the results are given in Table 44.

Morishita *et al.*[78] achieved good results in this field for chlorinated alkanes on PEG-20M and Apiezon L stationary phases at 90°C. Berezkin and Retunsky[163] checked the linearity of the *n*-alkane plot on four different stationary phases and the temperature dependence of the *b* value, using *n*-alkanes, 1-alkanols and their acetates as markers. The linearity of the *n*-alkane plot and the problem of the *b* value were studied on various stationary phases at different column temperatures by Hawkes[413], who obtained satisfactory results (Table 45).

Touabet *et al.*[430] studied methods for testing the linearity of retention time *versus* carbon number plots for *n*-alkanes. Through statistical evaluation of the results, four parameters models were generally found to be adequate. Engewald *et al.*[340] compared the *b* values with ΔG_{CH_2} values on different stationary phases at 100°C

TABLE 44

COMPARISON OF *b* VALUES MEASURED BY CHIEN *ET AL.*[54,55] AND CALCULATED BY VARIOUS METHODS ON OV-25 STATIONARY PHASE AT DIFFERENT COLUMN TEMPERATURES

Column temperature (°C)	*b Value*				
	Measured	*Calc. by linear equation*	*Difference*	*Calc. by Antoine equation*	*Difference*
40	0.4120	0.4122	−0.0002	0.4121	−0.0001
60	0.3590	0.3590	0	0.3590	0
80	0.3130	0.3119	0.0011	0.3130	0
100	0.2710	0.2698	0.0012	0.2728	−0.0018
120	0.2350	0.2320	0.0030	0.2374	−0.0024

TABLE 45

b VALUES FOR VARIOUS STATIONARY PHASES AT DIFFERENT COLUMN TEMPERATURES, AFTER HAWKES[413]

Stationary phase	*b Value*					
	50°C	*75°C*	*80°C*	*100°C*	*120°C*	*125°C*
Squalane	0.436	0.386	0.361	0.331	0.289	–
Apiezon L	0.432	0.370	–	0.315	–	0.263
OV-101	0.369	0.317	–	0.275	–	0.226
OV-3	0.388	0.323	–	0.277	–	0.239
OV-7	0.396	0.325	–	0.276	–	0.241
OV-61	0.340	0.272	–	0.239	–	0.207
OV-11	0.343	0.318	–	0.279	–	0.236
OV-17	0.379	0.310	0.318	0.276	0.261	0.228
OV-22	0.343	0.276	–	0.240	–	0.211
OV-25	0.306	0.246	–	0.227	–	0.188
OV-210	0.297	0.227	–	0.202	–	0.171
OV-225	0.339	0.253	–	0.226	–	0.186
Silar-5CP	0.321	0.276	–	0.216	–	0.180
Silar-10CP	0.261	0.221	–	0.177	–	0.137
PEG-20M	–	0.259	–	0.225	0.193	0.190
QF-1	–	0.289	0.262	–	0.209	–
DEGS	–	–	–	–	0.193	–

(Table 46). The *b* values measured by Chien *et al.*[54,55] and Hawkes[413] are summarized in Table 47. Finally, some *b* values measured by Chien *et al.*[54,55] on different OV stationary phases at different column temperatures are given in Table 48.

8. CONNECTION BETWEEN PHYSICO-CHEMICAL QUANTITIES AND RETENTION INDEX

In theory, this is one of the most important questions with respect to retention index system. A fundamental relationship exists between the specific retention volume (V_g) and the retention index (I):

$$\log V_g(s) = \frac{(I - K_c)b}{100} \tag{17}$$

TABLE 46

COMPARISON OF *b* VALUES AND ΔG_{CH_2} VALUES ON DIFFERENT STATIONARY PHASES AT 100°C, AFTER ENGEWALD *ET AL.*[340]

Stationary phase	*b Value*	ΔG_{CH_2} *(J mol⁻¹)*
Squalane	0.3196	2280
UCON LB-550X	0.2916	2080
UCON 50-HB-280X	0.2804	2000
OV-1	0.2776	1980
PEG-20M	0.2467	1760
Carbopack C (GTCB)	0.5860	4180

TABLE 47

COMPARISON OF *b* VALUES MEASURED BY CHIEN *ET AL.*[54,55] AND HAWKES[413] ON DIFFERENT OV STATIONARY PHASES AT 50°C

Stationary phase	*b Value*		
	Chien et al.[54,55]	*Hawkes*[413]	*Difference*
OV-101	0.3847	0.369	0.0157
OV-3	0.3924	0.388	0.0044
OV-7	0.3947	0.396	−0.0013
OV-11	0.3951	0.343	0.0521
OV-17	0.3886	0.379	0.0096
OV-22	0.3826	0.343	0.0396
OV-25	0.3846	0.306	0.0786

where K_c is the Kováts coefficient[429b]:

$$K_c = 100\left[z - \frac{\log V_g(z)}{b}\right] \tag{17a}$$

and b is the slope of the linear section of the n-alkane plot:

$$b = \log V_g(z + 1) - \log V_g(z) \tag{17b}$$

A useful relationship is available, if the following data for the GLC system used are known:

$$I_{s1}^{\text{st.ph.}}(T) - I_{s2}^{\text{st.ph.}}(T) = \frac{100}{b} \cdot \log \alpha \tag{18}$$

TABLE 48

b VALUES FROM DATA MEASURED BY CHIEN *ET AL.*[54,55] ON DIFFERENT STATIONARY PHASES AT DIFFERENT COLUMN TEMPERATURES

Stationary phase	*Phenyl (%)*	*b Value*			
		30°C	*50°C*	*70°C*	*90°C*[a]
OV-101	0	0.4323	0.3847	0.3427	0.3055
OV-1	0	0.4226	0.3785	0.3395	0.3048
OV-3	10	0.4415	0.3924	0.3498	0.3124
OV-7	20	0.4396	0.3947	0.3530	0.3141
OV-11	35	0.4430	0.3951	0.3530	0.3157
OV-17	50	0.4311	0.3886	0.3478	0.3086
OV-22	65	0.4327	0.3826	0.3383	0.2988
OV-25	75	0.4419	0.3846	0.3352	0.2922

[a] Values calculated by Antoine equations from measured data.

where α is relative volatility. In this rather broad area of research, numerous papers have been devoted clarifying the relationship between the boiling point and the retention index. Without aiming at completeness, we cite the contributions of Bermejo and Guillen[42], Calixto *et al.*[51], Chelghoum *et al.*[258], Nabivach and Vasiliev[365].

A method for calculating "solubility factors" in GLC by using retention indices was developed by Patte *et al.*[28a]. This method was refined and applied to 240 selected compounds covering a wide range of functional groups and molecular structures. Retention indices of mono- and bifunctional molecules on SE-30, squalane, PEG-20M and DEGS at 120°C were related to structural parameters by means of multiple regression and factor analysis by Buydens and co-workers[49,50].

Golovnya and Grigoryeva[58] derived a universal equation for members of homologous series of some organic compounds permitting the calculation of specific retention volume (V_g), retention index (I), partial free energy of sorption and the change in the energy contribution of a methylene unit. A significant correlation was found between the retention indices and the average molecular polarizabilities of ten polycyclic aromatic hydrocarbons by Lamparczyk *et al.*[72] on SE-30, OV-101, SE-52, OV-7 and OV-17 at 250°C. Szász *et al.*[84] demonstrated a relationship between molecular connectivity index, partition coefficient and chromatographic parameters. Berezkin and Retunsky[99] derived a modified equation for the calculation of the theoretical plate number and selection of the sorbent on the basis of retention indices.

Bermejo *et al.*[101] studied the relationships between parameters related to electronic polarizability, such as molar refraction, refractive index, Van der Waal's volume and molar volume, and the retention indices of alkylbenzenes on squalane and PEG-20M at 100°C. Good correlations were found by Calixto *et al.*[104] between retention indices and the total and binding energies. An interesting paper was published by Lamparczyk and Radecki[126] on correlations between retention and molecular physico-chemical properties such as polarizability and dipole moment.

Molecular orbital calculations were used to study the retention of *n*-alkenes by Garcia-Raso *et al.*[138]. Using the retention index, the influence of molecular parameters such as total energy, binding energy, excess charge distribution and values of the energy and coefficients of the highest occupied and lowest unoccupied molecular orbitals were considered. According to Klopman's equation, these parameters are directly related to the solute–stationary phase interaction term of the retention index. General equations including several homologous series were presented.

Sabljić[141] studied the calculation of the retention indices of chlorinated alkanes by molecular topology. The comparison of the results obtained with the molecular connectivity model and the empirical additive scheme revealed important advantages of the molecular connectivity approach[214].

Buydens *et al.*[169] presented a relationship between GC behaviour and topological, physico-chemical and quantum chemically calculated charge parameters for neuroleptica. Retention indices of some neuroleptic drugs were subsequently measured on OV-101 and OV-17 at 260°C[255].

Based on the influence of the binding energy on retention, relationships between the retention indices on squalane and the heats of formation of some hydrocarbons were found by Calixto *et al.*[170a]. Terms taken from the information theory[456] were used in order to improve the correlation coefficients of the equations of retention index *versus* heat of formation.

For a structurally diverse set of primary, secondary and tertiary heterocyclic amines, correlations were found by Osmialowski *et al.*[209] between retention indices and quantum chemically calculated parameters. Golovnya[267a] suggested a universal equation describing the deviation from linearity of the plots for *n*-alkanes and other homologous series. She demonstrated the principle of non-additivity of the sorption energy and its application to the precalculation of retention indices. Retention indices for seven straight-chain liquid-phase solvents (*n*-heptadecane, 1-hexadecene, 1-hexadecyl chloride, 1-hexadecyl bromide, 1-hexadecyl iodide, di-*n*-octyl ether and di-*n*-octyl thioether) of comparable length and 49 straight- and branched-chain solutes were target factor analysed by Howery and Soroka[279]. (Target factor analysis is a mathematical computer method for analysis of experimental errors. It was introduced in the research of retention indices, McReynolds system, etc. by Malinowski and Howery[490]; *cf.* refs. 47 and 567–570).

Robbat *et al.*[301] derived a multivariate relationship between the retention indices and molecular connectivities of mononitrated polycyclic aromatic hydrocarbons. Bermejo and Guillen[326] obtained valuable results by applying the regular solution model to the solution processes that take place in GLC. Equations were obtained that relate the specific retention volume of solutes to their molecular volume and latent heat of vaporization. Papp and co-workers[367,368] studied the correlations between molar refraction and retention indices measured on OV-1 and OV-225 at 240°C. They reported[368] some problems in the correlation of molecular parameters and the connectivity index. Sanchez *et al.*[378] studied the effect of the number of McReynolds constants on the reproducibility on 250 stationary phases.

Model non-ionic surfactants were analysed by Voelkel[387] on four stationary phases (SE-30, Apiezon K, OV-17 and QF-1) at different column temperatures. The retention indices and the partial molar thermodynamic parameters of solution, *i.e.*, Gibbs free energy, enthalpy and entropy, and their increments for characteristic structural fragments were calculated.

For further details, see refs. 22, 31, 35, 37, 69, 73, 98, 107, 139, 164, 212, 212a, 231, 242, 287, 294, 317, 328, 359, 359a, 360, 373, 390 and 397.

9. RETENTION INDEX AND MOLECULAR STRUCTURE

The relationship between molecular structure and retention index is the most frequently discussed aspect of retention index systems and remains at the centre of interest. Research activity in this area can be classified according to the basic idea from which the calculations and experimental studies started.

In the simplest case, the basis of research is the various differences between the values of the retention index of the many studies of this type we refer to those made by Boneva, Dimov and co-workers[44,249,260,329], Engewald and co-workers[339,340,409] and Haken, Korhonen and co-workers[60–63,111–113,119–125,177–179,180,185–196,282–284].

Useful retention indices published by Supelco[225a] are given in Table 49.

Retention indices of alkylbenzenes measured on various stationary phases at different column temperatures are of continuous interest for researchers and research teams. Remarkable results are shown in Tables 50–57.

Structure–retention correlations were derived from retention index differences

TABLE 49

RETENTION INDICES OF VARIOUS COMPOUNDS ON SP-1700 at 70°C[225a]

Compound	*Retention index (i.u.)*	*Compound*	*Retention index (i.u.)*
Ethylene	270	1,3-Butadiene	479
Carbon dioxide	281	Pentene-1	517
Propylene	329	*trans*-2-Pentene	530
Acetylene	336	2-Methyl-1-butene	530
Isobutane	366	*cis*-2-Pentene	546
Carbonyl sulphide	380	2-Methyl-2-butene	558
Isobutene/1-butene	420	2-Methylpentane	566
trans-2-Butene	443	3-Methylpentane	585
cis-2-Butene	460	3-Methylhexane	655
Isopentane	470		

by Engewald *et al.*[340]. It was shown that the combined application of retention index differences obtained in GLC and gas–solid chromatography (GSC) provides more detailed structural information (Table 58).

The GC retention behaviour of a series of chlorinated phenyl acetates was studied by Haken and Korhonen[61] on SE-30 and OV-351 at different column temperatures (Table 59). Haken and Korhonen[62] also dealt with the determination of isomeric chlorobenzenes on SE-30 and PEG-20M at different column temperatures and some of the retention indices measured are presented in Table 60. Retention indices of some aromatic esters measured by Haken *et al.*[65] on SE-30, OV-25, QF-1 and Silar 10C stationary phases at different column temperatures, *e.g.*, 200°C, are shown in Table 61. Retention indices of perfluoro-*n*-alkanes measured by Müller *et al.*[79] are listed in Table 62.

By means of GLC with a combination of SE-30 with three different stationary phases (Wax-51, Siponate DS-10 and OV-215), various compounds and chemical classes were identified from differences in retention indices by Winskowski[93]. Some of

TABLE 50

RETENTION INDICES OF SOME AROMATICS MEASURED BY BREDAEL[7] ON SE-30 AT 80 AND 130°C

Compound	*Retention index (i.u.)*	
	80°C	*130°C*
Benzene	659	670
Toluene	761	774
Ethylbenzene	854	867
m-Xylene	864	876
p-Xylene	864	876
o-Xylene	885	900
1,3,5-Trimethylbenzene	960	972
1,2,4-Trimethylbenzene	984	1000
1,2,3-Trimethylbenzene	1009	1029

TABLE 51

RETENTION INDICES (i.u.) OF SOME GEOMETRIC ISOMERS IN THE NEMATIC RANGE OF SOME SPECIAL STATIONARY PHASES AND ON OV-225 AT 99°C, AFTER ISENBERG *ET AL.*[117]

Substance	*Stationary phase*		
	4-n-Dodecyl-benzoic acid	*2-Chlorohydro-quinonebis(4-n-octyloxy benzoate)*	*OV-225*
m-Xylene	932	985	1058
p-Xylene	931	994	1056
o-Xylene	958	1017	1099
m-Chlorotoluene	1033	1101	1190
p-Chlorotoluene	1035	1116	1194
o-Chlorotoluene	1026	1091	1178
m-Diethylbenzene	1089	1126	1228
p-Diethylbenzene	1102	1150	1235
o-Diethylbenzene	1106	1148	1255
trans-Decalin	1103	1127	1151
cis-Decalin	1143	1163	1210

TABLE 52

RETENTION INDICES OF SOME AROMATIC HYDROCARBONS MEASURED BY ENGEWALD *ET AL.*[339] ON OV-1 AND UCON LB-550X AT 100°C

Compound	*Retention index (i.u.)*	
	OV-1	*UCON LB-550X*
Benzene	663.7	759.2
Toluene	767.2	862.1
Ethylbenzene	859.1	950.3
Vinylbenzene	885.4	1008.7
n-Propylbenzene	949.5	1036.6
Isopropylbenzene	920.5	1004.4
n-Butylbenzene	1047.2	1134.0
Allylbenzene	938.6	1044.1
Isopropenylbenzene	972.6	1089.6

TABLE 53

RETENTION INDICES OF SOME ALKYLBENZENES ON SQUALANE AT 100°C MEASURED BY NABIVACH AND VASILIEV[365]

Compound	*Retention index (i.u.)*	*Compound*	*Retention index (i.u.)*
Benzene	651.1	*o*-Xylene	883.9
Toluene	757.9	1,3,5-Trimethylbenzene	967.9
Ethylbenzene	848.7	1,2,3-Trimethylbenzene	1011.6
p-Xylene	862.1	1,2,3,4-Tetramethylbenzene	1136.3
m-Xylene	864.1	Pentamethylbenzene	1260.5

TABLE 54

RETENTION INDICES OF SOME ALKYLBENZENES ON SQUALANE AT 100°C, AFTER MATISOVÁ[418]

Compound	*Retention index (i.u.)*					
	Ref. 480	*Ref. 481*	*Ref. 482*	*Ref. 483*	*Ref. 484*	*Ref. 485*
Benzene	648.0	650.4	647.9	649.2	650.5	651.1
Toluene	755.7	758.0	756.9	756.6	760.1	757.9
Ethylbenzene	846.1	847.7	847.7	846.9	850.0	848.7
1,4-Dimethylbenzene	860.0	861.8	862.9	860.8	864.6	862.2
1,3-Dimethylbenzene	861.5	863.2	865.7	862.7	864.8	864.1
1,2-Dimethylbenzene	882.5	883.7	885.6	882.9	886.0	883.9
Isopropylbenzene	905.6	908.0	907.1	906.3	908.4	907.7
n-Propylbenzene	934.7	936.1	936.2	935.4	938.0	936.1
1-Methyl-4-ethyl-benzene	950.0	951.3	950.8	950.6	954.3	951.3
1-Methyl-2-ethyl-benzene	963.1	964.7	966.5	963.9	966.0	964.3
1,3,5-Trimethylbenzene	966.8	967.6	969.8	967.5	969.0	967.9
1,2,4-Trimethylbenzene	984.7	988.2	–	985.5	987.0	986.3
1,2,3-Trimethylbenzene	1010.1	1011.9	1013.0	1011.1	1012.9	1011.6
tert.-Butylbenzene	972.3	973.3	973.2	972.9	971.7	973.5
sec.-Butylbenzene	988.6	989.8	989.5	989.3	990.2	990.2

TABLE 55

RETENTION INDICES OF SOME ALKYLBENZENES ON SE-30 AND OV-101 AT 100°C, AFTER MATISOVÁ[418]

Compound	*Retention index (i.u.)*		
	SE-30		*OV-101*
	Ref. 486	*Ref. 487*	
Benzene	661.8	663.1	663.6
Methylbenzene	764.4	765.9	766.4
Ethylbenzene	865.5	857.7	858.9
1,4-Dimethylbenzene	865.5	867.4	867.7
1,2-Dimethylbenzene	888.9	890.0	890.3
n-Propylbenzene	946.9	949.3	949.3
1-Methyl-3-ethylbenzene	956.6	956.2	955.9
1-Methyl-4-ethylbenzene	957.0	958.1	958.2
1,3,5-Trimethylbenzene	960.2	963.1	963.3
1-Methyl-2-ethylbenzene	973.4	973.3	972.8
1,2,4-Trimethylbenzene	984.7	985.9	988.4
tert.-Butylbenzene	985.9	989.0	987.6
sec.-Butylbenzene	1003.6	1006.0	1005.7
1,2,3-Trimethylbenzene	1018.9	1017.7	1015.9
1-Methyl-3-isopropylbenzene	1005.8	1013.2	1011.9
1-Methyl-4-isopropylbenzene	1012.0	1017.0	1017.8
1-Methyl-2-isopropylbenzene	1026.0	1028.4	1032.3
1-Methyl-3-*n*-propylbenzene	1041.4	1043.2	1043.4
1,3-Diethylbenzene	1042.4	1044.1	1040.4
1-Methyl-4-*n*-propylbenzene	1045.9	1047.1	1047.5
n-Butylbenzene	1046.5	1047.4	1048.1

TABLE 56

RETENTION INDICES OF SOME ALKYLBENZENES ON UCON LB-550X AND CITROFLEX A-4 STATIONARY PHASES AT 90°C, AFTER MATISOVÁ[418]

Compound	*Retention index (i.u.)*			
	UCON LB-550X		*Citroflex A-4*	
	Ref. 488	*Ref. 484*	*Ref. 483*	*Ref. 481*
Benzene	757.6	757.4	782.6	783.7
Ethylbenzene	948.8	947.7	975.8	975.7
1,4-Dimethylbenzene	959.9	957.8	982.6	982.8
1,3-Dimethylbenzene	963.6	961.1	986.1	985.7
1,2-Dimethylbenzene	995.1	988.5	1013.5	1013.0
Isopropylbenzene	1003.9	1001.2	1034.6	1033.7
1-Methyl-3-ethylbenzene	1047.2	1045.5	1072.7	1073.1
1-Methyl-4-ethylbenzene	1047.2	1045.5	1073.1	1072.9
1,3,5-Trimethylbenzene	1064.3	1063.4	1086.5	1082.7
1-Methyl-2-ethylbenzene	1068.1	1066.3	1094.8	1095.2
tert.-Butylbenzene	1069.7	1065.3	1101.9	1100.8
Isobutylbenzene	1080.7	1080.9	1111.4	1110.6
sec.-Butylbenzene	1084.7	1082.0	1114.7	1113.6
1,2,4-Trimethylbenzene	1087.6	1086.7	1110.1	1100.6
1-Methyl-3-isopropylbenzene	1094.4	1099.5	1126.6	1122.6
1,2,3-Trimethylbenzene	1120.8	1119.7	1143.7	1140.8
1,3-Diethylbenzene	1125.0	1123.1	1153.4	1153.4
1-Methyl-4-*n*-propylbenzene	1130.0	1131.6	1159.5	1158.0
1,4-Diethylbenzene	1133.3	1132.5	1162.9	1162.9
n-Butylbenzene	1134.8	1132.5	1162.8	1162.3
1-Methyl-2-*n*-propylbenzene	1144.1	1144.5	1174.5	1173.3

his results are presented in Table 63. Jánosi[118] determined retention indices of methylnaphthalenes on OV stationary phases (Table 64). Electronic and conformational effects of substituents on the retentions of Z/E isomeric olefins were rationalized by Priboth *et al.*[137].

Some interesting results for retention indices are given in Tables 65–70.

The retention behaviour of 32 synthesized C_6–C_{15} monoalkylcyclopentadienes on squalane and PEG-20M at 64°C was studied by Soják *et al.*[381] (Table 71). Specific interactions of alkanes with different metal ion forms of ion exchangers in GSC were studied by Hirsch *et al.*[17]. Tóth[87], using GLC and specific chemical reactions, analysed complex petrochemical mixtures and obtained excellent retention index values on SE-30 and PEG-20M stationary phases. Buchman *et al.*[103] studied the structure of substituted cyclohexenes on the basis of retention indices.

We also draw readers' attention to papers by Szederkényi *et al.*[144], Wu[155], Horna *et al.*[182], Kuchar *et al.*[198], Morishita *et al.*[206], Andersson[243], Komárek *et al.*[281], and Premecz and Ford[372]. Further useful results are summarized in Tables 72–76.

A further group of studies on retention index–molecular structure correlations are concerned with the determination of increments connected with different functional groups. Without trying to be exhaustive, of the many papers of this type we

TABLE 57

RETENTION INDICES OF SOME ALKYLBENZENES ON PEG-20M AND PEG-1540 STATIONARY PHASES AT 90°C, AFTER MATISOVÁ[418]

Compound	*Retention index (i.u.)*			
	PEG-20M			*PEG-1540 (ref. 285)*
	Ref. 488	*Ref. 484*	*Ref. 486*	
Benzene	933.4	941.3	960.3	960.2
Ethylbenzene	1111.1	1119.4	1141.3	1139.0
Isopropylbenzene	1154.9	1162.5	1186.3	1188.2
n-Propylbenzene	1190.3	1197.3	1220.5	1221.3
1,3,5-Trimethylbenzene	1220.3	1228.2	1253.6	1256.3
tert.-Butylbenzene	1215.1	1222.5	1237.5	1250.0
Isobutylbenzene	1215.9	1230.0	1251.7	1252.5
1,2,4-Trimethylbenzene	1253.1	1262.7	1289.0	1290.6
1,3-Diethylbenzene	1275.8	1282.1	1308.1	1308.0
1-Methyl-3-propylbenzene	1277.2	–	1310.0	1309.9
1-Methyl-4-propylbenzene	1279.9	1287.5	1310.8	1312.9
1,4-Diethylbenzene	1283.6	1281.3	1316.4	1316.6
n-Butylbenzene	1284.0	1293.4	1319.1	1318.6
1-Methyl-2-propylbenzene	1305.4	1312.9	1337.5	1339.7
sec.-Butylbenzene	1227.2	1234.6	1259.1	1260.3
1-Methyl-3-isopropylbenzene	1244.3	1253.0	1275.7	1275.1
1,2,3-Trimethylbenzene	1301.8	1311.0	1339.8	1340.0

can cite those by Haken *et al.*[65], Anders *et al.*[160], Peetre *et al.*[211], Szymanowski *et al.*[228], Haken and Korhonen[269,270] and Haken and Vernon[271].

The influence of increasing stationary phase polarity on the retention index increments of homologous aromatic esters, RCOOR′, where R and R′ represent the acid (acyl) and alcohol chains, respectively, was reported by Haken *et al.*[65]. Their

TABLE 58

RETENTION INDICES OF SOME ALICYCLIC HYDROCARBONS MEASURED BY ENGEWALD *ET AL.*[340] ON OV-1 AND UCON LB-550X AT 100°C

Compound	*Retention index (i.u.)*	
	OV-1	*UCON LB-550X*
Cyclooctane	927.2	957.7
Cyclononane	1035.7	1070.0
Cyclodecane	1133.9	1168.5
Cycloundecane	1225.4	1260.7
Cyclododecane	1323.7	1344.5
cis-Cyclododecane	1306.1	1356.0
trans-Cyclododecane	1291.5	1340.7

TABLE 59

RETENTION INDICES OF SOME CHLORINATED PHENYL ACETATES MEASURED BY HAKEN AND KORHONEN[61] ON SE-30 AND OV-351 AT 180°C

Compound	*Retention index (i.u.)*	
	SE-30	*OV-351*
Phenyl acetate	1025	1639
2-Chlorophenyl acetate	1192	1838
3-Chlorophenyl acetate	1219	1856
4-Chlorophenyl acetate	1224	1878
2,4- and 2,5-dichlorophenyl acetate	1351	1998
2,6-Dichlorophenyl acetate	1330	1985
2,3-Dichlorophenyl acetate	1384	2067
3,4-Dichlorophenyl acetate	1410	2086

TABLE 60

RETENTION INDICES OF CHLOROBENZENES MEASURED BY HAKEN AND KORHONEN[62] ON SE-30 AND PEG-20M AT 160°C

Compound	*Retention index (i.u.)*	
	SE-30	*PEG-20M*
Chlorobenzene	840	1270
1,3-Dichlorobenzene	1016	1434
1,4-Dichlorobenzene	1016	1471
1,2-Dichlorobenzene	1050	1514
1,3,5-Trichlorobenzene	1150	1545
1,2,4-Trichlorobenzene	1193	1653
1,2,3-Trichlorobenzene	1228	1735
1,2,3,5-Tetrachlorobenzene	1344	1786
1,2,4,5-Tetrachlorobenzene	1344	1793
1,2,3,4-Tetrachlorobenzene	1388	1908
Pentachlorobenzene	1525	1999
Hexachlorobenzene	1695	2178

TABLE 61

RETENTION INDICES OF SOME AROMATIC ESTERS MEASURED BY HAKEN *ET AL.*[65] ON DIFFERENT STATIONARY PHASES AT 200°C

Compound	*Retention index (i.u.)*			
	SE-30	*OV-25*	*QF-1*	*Silar-10C*
Benzyl acetate	1154	1450	1557	2330
Benzyl propionate	1245	1537	1620	2380
Benzyl butyrate	1337	1622	1700	2442
Benzyl hexanoate	1531	1807	1893	2618
Benzyl isobutyrate	1288	1557	1636	2330
Benzyl isopentanoate	1382	1651	1745	2437

TABLE 62

RETENTION INDICES OF SOME PERFLUOROCARBONS MEASURED BY MÜLLER *ET AL.*[79] ON DIFFERENT STATIONARY PHASES AT 50°C

Compound	*Retention index (i.u.)*				
	Squalane	*QF-1*	*PEG-1000*	*DEGS*	*OV-275*
Perfluoro-*n*-heptane	300	500	225	315	304
Perfluoro-*n*-octane	341	565	252	425	404
Perfluoro-*n*-decane	425	694	380	645	587
Perfluoro-*n*-undecane	473	771	473	768	668
Perfluoro-*n*-dodecane	528	857	558	877	772

TABLE 63

RETENTION INDICES OF VARIOUS COMPOUNDS MEASURED BY WINSKOWSKI[93] ON SE-30 AT 100°C AND ON OV-215 AT 80°C

Compound	*Retention index (i.u.)*	
	SE-30	*OV-215*
Methanol	384	550
Ethanol	427	618
1-Propanol	530	718
1-Butanol	637	827
1-Pentanol	754	–
Nitromethane	536	926
1-Nitropropane	712	1106
Pyridine	743	1009
Methyl ethyl ketone	579	888
2-Pentanone	671	980

TABLE 64

RETENTION INDICES OF SOME ALKYLNAPHTHALENES MEASURED BY JÁNOSI[118] ON DIFFERENT OV STATIONARY PHASES AT 150°C

Compound	*Retention index (i.u.)*					
	OV-1	*OV-3*	*OV-7*	*OV-11*	*OV-17*	*OV-25*
Naphthalene	1194	1235	1273	1330	1384	1471
1-Methylnaphthalene	1306	1348	1390	1450	1508	1602
2-Methylnaphthalene	1294	1335	1373	1430	1484	1571
2-Ethylnaphthalene	1382	1423	1461	1518	1572	1659
2-*n*-Propylnaphthalene	1470	1511	1549	1606	1660	1747
2-*n*-Butylnaphthalene	1570	1611	1649	1706	1760	1847

TABLE 65

RETENTION INDICES OF SOME 1-ALKENES AND *n*-ALKYLCYCLOPENTANES ON OV-1 AT 100°C, AFTER ANDERS *ET AL.*[160]

Compound	*Retention index (i.u.)*	*Compound*	*Retention index (i.u.)*
1-Butene	388.7	Propylcyclopentane	839.2
1-Pentene	488.8	Butylcyclopentane	938.3
1-Hexene	588.9	Pentylcyclopentane	1037.6
1-Heptene	689.0	Hexylcyclopentane	1137.9
1-Octene	789.0	Octylcyclopentane	1338.0
1-Nonene	888.7	Nonylcyclopentane	1438.0
1-Decene	988.6	Decylcyclopentane	1536.3
1-Undecene	1088.0	Undecylcyclopentane	1636.4
1-Dodecene	1187.9	Cyclohexane	673.6
1-Tetradecene	1387.9	Methylcyclohexane	734.6
Cyclopentane	574.5	Ethylcyclohexane	842.8
Methylcyclopentane	638.1	Propylcyclohexane	936.4
Ethylcyclopentane	743.4	Butylcyclohexane	1036.0

results gave retention plots with excellent regressions. As an example, the equation for phenyl esters on SE-30 stationary phase was

$$I = 957 + 96.5R \tag{19}$$

where R is the number of carbon atoms in the R groups, with a regression coefficient of 0.9999.

By application of the temperature coefficients of the retention index and the additivity principle of retention index increments, the structures of alkenylcycloalkanes and the positions of the double bonds were identified by Anders *et al.*[160]. Several equations for the calculation of the retention indices of alkylalkoxysilanes on Apiezon M and XE-60 at 160°C were given and discussed by Peetre *et al.*[211].

TABLE 66

RETENTION INDICES OF SOME PHENYLACETIC AND PHENYLPROPIONIC ACID DERIVATIVES MEASURED BY MACEK AND SMOLKOVÁ-KEULEMANSOVÁ[204] ON OV-101 AND OV-17 AT 200°C

Compound	*Retention index (i.u.)*	
	OV-101	*OV-17*
2-Phenylpropionic acid	1299.7	1453.0
Phenylacetic acid	1269.4	1442.8
4-Ethylphenylacetic acid	1452.2	1571.2
2-(4-Bromophenyl)propionic acid	1574.0	1751.3
4-Isopropoxy-3-chloro-phenylacetic acid	1766.5	1966.6

TABLE 67

RETENTION INDICES OF VARIOUS COMPOUNDS MEASURED BY SÂNCHEZ *ET AL.*[218] ON SQUALANE AND PEG-1540 AT 80°C

Compound	*Retention index (i.u.)*	
	Squalane	*PEG-1540*
Isopropyl formate	518	863
Methyl ethyl ketone	538	922
Ethyl acetate	548	900
sec.-Butanol	555	1041
Isobutanol	575	1109
n-Butanol	610	1166
Ethyl isobutyl ether	628	801
Diethyl ketone	640	997
Benzene	646	959
Cyclohexane	669	742
Ethyl *n*-butyl ether	669	863
Isooctane	693	675
Diisopropyl ketone	742	1020
Toluene	753	1057
Di-*n*-propyl ketone	817	1145

TABLE 68

RETENTION INDICES OF SOME ESTERS OF LOWER CARBOXYLIC ACIDS ON SP-400 AT 80°C, AFTER KOMÂREK *ET AL.*[281]

Compound	*Retention index (i.u.)*	*Compound*	*Retention index (i.u.)*
n-Propyl acetate	708.1	*n*-Butyl acetate	809.0
n-Propyl propionate	803.8	*n*-Butyl propionate	903.4
n-Propyl butyrate	893.2	*n*-Butyl butyrate	992.3
n-Propyl pentanoate	993.0	*n*-Butyl pentanoate	1088.9
n-Propyl hexanoate	1092.1	*n*-Butyl hexanoate	1189.0

TABLE 69

RETENTION INDICES OF SOME ALKYL ESTERS ON SP-400 AT 80°C, AFTER KOMÂREK *ET AL.*[281]

Ester	*Retention index (i.u.)*
Methyl propionate	626.8
Ethyl propionate	704.7
n-Propyl propionate	803.8
n-Butyl propionate	903.4
n-Pentyl propionate	1003.1

TABLE 70

RETENTION INDICES OF ETHYL 2,3-EPOXY-3-PHENYLPROPIONATE ON UCON 50-LB-550X STATIONARY PHASE AT DIFFERENT COLUMN TEMPERATURES MEASURED BY RIEGO AND GARCÍA-RASO[300]

Column temperature (°C)	*Retention index (i.u.)*
160	1352
180	1360
200	1370
220	1375
240	1390

GLC was used by Szymanowski *et al.*[228] to determine the polarity of pure model polyoxyethylene glycol dialkyl ethers and some of their sulphur analogues. The polarity parameters were correlated with the surfactant structure and increments for characteristic groups were determined at different column temperatures. Retention indices of halogenated derivatives of cyclohexane, benzene and anisole on Apolane-87 and PEG-20M at 150°C were reported by Haken and Vernon[271]. Retention increments due to the molecular structure and the size of the pendant groups together with the effect of increasing stationary phase polarity and concepts of additivity were discussed.

The most important aspect of the relationship between molecular structure and retention index is based on structural increments, the determination and application of which have been the subject of numerous reports, of which the contributions of the

TABLE 71

RETENTION INDICES OF SOME MONOALKYLCYCLOPENTADIENES MEASURED BY SOJÁK *ET AL.*[381] ON SQUALANE AND PEG-20M AT 64°C

Compound[a]	*Retention index (i.u.)*	
	Squalane	*PEG-20M*
1,3-CP	523.1	745.7
2-Methyl-1,3-CP	624.4	834.2
1-Methyl-1,3-CP	626.2	844.5
5-Methyl-1,3-CP	645.9	870.4
2-Ethyl-1,3-CP	723.8	930.3
1-Ethyl-1,3-CP	727.6	940.4
5-Ethyl-1,3-CP	747.6	966.7
2-*n*-Propyl-1,3-CP	812.6	1010.0
1-*n*-Propyl-1,3-CP	816.4	1020.2
5-*n*-Propyl-1,3-CP	835.1	1046.6
2-*n*-Butyl-1,3-CP	912.6	1108.2
1-*n*-Butyl-1,3-CP	916.5	1118.1
5-*n*-Butyl-1,3-CP	933.9	1144.5

[a] CP = cyclopentadiene.

TABLE 72

RETENTION INDICES OF SOME HYDROCARBONS MEASURED BY BERMEJO *ET AL.*[327] ON SQUALANE, OV-101, SE-54, OV-215 AND OV-210 AT 80°C

Compound	*Retention index (i.u.)*				
	Squalane	*OV-101*	*SE-54*	*OV-215*	*OV-210*
1,3-Cyclopentadiene	510.5	541.5	549.5	604.2	613.0
Cyclopentene	547.7	559.7	566.5	574.3	591.3
1-Methylcyclopentane	646.3	653.5	659.9	670.1	677.6
Cyclohexene	676.8	683.2	693.0	708.6	721.2
2,5-Norbornadiene	686.3	706.9	718.3	759.9	770.3
2-Norbornene	714.6	725.7	735.2	766.1	775.1
3-Methylcyclohexene	737.7	742.3	749.7	771.3	778.6
Methylenecyclohexane	737.8	744.5	754.1	779.0	791.0
4-Methylcyclohexene	739.9	744.3	751.2	771.4	785.8
1-Methylcyclohexene	768.5	771.2	780.4	793.0	802.7
Vinylcyclohexane	821.4	823.2	831.9	861.9	869.9
4-Vinylcyclohexene	825.1	832.8	843.6	875.4	885.8
Ethylidenecyclohexane	861.8	868.8	878.0	895.6	905.3
cis-Cyclodecene	1111.3	1112.6	1126.5	1169.9	1183.5

groups of Bata[1,41,97,147], Boneva[5,43,44,249–253,259,329,330,407], Brooks[45,46,102a,331,402,403], Calixto[8,9,51,52,104,104a,138,170a] and Castello[10,53,105,257,404] and those listed in the Introduction can be considered as the most valuable sources.

After having completed studies on the relationship between structure and retention index increments for normal and isomeric alkanes[451,452], our group developed a method that made it possible to study the C–H bonds in the methyl groups in alkanes[385]. The fundamental equations in the calculation method were discussed in our previous review[47] (eqns. 74, 82 and 90–99).

TABLE 73

RETENTION INDICES OF SOME ALKYLQUINOLINES MEASURED BY BURYAN *ET AL.*[332] ON DIFFERENT STATIONARY PHASES AT 160°C

Quinoline[a]	*Retention index (i.u.)*		
	OV-101	*UCON LB-550X*	*PEG-20M*
Q	1246	1478	1924
IsoQ	1269	1503	1958
2-MQ	1308	1527	1946
8-MQ	1319	1527	1943
7-MQ	1354	1581	2020
6-MQ	1358	1582	2020
3-MQ	1361	1590	2042
2,8-M_2Q	1374	1563	1945
4,6-M_2Q	1487	1712	2159
2,6,8-M_3Q	1475	1667	2042

[a] Q = quinoline; M = methyl.

TABLE 74

RETENTION INDICES OF SOME CYCLOHALOGENS MEASURED BY EVANS AND HAKEN[341] ON APOLANE-87 AND PEG-20M AT 150°C

Compound	*Retention index (i.u.)*	
	Apolane-87	*PEG-20M*
Benzene	687	971
Fluorobenzene	680	996
Chlorobenzene	880	1231
Bromobenzene	974	1351
Iodobenzene	1088	1504
Anisole	928	1340
Fluoroanisole	916	1367
Chloroanisole	1120	1592
Bromoanisole	1212	1706
Iodoanisole	1326	1852
Cyclohexane	680	740
Fluorocyclohexane	735	990
Chlorocyclohexane	918	1173
Bromocyclohexane	1009	1288
Iodocyclohexane	1117	1405

The bond energies are used as a basis for calculation of the bond index increments. Bond energy data, E (kJ), can be found in the literature or calculated from equations as follows:

$$E_{\mathrm{C-H}} = 45.27/d \qquad (20)$$

TABLE 95

COMPARISON OF RETENTION INDICES OF ALKYLALKOXYSILANES MEASURED AND CALCULATED BY PEETRE *ET AL.*[211] ON APIEZON M AT 160°C

Compound	*Retention index (i.u.)*			
	160°C			*180°C on SE-54*
	OV-17	*OV-215*	*PEG-20M*	
α-Ribofuranose	1624	1675	1528	1626
β-Ribofuranose	1647	1688	1550	1636
α-Ribopyranose	1651	1775	1550	1663
β-Ribopyranose	1626	1709	1531	1642
α-Arabinofuranose	1597	1609	1531	1596
β-Arabinofuranose	1682	1738	1603	1666
α-Arabinopyranose	1597	1690	1524	1601
β-Arabinopyranose	1643	1717	1586	1635

TABLE 76

RETENTION INDICES OF SOME NON-IONIC SURFACTANTS MEASURED BY VOELKEL[387] ON DIFFERENT STATIONARY PHASES AT 170°C

Basic structure: $RX(CH_2CH_2O)_nR'$.

R	*R'*	*X*	*n*	*Retention index (i.u.)*		
				Apiezon K	*SE-30*	*QF-1*
C_4H_9	H	O	0	675	675	867
	H	O	2	1150	1193	1469
	H	O	3	1437	1479	1797
C_6H_{13}	H	S	0	931	918	1043
	H	S	1	1318	1317	1621
	H	S	2	1564	1578	1952
	H	S	3	1829	1844	2273
	H	O	0	815	822	1003
	H	O	1	1054	1090	1534
	H	O	2	1325	1363	1662
	H	O	3	1576	1631	1983
	H	NH	0	815	829	993
	H	NH	1	1183	1197	1475
	H	NH	2	1424	1443	1757
	H	NH	3	1656	1703	2082
C_8H_{17}	H	S	0	1200	1140	1298
	H	S	1	1603	1562	1918
	H	S	2	1971	1830	2277
	H	S	3	2045	2123	2604
	H	O	0	1044	999	1299
	H	O	1	1274	1282	1569
	H	O	2	1552	1568	1928
	H	O	3	1822	1855	2272
	H	NH	0	1091	993	1230
	H	NH	1	1408	1333	1711
	H	NH	2	1645	1608	2062
	H	NH	3	1913	1917	2355
C_6H_{13}	CH_3	O	3	1592	1660	1903
C_8H_{17}	CH_3	O	3	1837	1880	2175
$C_{10}H_{21}$	CH_3	O	3	2028	2121	2435

and

$$E_{C\text{–}C} = 53.56/d \qquad (21)$$

where C–H denotes the carbon–hydrogen bond in alkanes, C–C the carbon–carbon bond in alkanes and d is the bond distance (nm). The bond distance can be approximated by

$$d = 0.819 \sum_{i=1}^{2} a_0(i) + 0.157 \sum_{j=1}^{p} a_1(j) + 0.024 \sum_{k=1}^{q} a_2(k) \qquad (22)$$

where

i = serial number of the atoms in the bond examined;
j = serial number of the atoms of the bond in the primary environment;
k = serial number of the atoms of the bond in the secondary environment;
p = total number of atoms of the bond in the primary environment;
q = total number of atoms of the bond in the secondary environment;
0.819 = bond factor;
0.157 = primary environment factor;
0.024 = secondary environment factor;
a_0 = the atomic code number in the bond;
a_1 = the atomic code number in the primary environment;
a_2 = the atomic code number in the secondary environment [the atomic code numbers of alkanes are single-digit numbers (see Table 77)].

The calculation of the bond index increments from the bond distances is based on following equations:

$$i_b(\text{C–H bonds}) = 0.815/d \tag{23}$$

$$i_b(\text{C–C bonds}) = 0.964/d \tag{24}$$

Coding rules for the bonds in alkanes are summarized in the original paper[385].

Similarly to the case of the retention index increments of alkanes, the molecular structures of benzene and alkylbenzenes can be coded and described[77a,510]. For example, let us calculate the relevant data for benzene. The retention index of benzene on OV-3 stationary phase at 80°C is 681.9 i.u.[55], the C–C bond length is 0.1397 nm with a bond energy of 119.86 kcal and the C–H bond length is 0.1084 nm with a bond energy of 99.82 kcal[454,455]. Thus, the formation (atomization) energy of benzene is 1318.08 kcal/mol. The molecular structural coefficient of benzene on OV-3 at 80°C can be calculated as follows:

$$\begin{aligned} S^{\text{OV-3}}_{c,\text{benzene}}(80°\text{C}) &= \frac{100}{b}\log V_g = I - K_c = 681.9 - 149.1 \\ &= 532.8\ \{\log\,[\text{cm}^3(\text{He})/\text{g(OV-3)}]\} \end{aligned} \tag{25}$$

TABLE 77

BOND LENGTH INCREMENT VALUES OF ALKANES AND BOND CODES

Atom	*Bond code*	*Bond length increment value (nm)*
Primary carbon	1	0.07900
Secondary carbon	2	0.06500
Tertiary carbon	3	0.05565
Quaternary carbon	4	0.04978
Hydrogen bound to primary carbon	5	0.02700
Hydrogen bound to secondary carbon	6	0.03100
Hydrogen bound to tertiary carbon	7	0.03500

where S_c is the molecular structural coefficient: log [cm^3(carrier gas)/g(stationary phase); K_c is the Kováts coefficient {– log [cm^3(carrier gas)/g(stationary phase)]};

$$K_c^{\text{OV-3}}(80°\text{C}) = 149.1\ \{-\ \log\ [\text{cm}^3(\text{He})/\text{g}(\text{OV-3})]\} \tag{26}$$

The bond index increments are calculated in i.u. from the bond energy using the factor[385]

$$f_c = 0.0513\ \text{i.u./kcal.} \tag{27}$$

From S_c:

$$f_S = \frac{\text{molecular structural coefficient}}{\text{formation (atomization) energy}}\ . \qquad \left(\frac{\log\ [\text{cm}^3(\text{carrier gas})/\text{g}(\text{stationary phase})]\ \text{mol}}{\text{kcal}}\right) \tag{28}$$

Structural increments are calculated in log [cm^3(carrier gas)/g(stationary phase)] mol from the bond energy by f_S as follows:

$$f_{S,\text{benzene}}^{\text{OV-3}}(80°\text{C}) = 532.8/1318.08$$
$$= 0.4042\ \log\ [\text{cm}^3(\text{carrier gas})/\text{g}(\text{stationary phase})]\ \text{mol/kcal} \tag{29}$$

Hence

$$i_b(\text{C–C}) = 119.86 \cdot 0.0513 = 6.15\ \text{i.u.} \tag{30}$$

$$i_b(\text{C–H}) = 99.82 \cdot 0.0513 = 5.12\ \text{i.u.} \tag{31}$$

where i_b = bond index increment (i.u.).

$$i_{s1}^{\text{OV-3}}(80°\text{C}) = 119.86 \cdot 0.4042$$
$$= 48.45\ \log\ [\text{cm}^3(\text{carrier gas})/\text{g}(\text{stationary phase})]\ \text{mol} \tag{32}$$

$$i_{s2}^{\text{OV-3}}(80°\text{C}) = 99.82 \cdot 0.4042$$
$$= 40.35\ \log\ [\text{cm}^3(\text{carrier gas})/\text{g}(\text{stationary phase})]\ \text{mol} \tag{33}$$

for two different bonds in benzene, where i_s = structural increment log [cm^3(carrier gas)/g(stationary phase)] mol. Atomic code numbers[47] of benzene and alkylbenzenes are summarized in Table 78.

The application of bond increment values gives a new possibility for studying the relationship between molecular structure and retention index. The effect of the primary and secondary atomic environments on the interactions of some alkane C–H bonds on a squalane stationary phase at different column temperatures was studied by Tekler *et al.*[385] and the results are given in Table 79.

Research based on structural increments is expected to make significant progress in the future. Development will be extremely rapid in those fields in which, in addition to literature sources, one can set up additional relationships which provide the

TABLE 78

BOND LENGTH INCREMENT VALUES OF BENZENE AND METHYLBENZENES AND BOND CODES

Atom	*Bond code*	*Bond length increment value (nm)*
Carbon in the methyl group	A1	0.08755
Hydrogen in the methyl group	A2	0.02360
Tertiary carbon in the ring	A3	0.06267
Quaternary carbon in the ring	A4	0.05240
Hydrogen bound to ring	A5	0.03966

TABLE 79

INTERACTION INDEX INCREMENTS OF SOME ALKANE C–H BONDS ON SQUALANE STATIONARY PHASE AT DIFFERENT COLUMN TEMPERATURES AND FOR DIFFERENT ATOMIC ENVIRONMENTS, AFTER TEKLER *ET AL.*[385]

Hydrogen was used as the carrier gas. C_3 = propane; C_4 = butane; C_5 = pentane; M = methyl; E = ethyl.

Compound	*Bond code*	*Interaction index increment*				
		30°C	*50°C*	*70°C*	*100°C*	*120°C*
Primary C–H bonds						
CH_4	[C–H]	17.12	17.12	17.12	17.12	17.12
$22M_2C_3$	15:4 (111) 55; 0.	19.01	19.08	19.16	19.29	19.39
C_2H_6	15:1 (555) 55; 0.	21.37	21.37	21.37	21.37	21.37
$2MC_3$	15:3 (117) 55; 0.	21.53	21.57	21.60	21.62	21.63
$22M_2C_4$	15:4 (112) 55; 0.	21.75	21.84	21.93	22.06	22.15
	15:2 (466) 55; 0.	21.80	21.89	21.98	22.11	22.20
$223M_3C_4$	15:4 (113) 55; 0.	22.65	22.80	22.95	23.17	23.32
	15:3 (147) 55; 0.	22.70	22.85	23.00	23.22	23.37
C_3H_8	15:2 (166) 55; 0.	23.28	23.28	23.28	23.28	23.28
$2233M_4C_4$	15:4 (114) 55; 0.	22.60	22.82	23.04	23.37	23.59
$2MC_4$	15:2 (366) 55; 0.	23.25	23.30	23.35	23.41	23.44
	15:3 (127) 55; 0.	23.25	23.30	23.35	23.41	23.44
$2234M_4C_5$	15:3 (347) 55; 0.	23.15	23.32	23.49	23.75	23.92
$23M_2C_4$	15:3 (137) 55; 0.	23.46	23.58	23.70	23.90	24.04
$223M_3C_4$	15:3 (247) 55; 0.	23.65	23.79	23.92	24.12	24.25
n-C_4H_{10}	15:2 (266) 55; 0.	24.29	24.29	24.29	24.29	24.29
$234M_3C_5$	15:3 (337) 55; 0.	24.32	24.45	24.58	24.75	24.86
$33M_2C_5$	15:4 (122) 55; 0.	24.35	24.49	24.64	24.88	25.06
$3MC_5$	15:3 (227) 55; 0.	24.68	27.74	24.81	24.92	25.00
$23M_2C_5$	15:3 (237) 55; 0.	24.99	25.09	25.20	25.32	25.40
$22334M_5C_5$	15:4 (134) 55; 0.	24.85	25.13	25.41	25.83	26.11
$233M_3C_5$	15:4 (123) 55; 0.	25.20	25.38	25.57	25.84	26.03
$2233M_4C_5$	15:4 (124) 55; 0.	25.66	25.87	26.07	26.36	26.54
$2334M_4C_5$	15:4 (133) 55; 0.	26.00	26.21	26.41	26.71	26.91
$3M3EC_5$	15:4 (222) 55; 0.	27.16	27.18	27.21	27.25	27.28
$23M_23EC_5$	15:4 (223) 55; 0.	27.38	27.59	27.79	28.10	28.31
$223M_33EC_5$	15:4 (224) 55; 0.	27.66	27.94	28.22	28.66	28.96
$234M_33EC_5$	15:4 (233) 55; 0.	27.84	28.10	28.35	28.72	28.96

(*Continued on p. 48*)

TABLE 79 (*continued*)

Compound	*Bond code*	*Interaction index increment*				
		30°C	*50°C*	*70°C*	*100°C*	*120°C*
Secondary C–H bonds						
$22M_2C_4$	26:1 (555) 4 (111) 6; 0.	21.19	21.27	21.36	21.49	21.58
C_3H_8	26:1 (555) 1 (555) 6; 0.	22.60	22.60	22.60	22.60	22.60
$2MC_4$	26:1 (555) 3 (117) 6; 0.	22.66	22.71	22.75	22.81	22.84
$223M_3C_5$	26:1 (555) 3 (147) 6; 0.	23.04	23.18	23.31	23.50	23.62
n-C_4H_{10}	26:1 (555) 2 (166) 6; 0.	23.67	23.67	23.67	23.67	23.67
$33M_2C_5$	26:1 (555) 4 (112) 6; 0.	23.71	23.85	23.99	24.23	24.40
$3MC_5$	26:1 (555) 3 (127) 6; 0.	24.05	24.11	24.17	24.28	24.36
$23M_2C_5$	26:1 (555) 3 (137) 6; 0.	24.34	24.44	24.53	24.66	24.74
$233M_3C_5$	26:1 (555) 4 (113) 6; 0.	24.55	24.73	24.90	25.17	25.35
$2233M_4C_5$	26:1 (555) 4 (114) 6; 0.	24.99	25.19	25.39	25.67	25.85
$3M3EC_5$	26:1 (555) 4 (122) 6; 0.	26.45	26.48	26.50	26.54	26.57
$23M_23EC_5$	26:1 (555) 4 (123) 6; 0.	26.67	26.87	27.07	27.37	27.57
$223M_33EC_5$	26:1 (555) 4 (124) 6; 0.	26.93	27.21	27.49	27.91	28.20
Tertiary C–H bonds						
$2MC_3$	37:1 (555) 1 (555) 1 (555); 0.	19.95	19.99	20.01	20.03	20.04
$223M_3C_4$	37:1 (555) 1 (555) 4 (111); 0.	21.05	21.19	21.33	21.54	21.68
$2MC_4$	37:1 (555) 1 (555) 2 (166); 0.	21.61	21.66	21.70	21.76	21.79
$2234M_4C_5$	37:1 (555) 3 (117) 4 (111); 0.	21.54	21.70	21.86	22.10	22.26
	37:1 (555) 1 (555) 3 (147); 0.	21.50	21.66	21.82	22.06	22.22
$23M_2C_4$	37:1 (555) 1 (555) 3 (117); 0.	21.82	21.92	22.04	22.22	22.35
$223M_3C_5$	37:1 (555) 2 (166) 4 (111); 0.	22.01	22.14	22.27	22.45	22.57
$234M_3C_5$	37:1 (555) 1 (555) 3 (137); 0.	22.60	22.73	22.84	23.00	23.10
	37:1 (555) 3 (117) 3 (117); 0.	22.68	22.80	22.92	23.08	23.18
$3MC_5$	37:1 (555) 2 (166) 2 (166); 0.	23.03	23.08	23.14	23.25	23.33
$23M_2C_5$	37:1 (555) 1 (555) 3 (127); 0.	23.22	23.32	23.41	23.53	23.60
	37:1 (555) 2 (166) 3 (117); 0.	23.30	23.40	23.49	23.61	23.68
$22334M_5C_5$	37:1 (555) 1 (555) 4 (114); 0.	23.09	23.35	23.61	24.00	24.26
$233M_3C_5$	37:1 (555) 1 (555) 4 (112); 0.	23.42	23.59	23.76	24.01	24.18
$2334M_4C_5$	37:1 (555) 1 (555) 4 (113); 0.	24.16	24.35	24.54	24.82	25.01
$23M_23EC_5$	37:1 (555) 1 (555) 4 (122); 0.	25.45	25.64	25.83	26.12	26.31
$234M_33EC_5$	37:1 (555) 1 (555) 4 (123); 0.	25.86	26.10	26.33	26.68	26.91

necessary data (bond distance and energy, specific retention volume, etc.) for calculation of the structural increments.

For further information about molecular structure–retention index relationships, see refs. 1, 2, 4, 5, 19a, 23, 25, 27, 28, 35a, 35b, 36, 37a, 39a, 40a, 41, 45, 54, 55, 71, 75, 91, 92, 95, 94, 97, 109, 114, 115, 118, 126, 136, 151, 158, 159, 170, 181, 197, 201, 204, 208, 210, 212, 213, 219, 226, 232, 236, 238, 246, 247, 250, 257, 265, 285, 287a, 292, 295–297, 300, 309, 327, 330–333, 337, 344, 361, 363, 364, 366, 374, 382, 384, 398, 403, 410, 414, 415, 417, 421, 424a, 428, 433 and 475.

10. ROHRSCHNEIDER'S CONCEPT AND CALCULATION METHOD

As nearly all the important questions pertaining to the Rohrschneider concept and calculation method were been dealt with in our previous review[47], here we discuss only the newest results in this very significant area. In recent years researchers seem to have focused on the problems of the precalculation of retention indices.

The ΔI value can be calculated by Rohrschneider's equation in classical GLC. For example, let us calculate the ΔI value of pyridine on PEG-4000 at 120°C by Rohrschneider's equation from McReynolds constants[439]. We can write the following system of equations:

$$\begin{aligned}
&\text{on Apiezon L:} & 42 &= 0.13a^{R} + 0.35b^{R} + 0.11c^{R} + 0.31d^{R} + 0.33e^{R} && (34)\\
&\text{on OV-3:} & 88 &= 0.55a^{R} + 0.39b^{R} + 0.46c^{R} + 0.84d^{R} + 0.17e^{R} && (35)\\
&\text{on OV-17:} & 202 &= 1.12a^{R} + 1.19b^{R} + 1.05c^{R} + 1.84d^{R} + 0.69e^{R} && (36)\\
&\text{on PEG-20M:} & 510 &= 3.87a^{R} + 2.82b^{R} + 2.21c^{R} + 4.34d^{R} + 1.48e^{R} && (37)\\
&\text{on DEGS:} & 860 &= 5.95a^{R} + 4.22b^{R} + 3.23c^{R} + 7.25d^{R} + 2.40e^{R} && (38)
\end{aligned}$$

where a^{R}, b^{R}, c^{R}, d^{R} and e^{R} = substance-specific factors according to Rohrschneider[47]. On solving this system of equations the values $a^{R} = -18.509$, $b^{R} = 150.997$, $c^{R} = -138.944$, $d^{R} = 146.524$ and $e^{R} = -116.914$ were obtained.

Using these substance-specific factors and McReynolds constants on PEG-4000 at 120°C, we can write

$$\begin{aligned}
\Delta I^{\text{PEG-4000-squalane}}_{\text{pyridine}}(120^{\circ}\text{C}) &= (3.99 \cdot -18.509) + (2.85 \cdot 150.997) + \\
&+ (2.24 \cdot -138.944) + (4.43 \cdot 146.524) + (1.48 \cdot -116.914) = 521.3\ \text{i.u.} \qquad (39)
\end{aligned}$$

The value as measured by McReynolds[439] was 520.0 i.u.

It could also be established from Rohrschneider's paper[44] that the minimum number of standard substances is three and the optimum is five. As an example, the calculation of the interaction index increment of the C–H bond [37:1 (555) 1 (555) 1 (555); 0.] (for an explanation of the code, see ref. 385) on squalane stationary phase at 100°C with three standard substances is performed using the following system of equations:

$$\begin{aligned}
19.95 &= 21.05s_1 + 21.61s_2 + 21.54s_3 && (40)\\
20.01 &= 21.33s_1 + 21.70s_2 + 21.86s_3 && (41)\\
20.04 &= 21.68s_1 + 21.79s_2 + 22.26s_3 && (42)
\end{aligned}$$

On solving these equations the values $s_1 = -6.90$, $s_2 = 2.00$ and $s_3 = 5.66$ were obtained.

Using s_i values and suitable data from the paper of Tekler *et al.*[385], we can write

$$i_i^{\text{Sq}}(100^{\circ}\text{C}) = (21.54 \cdot -6.90) + (21.76 \cdot 2.0) + (22.10 \cdot 5.66) = 19.98\ \text{i.u.} \qquad (43)$$

where i_i is the interaction index increment value (i.u.)[385]. The increment value measured was 20.03 i.u.

Recently, our group has come to the conclusion that those papers by Rohrschneider which deal with specific retention volume are at least as important as those connected with the retention index, which prompted us to begin extensive research in this field. Early results of these investigations are summarized in Tables 2–6. The basic ideas in our calculation method are presented below for the case of *cis*-3-methyl-2-pentene. From the papers by Chien *et al.*[54,55], the following equation systems can be written:

System I: log V_g values

Guiding principle:

$$\log V_g(s) = \log V_g(nC_5) \cdot s_1 + \log V_g(nC_6) \cdot s_2 + \log V_g(nC_7) \cdot s_3 + \\ + \log V_g(nC_8) \cdot s_4 + \log V_g(nC_9) \cdot s_5 \quad (44)$$

where V_g = specific retention volume [cm^3 (carrier gas)/g(st.ph.)], s = substance examined, s_i = substance-specific factor and nC_z = n-alkane with carbon number z. Then,

$$\text{on OV-1: } 97.48 = 36.87s_1 + 88.47s_2 + 211.4s_3 + 504.5s_4 + 1202s_5 \quad (45)$$
$$\text{on OV-3: } 90.97 = 32.15s_1 + 79.29s_2 + 195.6s_3 + 482.3s_4 + 1190s_5 \quad (46)$$
$$\text{on OV-7: } 85.15 = 28.56s_1 + 71.26s_2 + 176.3s_3 + 437.9s_4 + 1090s_5 \quad (47)$$
$$\text{on OV-17: } 62.89 = 18.94s_1 + 46.60s_2 + 114.10s_3 + 282.50s_4 + 693.60s_5 \quad (48)$$
$$\text{on OV-25: } 41.28 = 11.60s_1 + 28.15s_2 + 68.36s_3 + 165.80s_4 + 405.90s_5 \quad (49)$$

On solving these equations the values $s_1 = -5.743, s_2 = 1.939, s_3 = 5.067, s_4 = 7.313$ and $s_5 = -7.901$ at 50°C were obtained. Using these s_i values and suitable data from the papers by Chien *et al.*[54,55], we can write

$$\log V_g^{\text{OV-11}}(50°\text{C}) = (23.26 \cdot -5.743) + (57.78 \cdot 1.939) + (143.4 \cdot 5.067) + \\ + (355.9 \cdot 7.313) + (883.3 \cdot -7.901) = 1.87407 \quad (50)$$

Hence $V_g^{\text{OV-11}}(50°\text{C})_{\text{calculated}}$ = antilog 1.87407 = 74.83 cm^3 He/g OV-11. The specific retention volume measured was 73.28 cm^3 He/g OV-11.

System II: log $V_g(s)^{\text{st.ph.}}$/log $V_g(s)^{OV\text{-}1}$ values

Guiding principle:

$$\frac{\log V_g(s) \text{ on st.ph. } i}{\log V_g(s) \text{ on OV-1}} = \sum_{i=1}^{5} \left[\frac{\log V_g(nC_{i+4})^{\text{st.ph.}}}{\log V_g(nC_{i+4})^{\text{OV-1}}}\right] \cdot s_i \quad (51)$$

$$\text{OV-3/OV-1: } 0.985 = 0.962s_1 + 0.976s_2 + 0.985s_3 + 0.993s_4 + 0.999s_5 \quad (52)$$
$$\text{OV-7/OV-1: } 0.970 = 0.929s_1 + 0.952s_2 + 0.966s_3 + 0.977s_4 + 0.986s_5 \quad (53)$$
$$\text{OV-11/OV-1: } 0.938 = 0.872s_1 + 0.905s_2 + 0.928s_3 + 0.944s_4 + 0.957s_5 \quad (54)$$
$$\text{OV-17/OV-1: } 0.904 = 0.815s_1 + 0.857s_2 + 0.885s_3 + 0.907s_4 + 0.922s_5 \quad (55)$$
$$\text{OV-25/OV-1: } 0.812 = 0.679s_1 + 0.745s_2 + 0.789s_3 + 0.821s_4 + 0.847s_5 \quad (56)$$

On solving these equations the values $s_1 = -0.928, s_2 = 1.441, s_3 = -2.024, s_4 = 6.000$ and $s_5 = -3.491$ were obtained. The sum of substance-specific factors can be calculated as follows:

$$\sum_{i=1}^{5} s_i = -0.928 + 1.441 - 2.024 + 6.0 - 3.491 = 0.998 \tag{57}$$

The theoretical value[47] of the sum of substance-specific factors is 1.000.

Some Rohrschneider constants are given in Tables 80 and 81.

11. McREYNOLDS' SYSTEM. POLARITY OF STATIONARY PHASES

In recent years it has been established that of the ten McReynolds constants[439] the first five (for benzene, *n*-butanol, 2-pentanone, nitropropane and pyridine) are sufficient for both research and everyday practice.

Widespread use of the McReynolds system is hindered partly by some erroneously measured data, and especially by the fact that these constants were determined only at 120°C. Combination of the Rohrschneider[441] and McReynolds[439] systems supplemented with data measured at 80 and 140°C would ensure greater development of this area in the future. The question of the polarity of stationary phases is also being studied extensively and various aspects of this problem have been dealt with by many investigators in recent years.

TABLE 80

ROHRSCHNEIDER CONSTANTS OF SOME STATIONARY PHASES USED IN GLC, AFTER HAKEN AND KHEMANGKORN[442] AND CSIZMADIÁNÉ[443]

Stationary phase	*Rohrschneider constant*				
	x	*y*	*z*	*u*	*s*
F-61	0.31	0.49	0.82	1.08	0.83
85% Phenyl	1.88	2.33	2.15	3.80	2.95
Hallcomid M-18-OL	0.96	2.93	1.59	2.99	1.77
Citroflex A-4	1.36	2.66	2.11	3.70	2.33
Zonyl E-7	2.37	4.37	5.16	5.84	–
Hyprose SP-80	2.96	5.57	4.22	6.53	5.91
Diethylene glycol succinate (DEG 5)	4.93	7.58	6.14	9.50	8.37
PEG-5000 K_2	2.69	5.11	3.38	6.53	4.40

TABLE 81

RETENTION INDICES OF ROHRSCHNEIDER STANDARDS ON OV-225 AT 90°C, AFTER ISENBERG *ET AL.*[117]

Compound	*Retention index (i.u.)*
Benzene	854
Butanone	705
Ethanol	911
Nitromethane	968
Pyridine	1068

Vigdergauz *et al.*[464] developed a technique for the classification of liquid crystalline stationary phases for the GC analysis of positional isomers. The influence of the polarity of stationary phases on the retention of solutes with different molecular structures was studied by Calixto and Raso[9].

A compilation of solubility data for 240 substances on 207 stationary phases was published by Patte *et al.*[28a]. Correlation between polarity of stationary phases and the retention data of solutes with various numbers of methylene groups was examined by Sidorov[34a] and Stolyarov and Kartsova[35c]. An optimization method for selecting stationary phases was described by Vigdergauz and Bankoskaya[38a]. A classification of the "polarity" of porous polymer bead stationary phases by comparison with squalane and Apolane-87 was given by Castello and D'Amato[53]. Markides *et al.*[76,77] studied cyanosilicones as stationary phases in GLC.

Fernandez-Sanchez *et al.*[142] obtained interesting results using McReynolds constants relative to *n*-decane. The interactions involved were studied with the help of Snyder's selectivity triangle, using the retention indices and the selectivity parameters[220,248]. A procedure was described by Krupčik *et al.*[286] for the computer optimization of the selectivity of capillary columns in series for the GC separation of cyclic and aromatic hydrocarbons. Useful results on siloxane–silarylene copolymer stationary phases were presented by Bemgård *et al.*[322]. A new method of classification was applied to 233 stationary phases used in GLC by García-Dominguez *et al.*[336]. A classification of GC stationary phases by a new variant of the Kováts retention index system was reported by Evans and Haken[342].

Solute–solvent interactions in liquid alkylammonium-4-toluenesulphonate salts were studied by Furton and Poole[345]. GC stationary phase properties of two room-temperature liquid organic salts were demonstrated with interesting results by Furton *et al.*[346]. Two valuable methods were used by Kersten and co-workers[354,355] to establish the influence of concurrent retention mechanisms (GSC and GLC) on the

TABLE 82

McREYNOLDS STANDARDS OF SOME LIQUID CRYSTALLINE STATIONARY PHASES MEASURED BY SZULC AND WITKIEWICZ[85] AT 120°C

Symbol[a] of stationary phase	*Retention index (i.u.)*				
	Benzene	*n-Butanol*	*2-Pentanone*	*1-Nitopropane*	*Pyridine*
A_1	809	858	860	980	1010
A_2	802	848	855	966	1016
A_3	884	936	929	1086	1103
A_4	894	918	942	1079	1174
A_5	838	891	891	1019	1053
B_1	803	815	835	927	1019
B_2	831	853	863	980	1036
B_3	824	825	844	937	1019
C_1	858	910	913	1049	1081
C_2	838	866	888	1021	1063
C_3	837	844	852	985	1023

[a] Symbols as in original paper[85].

TABLE 83

RETENTION INDICES OF McREYNOLDS STANDARDS MEASURED AND CALCULATED BY FERNANDEZ-SANCHEZ *ET AL.*[379] ON DIFFERENT STATIONARY PHASES AT 120°C

McReynolds standard	*Retention index (i.u.)*				
	OV-101	*OV-25*	*PEG-20M*	*OV-225*	*SP-2340*
Benzene	672	828	992	871	1189
n-Butanol	663	796	1178	951	1362
2-Pentanone	685	840	1053	957	1262
1-Nitropropane	724	954	1279	1130	1586
1-Iodobutane	821	986	1111	1035	1287
cis-Hydrindane	1004	1117	1156	1115	1246

accuracy of McReynolds constants. Interesting results were presented by Pomaville and Poole[369] on thermally stable, highly fluorinated stationary phases in GLC. Poole *et al.*[371,424], re-examined Rohrschneider and McReynolds constants. The polarity of OV and SE series stationary phases was estimated by García-Raso *et al.*[375]. Some McReynolds constants on different stationary phases at different temperatures are summarized in Tables 82–87.

Complementing the polarity table published in our previous review[47], the retention polarity values of the most frequently used stationary phases, mostly based on McReynolds constants obtained at 120°C[439], are summarized in Table 88.

For further information, see also refs. 52, 79, 117, 140, 143a, 162, 263, 299, 350, 351, 352, 370, 423, 388, 389, 406 and 425.

11.1. Mixed stationary phases

Researchers working in different areas of GLC soon realized the significance of using mixed stationary phases (tandem, mixed stationary phases, mixing packings,

TABLE 84

RETENTION INDICES OF ROHRSCHNEIDER AND McREYNOLDS STANDARDS MEASURED BY CASTELLO AND D'AMATO[53] ON SQUALANE AT DIFFERENT COLUMN TEMPERATURES

Compound	*Retention index (i.u.)*	
	100°C	*125°C*
Ethanol	396	391
Methyl ethyl ketone	533	534
Nitromethane	467	463
Benzene	647	652
n-Butanol	588	590
2-Pentanone	624	626
Pyridine	707	711
1-Nitropropane	647	652

TABLE 85

RETENTION INDICES OF ROHRSCHNEIDER AND McREYNOLDS STANDARDS MEASURED BY CASTELLO AND D'AMATO[53] ON APOLANE-87 AT DIFFERENT COLUMN TEMPERATURES

Compound	*Retention index (i.u.)*	
	100°C	*200°C*
Ethanol	413	397
Methyl ethyl ketone	541	542
Nitrometane	500	500
Benzene	670	702
n-Butanol	603	610
Methyl propyl ketone	630	636
Pyridine	719	757
1-Nitropropane	662	678

etc.) and this idea led to important results from both theoretical and practical points of view.

There is steadily growing interest in this field even now, in spite of the fact that the development and marketing of a standard apolar stationary phase (Apolane-87) was not followed by the development of a standard polar stationary phase, although this was attempted. Although some important results have been achieved without using the polar counterpart, the special advantages offered by mixed stationary phases (*e.g.*, computer-assisted polarity design, resolution optimization by mixed stationary phases) could be exploited only if both polar and apolar stationary phases are applied together.

For detailed information, see refs. B10, 10, 85, 86, 176, 216, 218, 256, 306, 379, 379a and 465.

TABLE 86

CORRECTED RETENTION INDICES OF McREYNOLDS STANDARDS OBTAINED BY KERSTEN AND POOLE[354] ON DIFFERENT STATIONARY PHASES AT 80°C

Standard	*Retention index (i.u.)*			
	Squalane	*OV-225*	*PEG-20M*	*OV-275*[a]
Benzene	642	861	973	1104
n-Butanol	580	953	1151	1285
2-Pentanone	620	951	1000	1205
Nitropropane	642	1117	1232	1437
Pyridine	685	1052	1201	1397
2-Methyl-2-pentanol	682	979	1101	1217
Iodobutane	806	1017	1094	1172
2-Octyne	842	990	1074	1071
1,4-Dioxane	643	971	1089	1294
cis-Hydrindane	989	1090	1135	1116

[a] Uncorrected values.

TABLE 87

COMPARISON OF CORRECTED AND UNCORRECTED RETENTION INDICES OF McREYNOLDS STANDARDS OBTAINED BY KERSTEN AND POOLE[354] ON OV-225 AT 80°C

Standard	*Retention index (i.u.)*		
	Corrected	*Uncorrected*	*Difference*
Benzene	861	853	8
n-Butanol	953	953	0
2-Pentanone	951	947	4
Nitropropane	1117	1112	5
Pyridine	1052	1050	2
2-Methyl-2-pentanol	979	970	9
Iodobutane	1017	1013	4
2-Octyne	990	987	3
1,4-Dioxane	971	970	1
cis-Hydrindane	1090	1086	4

TABLE 88

RETENTION POLARITY OF SOME STATIONARY PHASES AT 120°C, ON THE BASIS OF McREYNOLDS CONSTANTS[439]

McReynolds code number	*Stationary phase*	*Retention polarity (polarity units)*
2000	Squalane	0.00
2226	Hexatriacontane	0.69
2063	Nujol	1.01
2298	Mineral oil	1.16
2270	Liquid paraffin	1.19
–	Apolane-87	2.30
2128	Apiezon M	4.24
2127	Apiezon L	4.39
2013	Apiezon B (treated)	4.49
2082	Polybutene-32	4.82
2081	Polybutene-128	4.90
2012	Apiezon L	5.11
2318	DC-330	6.37
2195	Apiezon L	6.38
2066	SE-96	6.43
2140	Apiezon N	6.67
2077	SE-30	6.80
2034	OV-1	6.95
–	OV-73	6.95
2050	M and B silicone oil	7.11
–	DC-200	7.11
–	SP-2100	7.17
–	ASI 100 methyl	7.17
2039	OV-101	7.17
2076	DC-410	7.33
2065	Versilube F-50	7.51

(*Continued on p. 56*)

TABLE 88 (*continued*)

McReynolds code number	*Stationary phase*	*Retention polarity (polarity units)*
2101	DC-11	8.69
2316	DC-510	9.24
2087	DC-200	10.18
2078	SE-52	10.42
2320	SE-54	10.51
–	SP-400	10.67
2314	DC-556	12.18
2204	OV-3	13.17
2100	Beeswax	13.18
–	OV-105	14.45
–	Dexil 300	14.72
2144	Fluorolube HG-1200	15.30
2194	Apiezon H	15.63
2080	Halocarbon wax	15.70
2171	Butoxyethyl stearate	15.89
2123	OV-7	18.39
2120	DC-550	19.25
2323	Apiezon W	19.41
2179	Dinonyl sebacate	19.90
2061	DC-703	20.32
2052	Dioctyl sebacate	20.39
2178	Di(2-ethylhexyl) sebacate	20.44
2056	Diisodecyl adipate	20.91
2169	Ditridecyl phthalate	21.46
2149	Diethoxy tetrachlorophthalate	21.47
2310	DEG stearate	21.74
2250	Dilauryl phthalate	22.01
2313	Octyl decyl adipate	22.04
–	SP-1200	22.08
2170	Diisooctyl adipate	22.20
–	Bis(2-ethylhexyl) tetrachlorophthalate	22.77
2024	TMP tripelargonate	22.77
2057	Diisooctyl adipate	23.01
2187	Diisodecyl phthalate	23.93
2124	OV-11	24.37
–	OV-1701	24.58
2070	Dinonyl phthalate	25.07
2229	DC-710	25.64
2060	Dioctyl phthalate	25.93
2276	Flexol GPE	25.94
–	Poly-I 110	26.03
2103	Hallcomid M-18	26.64
2116	Diisooctyl phthalate	26.77
2038	OV-17	27.40
–	SP-2250	27.40
2114	Hallcomid M-18 OL	28.83
2205	SP-392	29.60
2022	Flozol 8N8	29.88
2291	Span-60	30.17
2247	Hercoflex-600	30.28

TABLE 88 (*continued*)

McReynolds code number	*Stationary phase*	*Retention polarity (polarity units)*
2162	Versamid	30.46
2059	UCON LB-550-X	31.19
2069	Span-80	31.70
2049	UCON 50-HB-1800-X	31.93
2096	Castor wax	31.94
2254	Flexol B-400	32.88
2175	Estynox	33.29
2125	OV-22	33.29
2190	Trimer acid	33.66
–	Poly-A 103	33.69
2266	Atpet-200	33.92
2264	Pluracol P-2010	33.97
2113	UCON LB-1715	34.16
2182	Dibutoxyethyl adipate	34.28
–	Poly-A 101A	34.60
2253	Thanol PEG 1000	35.01
2044	OV-25	35.86
2160	Acetyl tributyl citrate	35.96
2007	Pluronic L-81	36.01
2177	Didecyl phthalate	36.14
2068	OS-124	36.37
2111	Tributyl citrate	37.01
2319	GE SR-119	37.71
2017	OS-138	38.06
2147	Diethoxyethyl sebacate	38.39
2048	Dibutoxyethyl phthalate	38.73
–	SP-1220	39.35
2174	Dibutoxyethyl phthalate	39.38
2108	NPG sebacate	39.43
2132	Squalane	40.60
–	Poly-A 135	41.66
2046	UCON 50-HB-280-X	43.41
2131	Polytergent J-300	43.74
2164	Paraplex G-25	44.27
2047	Tricresyl phosphate	44.34
2085	SAIB	44.34
2302	Ethomeen 18/25	44.50
2180	Polytergent J-400	44.75
2025	Oronite NIW	45.75
2086	QF-1	45.99
2252	UCON 50-HB-660	46.56
2093	PPG sebacate	46.63
2126	OV-210	46.78
2021	Ethofat 60/25	47.18
–	OV-202	47.18
–	SP-2401	47.18
2251	UCON 50-HB-3520	47.20
–	SP-2401	47.22
2062	Ethomeen S-125	47.53
2261	Igepal CO-630	47.77

(*Continued on p. 58*)

TABLE 88 (*continued*)

McReynolds code number	*Stationary phase*	*Retention polarity (polarity units)*
2092	LSX-3-0295	47.86
–	OV-215	47.95
2005	Pluronic P-65	48.32
2008	Pluronic P-85	48.43
2067	Tergitol NPX	48.74
2176	Emulphor ON-870	49.32
2183	Cresyl diphenyl phosphate	49.36
2003	Pluronic I-35	49.37
2184	Polytergent G-300	50.46
2228	Polyglycol 15-200	50.83
2122	Triton X-100	50.98
2129	Stepan DS-60	51.02
–	OV-330	52.08
2055	UCON 50-HB-5100	53.09
2146	Diethoxyethyl phthalate	53.15
2091	Siponate DS-10	53.24
2075	XE-60	53.83
2102	Renex-678	54.18
2045	OV-225	56.41
2185	Bis(ethoxyethoxyethyl phthalate	56.41
2138	NPGA	56.63
2300	UCON 75-H-90 000	57.57
2004	Pluronic F-88	58.70
2037	HI-EFF 8BP	60.22
2020	Igepal CO-880	60.45
2051	Triton X-305	61.14
2142	CW-4000 monostearate	62.40
2152	Zonyl E-7	63.97
2094	CW-4000 monostearate-2	64.79
2215	NPGS	65.23
2090	Quadrol	65.77
2098	Igepal CO-990	65.84
2042	EGSP-Z	67.51
2028	Carbowax(PEG)-20M	71.91
2084	Epon-1001	71.91
2029	Carbowax(PEG)-6000	71.95
2079	Ethylene glycol isophthalate	72.29
2315	Carbowax(PEG)-4000	73.32
–	OV-351	74.49
–	SP-1000	75.02
–	SP-2300	75.39
2153	XF-1150	75.43
–	Silar-5CP	75.51
2133	Sorbitol hexaacetate	77.68
2135	FFAP	78.86
2089	STAP	79.14
2026	Carbowax(PEG)-1000	79.84
2196	Sucrose octaacetate	80.59
–	PEG-1500	80.59
2334	MER-2	81.43

TABLE 88 (*continued*)

McReynolds code number	*Stationary phase*	*Retention polarity (polarity units)*
2119	PEG-600	81.90
2208	Butanediol succinate	82.46
2212	EGA	82.61
2139	Butanediol succinate-2	83.11
2219	PDEAS	84.19
2151	Reoplex-400	85.09
2157	LAC IR-296	85.50
2209	DEG adipate	85.61
2027	Carbowax(PEG)-1540	86.24
2304	Resoflex-R-296	86.63
2225	LAC-2-R-446	87.67
2041	EGSS-Y	88.11
2339	Hyprose SP-80	91.54
–	EGSP-A	92.37
–	SP-2310	99.31
–	Silar-7CP	99.55
–	ECNSS-S	99.62
2040	ECNSS-M	100.39
2338	Diglycerol	102.40
2107	DEGS Supelco-1045	102.55
2036	EGSS-X	105.30
2325	DEGS	106.63
2327	Ethylene glycol phthalate	106.69
2210	DEGS Supelco-1303	108.87
–	Silar-9CP	109.95
–	SP-2330	109.95
2303	DEGS-2	110.03
2224	LAC-3-R-728	110.43
–	SP-2340	114.39
–	Silar-10CP	114.51
2329	Glycol succinate	115.21
2110	THEED	116.20
2097	Tetracyanoethoxy PE	116.38
2213	EGS	116.77
–	SP-216-PS	122.53
–	1,2,3,4,5,6-Hexakis(cyclo-N)	123.86
2035	TCEP	128.91
–	OV-275	131.38
–	1,2,3,4-Tetrakis(cyclo-B)	131.78
2099	Cyanoethylsucrose	136.31
2117	BCEF	144.60

12. PRECALCULATION OF RETENTION INDEX

The widespread use of personal and home computers in the laboratory has given an impetus to such applications, but the progress is far from satisfactory. The problem is not connected with the computer software, but with the GLC itself. In spite of the fact that the theoretical background needed for the calculations is almost complete, there is a dearth of reliable GC data for use in calculations, especially in those instances where the calculations are to be extended over different column temperatures.

We consider as examples papers of Calixto *et al.*[52], Szulc *et al.*[86], Bermejo and Guillen[102], Jánosi[118], Morishita *et al.*[206], Peetre *et al.*[211], Podmaniczky *et al.*[212], Betts[248], Mihara and Masuda[363], Fernandez-Sanchez *et al.*[379], Papazova *et al.*[421] and Peng *et al.*[422]. Some of their most interesting results are summarized in Tables 89–103.

From the many studies in this field we refer to those involving different mathematical aspects. Equations for retention indices *versus* Van der Waals volume on squalane stationary phase were studied by Calixto and Raso[8] for alcohols, carbonyls, esters and ethers. A method of calculating the specific retention volumes of compounds from their retention indices was presented by Golovnya and Grigoryeva[58a]. Relationships between GC retention indices of aromatic hydrocarbons and several parameters were demonstrated by Calixto and Raso[104a]. Calculation of retention indices of chlorinated alkanes was presented by Sabljić[141]. A new equation for the calculation of the retention indices of aliphatic saturated esters on any stationary phases was derived by Bermejo and Guillen[166].

Retention indices of C_6 epoxides on OV-101 stationary phase at four column temperatures between 60 and 90°C were determined by Boneva and Dimov[253]. Linear regression equations permit the precalculation of the retention indices. Application of a three-factor model on 24 stationary phases was reported by Howery *et al.*[280]. Retention indices of 42 solutes showed good agreement with predictions. Precalculation of the retention indices of isoalkanes on squalane was proposed by Dimov[335]. Prediction of retention data using the slope of the log(adjusted retention time) *versus* carbon number plot for *n*-alkanes was discussed by Hawkes[413].

For further information, see also refs. 26, 40, 49, 50, 72, 74, 78, 102, 105a, 116, 138, 163, 167, 170a, 183, 206, 207, 267a, 278, 288, 291, 293, 303, 313, 323, 324, 343, 348, 357, 383, 391, 407, 422, 467 and 475.

TABLE 89

COMPARISON OF RETENTION INDICES OF SOME ALCOHOLS MEASURED AND CALCULATED BY CALIXTO *ET AL.*[52] ON PEG-1540 AT 90°C

Alcohol	*Retention index (i.u.)*					
	Measured	*Calculation by equation in ref. 52*				
		1	*2*	*3*	*4*	*5*
Propanol	1039.3	−2.2	2.6	−2.2	−2.2	−2.2
n-Butanol	1149.6	0.9	3.2	0.9	0.9	0.9
n-Pentanol	1258.1	2.2	0.4	2.2	2.2	2.2
n-Hexanol	1363.1	0	−9.3	0	0	0
n-Heptanol	1470.4	0.1	−1.7	0.1	0.1	0.1
n-Octanol	1577.2	−0.3	3.1	−0.3	−0.3	−0.3
n-Nonanol	1684.1	−0.6	4.2	−0.6	−0.6	−0.7

TABLE 90

COMPARISON OF RETENTION INDICES MEASURED AND CALCULATED BY SZULC *ET AL.*[86] ON MIXED LIQUID-CRYSTALLINE STATIONARY PHASES AT 120°C

Symbol[a] of stationary phase	*Compound[b]*	*Retention index (i.u.)*		
		Measured	*Calculated*	*Difference*
$A_1 + B_2$	*o*-E_2B	1068.0	1059.4	8.6
	m-E_2B	1148.7	1142.1	6.6
	p-E_2B	1195.5	1188.9	6.6
$B_2 + C_1$	*o*-E_2B	1203.5	1195.8	7.7
	m-E_2B	1183.3	1175.9	7.4
	p-E_2B	1233.7	1224.2	9.5
$A_1 + C_1$	*o*-E_2B	1171.4	1170.4	1.0
	m-E_2B	1153.4	1152.1	1.3
	p-E_2B	1199.6	1199.7	0.1
$A_1 + B_2 + C_1$	*o*-E_2B	1171.3	1160.1	11.2
	m-E_2B	1151.9	1143.3	8.6
	p-E_2B	1198.9	1190.6	8.3
$A_1 + C_3$	*o*-E_2B	1164.9	1165.2	0.3
	m-E_2B	1145.6	1146.9	1.3
	p-E_2B	1188.4	1191.8	3.4
$C_1 + C_3$	*o*-E_2B	1204.7	1202.6	2.1
	m-E_2B	1181.9	1181.0	0.9
	p-E_2B	1224.9	1226.2	1.3
$A_1 + C_1 + C_3$	*o*-E_2B	1168.4	1164.8	3.6
	m-E_2B	1149.0	1147.0	2.0
	p-E_2B	1192.5	1192.5	0.0
$B_2 + C_3$	*o*-E_2B	1194.7	1190.5	4.2
	m-E_2B	1171.8	1169.8	2.0
	p-E_2B	1215.7	1215.1	0.6
$A_1 + B_2 + C_3$	*o*-E_2B	1163.9	1150.8	13.1
	m-E_2B	1144.4	1134.1	10.3
	p-E_2B	1187.2	1180.1	7.1

[a] Symbols as in ref. 85.

[b] E_2B = diethylbenzene.

13. RETENTION INDEX AND COMPUTERS (GC–MS)

Although the use of computers is becoming increasingly popular and many researchers have applied them in chromatogram evaluation (GC–MS), the possibilities offered have not been fully exploited.

A computerized rapid analysis system and its application to two research problems were described by Demirgian[106]. From the results published in this field we

TABLE 91

COMPARISON OF RETENTION INDICES MEASURED AND CALCULATED BY BERMEJO AND GUILLÉN[102] ON SQUALANE AT 50°C

Compound[a]	*Retention index (i.u.)*				
	Measured	*Calculated*		*Difference*	
		Method 1	*Method 2*	*Method 1*	*Method 2*
2-MC_4	474.9	468.4	469.1	6.5	5.8
2,2-M_2C_4	536.6	527.7	528.2	8.9	8.4
2,3-M_2C_4	567.6	562.5	562.5	5.1	5.1
2-MC_5	569.5	571.1	571.1	−1.6	−1.6
3-MC_5	584.0	584.4	584.1	−0.4	−0.1
2,2-M_2C_5	625.9	626.6	626.0	−0.7	−0.1
2,4-M_2C_5	629.9	631.7	631.3	−1.8	−1.4
2,2,3-M_3C_4	639.8	634.6	634.1	5.2	5.7
3,3-M_2C_5	658.9	656.1	655.4	2.8	3.5

[a] M = methyl; C_4 = butane; C_5 = pentane.

can mention by way of illustration those of Brooks *et al.*[46], Burns and Tingey[48], Marriott *et al.*[129], Maurer and Pfleger[130,131], Tandon *et al.*[148], Tong *et al.*[152], Gill and co-workers[175,267], Wu[316], D'Agostino *et al.*[318], Harvey *et al.*[349], Sakamoto *et al.*[376], Hajšlová *et al.*[412], Köppel *et al.*[416] and Matisová[418].

For further information, see also refs. 102a, 225, 289, 304, 402 and 479.

14. RETENTION INDEX LIBRARY

Similarly to retention index review papers, attempts to organize a retention index library[30,143,396,429a] have been only of a recapitulatory type, *i.e.*, they contain very few critical elements, if any. Thus if may often happen that different retention index values are given for the same compound measured with a particular GC system. As

TABLE 92

COMPARISON OF RETENTION INDICES OF 2-METHYLNAPHTHALENE MEASURED AND CALCULATED BY JÁNOSI[118] ON DIFFERENT OV STATIONARY PHASES AT 150°C

Stationary phase	*Retention index (i.u.)*		
	Measured	*Calculated*	*Difference*
OV-1	1294.0	1293.7	0.3
OV-3	1335.0	1335.0	0
OV-7	1373.0	1374.5	−1.5
OV-11	1433.0	1431.0	2.0
OV-17	1484.0	1484.7	−0.7
OV-22	1536.0	1536.6	−0.6
OV-25	1571.0	1570.6	0.4

TABLE 93

COMPARISON OF RETENTION INDICES MEASURED AND CALCULATED BY BERMEJO AND GUILLÉN[166] OF ALIPHATIC SATURATED ESTERS ON DIFFERENT STATIONARY PHASES AT 120°C

Compound	*Retention index (i.u.)*					
	Diisodecylphthalate		*Pluronic P65*		*Bis(2-ethoxyethyl)-phthalate*	
	Measured	*Calc.*	*Measured*	*Calc.*	*Measured*	*Calc.*
Methyl formate	482	+14	627	+10	641	+37
Ethyl acetate	659	+3	772	−2	801	0
Propyl formate	684	+4	802	0	828	+7
Propyl acetate	757	+7	867	0	897	0
Isopropyl propionate	780	+9	868	+14	905	+4
Isobutyl acetate	817	+8	914	+8	948	+2
Propyl propionate	846	+5	947	+3	980	0
Pentyl formate	892	−7	1010	−5	1043	−7
Isobutyl propionate	909	−1	999	+2	1036	−7
2-Ethyl 1-butylacetate	1025	0	1127	−2	1164	−10

TABLE 94

COMPARISON OF RETENTION INDICES MEASURED BY MORISHITA *ET AL.*[206] AND CALCULATED ON PEG-20M STATIONARY PHASE AT 93°C

Compound[a]	*Retention index (i.u.)*		
	Measured	*Calculated*	*Difference*
1-C_5SH	1052.9	1054.4	−1.5
1-C_7SH	1253.8	1252.6	+1.2
2-C_5SH	967.9	969.2	−1.3
2-C_7SH	1165.5	1164.6	+0.9
3-C_5SH	979.5	976.0	+3.5
3-C_6SH	1062.5	1061.5	+1.0
3-C_7SH	1157.6	1158.6	−1.0
4-C_7SH	1144.1	1146.7	−2.6
C_1-SC_4	1032.6	1036.2	−3.6
C_1-SC_5	1132.3	1133.3	−1.0
C_1-SC_6	1232.1	1231.6	+0.5
C_1-SC_7	1332.1	1331.4	+0.7
C_1-SC_8	1431.7	1431.5	+0.2
C_2-SC_4	1096.1	1095.9	+0.2
C_2-SC_5	1193.0	–	–
C_2-SC_6	1291.2	1291.3	−0.1
C_2-SC_7	1390.7	1391.1	−0.4

[a] C_1 = Methyl; C_2 = ethyl; C_4 = *n*-butyl; C_5 = *n*-pentyl; C_6 = *n*-hexyl; C_7 = *n*-heptyl; C_8 = *n*-octyl.

TABLE 95

COMPARISON OF RETENTION INDICES OF ALKYLALKOXYSILANES MEASURED AND CALCULATED BY PEETRE *ET AL.*[211] ON APIEZON M AT 160°C

Compound	*Retention index (i.u.)*		
	Measured	*Calculated*	*Difference*
$CH_3Si(OCH_3)_3$	624	624	0
$CH_3Si(OC_4H_9)_3$	1271	1272	−1
$CH_3Si(OC_5H_{11})_3$	1538	1539	−1
$CH_3Si(OC_6H_{13})_3$	1808	1811	−3
$CH_3Si(OC_7H_{15})_3$	2085	2083	2
$(CH_3)_2Si(OC_2H_5)_2$	678	677	1
$(CH_3)_2Si(OC_3H_7)_2$	847	846	1
$(CH_3)_2Si(OC_4H_9)_2$	1024	1022	2

TABLE 96

COMPARISON OF RETENTION INDICES MEASURED AND CALCULATED BY PODMANICZKY *ET AL.*[212] ON PEG-20M AT DIFFERENT COLUMN TEMPERATURES

Compound	*Retention index (i.u.)*					
	80°C		*100°C*		*120°C*	
	Measured	*Δ*[a]	*Measured*	*Δ*[a]	*Measured*	*Δ*[a]
Benzene	960.7	−0.2	968.7	−0.7	976.9	+2.0
Toluene	1058.0	−0.5	1067.0	−1.1	1076.1	−0.8
p-Xylene	1149.9	−0.1	1159.9	−1.2	1169.8	−1.6
m-Xylene	1156.3	+0.7	1166.4	−0.1	1176.3	0.0
o-Xylene	1198.3	+1.2	1209.8	−0.6	1221.1	−1.4

[a] Difference between measured and calculated values.

TABLE 97

COMPARISON OF RETENTION INDICES MEASURED AND CALCULATED BY BETTS[248] ON DIFFERENT STATIONARY PHASES AT 120°C

Stationary phase	*Retention index (i.u.)*					
	n-Butanol		*Pyridine*		*2-Octyne*	
	Measured	*Δ*[a]	*Measured*	*Δ*[a]	*Measured*	*Δ*[a]
Squalane	590	+20	699	+6	841	+11
OV-1	645	+18	741	−4	864	−5
SE-30	643	+2	740	+3	863	+3
SP-2100	647	+4	742	+4	866	−6
OV-17	748	−1	901	−30	946	−16
SP-2550	748	−10	901	−14	946	−10
OV-210	828	−13	1009	+32	897	+6
OV-225	959	+20	1085	+39	991	+11
SP-2330	1315	+52	1477	+80	1153	+56
PEG 1000	1197	+38	1288	+60	1081	+29
PEG 20M	1126	+22	1209	+29	1062	+21
DEGS	1323	+94	1490	+127	1162	+47

[a] Difference between measured and calculated values.

TABLE 98

COMPARISON OF RETENTION INDICES OF SOME ALKYLPYRIDINES MEASURED AND CALCULATED BY MORISHITA *ET AL.*[291] ON OV-101 AND PEG-20M AT 150°C

Compound	*Retention index (i.u.)*			
	OV-101		*PEG-20M*	
	Measured	*Δ*[a]	*Measured*	*Δ*[a]
Pyridine	744.6	+3.4	1241.5	+1.7
2-Methylpyridine	814.0	−2.1	1268.3	−3.2
3-Methylpyridine	859.1	+0.8	1354.3	+0.6
4-Methylpyridine	862.7	−1.6	1363.5	+1.0
2,3-Dimethylpyridine	940.3	+9.2	1410.5	+13.8
2,5-Dimethylpyridine	925.9	−4.0	1377.6	−6.2
2,6-Dimethylpyridine	875.8	−2.1	1287.9	+0.2
3,4-Dimethylpyridine	999.9	−1.2	1528.3	−4.9
3,5-Dimethylpyridine	972.4	−2.7	1468.7	−1.6
2,4,6-Trimethylpyridine	982.4	+0.2	1409.1	+1.3
2,4-Dimethylpyridine	923.9	−1.0	1390.1	−2.9

[a] Difference between measured and calculated values.

TABLE 99

COMPARISON OF RETENTION INDICES MEASURED AND CALCULATED BY MIHARA AND MASUDA[363] ON OV-101 AND PEG-20M AT 70°C

Compound	*Retention index (i.u.)*			
	OV-101		*PEG-20M*	
	Measured	*Calculated*	*Measured*	*Calculated*
Methylpyrazine	801	800	1235	1235
2,3-Dimethylpyrazine	897	894	1309	1307
2,5-Dimethylpyrazine	889	890	1290	1293
2,6-Dimethylpyrazine	889	887	1300	1296
Trimethylpyrazine	981	981	1365	1367
Tetramethylpyrazine	1067	1072	1439	1441
Ethylpyrazine	894	891	1300	1300
2-Ethyl-5-methylpyrazine	980	981	1357	1357
2-Ethyl-6-methylpyrazine	977	973	1353	1351
2,5-Dimethyl-3-ethylpyrazine	1059	1059	1400	1403
2,6-Dimethyl-3-ethylpyrazine	1064	1064	1415	1412
2,3-Dimethyl-5-ethylpyrazine	1066	1067	1421	1422
2,3-Diethylpyrazine	1065	1060	1417	1413

TABLE 100

COMPARISON OF RETENTION INDICES MEASURED AND CALCULATED BY FERNÁNDEZ-SANCHEZ *ET AL.*[379] ON DIFFERENT MIXED STATIONARY PHASES AT 120°C

McReynolds standard	*Retention index (i.u.)*								
	OV-225 + SP-2340 (78.1:21.9)			*OV-225 + SP-2340 (51:49)*			*OV-225 + SP-2340 (10.3:89.7)*		
	Measured	*Calculated*	*Difference*	*Measured*	*Calculated*	*Difference*	*Measured*	*Calculated*	*Difference*
Benzene	893	893	0	953	958	−5	1125	1124	+1
1-Butanol	988	991	−3	1069	1073	−4	1290	1286	+4
2-Pentanone	981	983	−2	1044	1042	+2	1197	1198	−1
1-Nitropropane	1171	1173	−2	1259	1265	−6	1515	1503	+12
Pyridine	1114	1114	0	1198	1200	−2	1438	1430	+8
2-Methyl-2-pentanol	988	989	−1	1045	1051	−6	1233	1227	+6
1-Iodobutane	1047	1047	0	1088	1091	−3	1237	1233	+4
2-Octyne	997	995	+2	1013	1020	−7	1108	1106	+2
1,4-Dioxane	1021	1023	−2	1098	1100	−2	1320	1314	+6
cis-Hydrindane	1118	1119	−1	1141	1145	−4	1226	1222	+4

TABLE 101

COMPARISON OF MEASURED AND CALCULATED RETENTION INDICES ON SQUALANE AT 30°C, AFTER PAPAZOVA *ET AL.*[421]

Substance	*Retention index (i.u.)*		
	Measured	*Calculated*	*Difference*
cis-3-Hexene	592.3	591.5	+0.8
2-Ethyl-1-butene	592.0	590.5	+1.5
trans-2-Hexene	597.3	596.6	+0.7
trans-3-Hexene	592.8	594.2	+1.4
cis-2-Hexene	603.2	601.5	+1.7
3,3-Dimethyl-1-pentene	624.1	623.7	+0.4

TABLE 102

COMPARISON OF MEASURED (BY TPGC) AND CALCULATED RETENTION INDICES OF AROMATIC HYDROCARBONS ON SE-30, AFTER PENG *ET AL.*[422]

Compound	*Retention index (i.u.)*		
	Measured	*Calculated*	*Difference*
Benzene	654	658	−4
Toluene	764	768	−4
Ethylbenzene	858	858	0
o-Xylene	895	893	+2
m-Xylene	871	878	−7
p-Xylene	875	878	−3
n-Butylbenzene	1058	1058	0
Biphenyl	1375	1376	−1
Octahydroanthracene	1684	1654	+30
p-Terphenyl	2121	2094	+27

TABLE 103

COMPARISON OF MEASURED (BY TPGC) AND CALCULATED RETENTION INDICES OF ALCOHOLS ON SE-30, AFTER PENG *ET AL.*[422]

Compound	*Retention index (i.u.)*		
	Measured	*Calculated*	*Difference*
2-Methyl-1-propanol	626	626	0
3-Methyl-1-butanol	726	716	+10
3-Methoxy-1-butanol	814	816	−2
2-Ethyl-1-butanol	836	816	+20

TABLE 104

OUTLINE OF A PAGE IN A PROPOSED INTERNATIONAL RETENTION INDEX LIBRARY[a]

Substance: Benzene
Retention data:
I. 1 Stationary phase: OV-101.
2. Temperature range of appicability: 0–350°C.
3 Kováts coefficients at different frequently used column temperatures:

Column temperature (°C)	*Kováts coefficient [dim.]*[b]
0	53.24
10	61.10
30	78.17
50	97.29
70	118.77
90	143.03
100	156.22
110	170.34
120	185.43
130	201.44
150	237.84

4. *b* Values at different frequently used column temperatures:

Column temperature (°C)	*b Value*
0	0.5171
10	0.4868
30	0.4323
50	0.3847
70	0.3427
90	0.3055
100	0.2884
110	0.2722
120	0.2568
130	0.2422
150	0.2152

5. Retention indices at different frequlently used column temperatures:

Column temperature (°C)	*Retention index (i.u.)*
0	631.9
10	635.3
30	642.0
50	648.3
70	654.3
90	660.0
100	662.8
110	665.5
120	668.1
130	670.7
150	678.2

TABLE 104 (*continued*)

II. 1. Stationary phase: Apolane-87.
2. Temperature range of applicability: 30–280°C.
3. Kováts coefficients at different frequently used column temperatures:

Column temperature (°C)	*Kováts coefficient [dim.]*[b]
30	73.71
40	80.39
50	86.92
70	99.52
90	111.54
100	117.34
110	123.02
120	128.57
130	134.00
150	144.51

4. *b* Values at different frequently used column temperatures:

Column temperature (°C)	*b Value*
30	0.4299
40	0.4090
50	0.3894
70	0.3536
90	0.3217
100	0.3071
110	0.2932
120	0.2800
130	0.2675
150	0.2442

5. Retention indices at different frequently used column temperatures:

Column temperature (°C)	*Retention index (i.u.)*
30	646.1
40	649.4
50	652.7
70	659.2
90	665.7
100	669.0
110	672.3
120	675.5
130	678.8
150	685.3

III. 1. Stationary phase: Squalane.
2. Temperature range of applicability: 0–125°C.
etc.

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[a] The International Retention Index Library is sponsored.

[b] Carrier gas: helium.

a consequence, the user has to decide which value to take as the proper one. In other instances the published data and/or retention index library are reliable, but incomplete to a large extent.

The best solution would be the establishment of an international *ad hoc* committee sponsored by those companies which produce and sell stationary phases, supports, and open-tubular (capillary) columns. Moreover, it would be advantageous to obtain additional support from companies manufacturing gas chromatographs and integrators and/or computers for GLC.

Prior to the beginning of the extensive collection of data, this *ad hoc* committee should undertake the selection of those relationships which represent the theoretical basis (retention index calculations, measurement and calculation of the dead time, etc.), then make them available to those who participated in the measurement and collection of data.

Table 104 outlines a data sheet in a future International Retention Index Library.

For further information, see ref. 215.

15. LIST OF SYMBOLS USED

α	relative volatility;
a_0	atomic code number in the bond;
A	constant in eqn. 1;
a^R	substance-specific factor according to Rohrschneider;
a_1	atomic code number in the primary environment;
a_2	atomic code number in the secondary environment;
B	constant in eqn. 1;
b^R	substance-specific factor according to Rohrschneider;
b	slope of *n*-alkane plot;
C	constant in eqn. 1;
c^R	substance-specific factor according to Rohrschneider;
d	bond length;
d^R	substance-specific factor according to Rohrschneider;
D	constant in eqn. 9; dimension of S_c and/or K_c; [dim.] = log [cm^3 (carrier gas)/g (stationary phase)];
E	constant in eqn. 9;
e^R	substance-specific factor according to Rohrschneider;
E_{C-H}	bond energy of alkane C–H bond;
E_{C-C}	bond energy of alkane C–C bond;
f_c	index units/energy units conversion factor for alkanes;
f_s	[dim.]/energy units conversion factor for alkylbenzenes;
ΔG	partial molar free energy of solution;
I	isothermal retention index;
i.u.	retention index units;
i	serial number;
i_b	bond index increment;
i_i	interaction index increment;
i_s	structural increment;
ΔI	$I_s^{st.ph.}(T) - I_s^{SQ}(T)$;
j	serial number;

k	serial number;
K_c	Kováts coefficient, $\{-\log [\mathrm{cm}^3$ (carrier gas)/g (stationary phase)]};
n-C_z	n-alkane with carbon number z;
p	total number of atoms of the bond in the primary environment;
p.u.	polarity units;
q	total number of atoms of the bond in the secondary environment;
s	substance of interest;
s_c	molecular structural coefficient, $\{\log [\mathrm{cm}^3$ (carrier gas)/g (stationary phase)]};
st.ph.	stationary phase;
SQ	squalane stationary phase;
s_i	ith substance-specific factor;
t_M	gas holdup (dead) time;
t'_R	adjusted retention time;
t_N	net retention time;
T	the column-temperature;
TPGC or TP	temperature-programmed gas chromatography;
V_g	specific retention volume;
V_N	net retention volume;
X	retention value used in calculation;
z	carbon number of n-alkane.

16. LIST OF COMPOUNDS EXAMINED

To facilitate the use of this review, retention indices are grouped in Table 105 based on the type of chemical compound.

TABLE 105

REFERENCES TO RETENTION INDICES OF DIFFERENT COMPOUNDS

Compound type	*References*
Acids	422
Adamantanes	246
Alcohols	8, 19, 58a, 120, 281, 284, 324, 329, 343, 349, 422
Aldehydes	93
Aldoses	366
Alicyclic hydrocarbons	340
Aliphatic acids	281
Alkaloids	260
Alkanes	2, 7, 19, 35b, 36, 48, 54, 55, 75, 93a, 161, 173, 250, 258, 309, 325, 333, 335, 407, 413, 422, 428, 430
Alkanols	5
Alkenes	7, 17, 19, 54, 55, 93a, 138, 155, 173, 249, 258, 297, 316, 422
Alkenylbenzenes	160, 339
Alkyl acrylates	182
Alkylalkoxysilanes	211
Alkyl chlorides	257
Alkyldecenes	208
Alkylnaphthalenes	118
Alkylphenols	409
Alkylporphyrins	129, 175, 267
Alkylquinolines	332

(*Continued on p. 72*)

TABLE 105 (*continued*)

Compound type	*References*
Alkylserines	376
Alkynes	208
Amidines	292, 295, 296
Amines	145, 209, 225a, 403, 422
Amino ether alcohols	384, 388
Amino acids	219
Anthracenes	287
Anthraquinones	201
Antidepressants	130
Aromatics	7, 19, 42, 44, 54, 55, 58a, 101, 104a, 170a, 258, 285, 286, 309, 418, 422, 424a, 429a, 433
Arylaliphatic acids	198
Azaarenes	291
Barbituric acids	25
Benzodiazepines	414
Benzophenones	414
Benzothiophenes	243, 415
Benzylideneamines	210
Beta-adrenolytics	417
Beta-blockers	289
Bicyclo-2-alkenones	212b
Carbohydrates	374
Carbonyls	8
Chlorinated alkanes	78, 141
Chlorinated anisoles	123
Chlorinated benzenes	62, 167, 185, 214, 247
Chloroallyl compounds	137
Chloroanisoles	186
Chloroethanols	191
Chlorophenols	125, 192
Chlorovinyl compounds	137
Chlorinated dibenzo-*p*-dioxins	337
Chlorinated hydrocarbons	71
Chlorinated 4-hydroxybenzaldehydes	122
Chlorinated salicylaldehydes	124
Chlorinated veratroles	121
Cumene	23
Cyclic ferroceneboronates	331
Cyclic hydrocarbons	7, 19, 54, 55, 286
Cycloalkanes	102
Cyclohexenes	27, 103
Cycloolefins	327
Cyclopentadienes	381
Dibenzothiepins	232
Dichlorobenzyl alkyl ethers	238
Dienes	422
Dimethylbenzamidines	210
Dioxides	243
Diterpenes	136
Drugs	40a, 255, 364, 396
Esters	8, 58a, 60, 61, 63, 65, 93, 111–113, 119, 166, 177–179, 180, 188–190, 193, 194–196, 269, 270, 275, 276, 281–284, 343, 359, 388, 422

TABLE 105 (*continued*)

Compound type	*References*
Epoxides	253, 330
Essential oils	114, 115
Ethers	8, 58a, 228, 343, 384, 422
Fatty acids	349
Fusariotoxins	41
Glycidic esters	300
Halides	182
Halocarbons	10, 19a
Halogenated alkanes	404
Halogenated anisoles	271, 341
Halogenated benzenes	271, 341
Halogenated cyclohexanes	271, 341
Halogenated olefins	404
Halogenated phenols	422
Halogenocarboxylic acids	236
Halopropionates	281
Heterocyclics	422
Hydrazones	144
Hydroxy acids	102a
Irritants	158
Ketones	58a, 93, 213, 343, 422
Ketonic bile acids	148
Lemon oil	256
Monocyclic terpene alcohols	159
Mycotoxins	1
Naphthalenes	7, 118
Neuroleptics	131, 170
Nitrated polyaromatic hydrocarbons	92, 187, 301–303
Non-ionic surfactants	310, 387
Olefins	127
Organic acids	37a
Organophosphorus compounds	158
Perfluorocarbons	79
Permethylated oligosaccharide alditols	91
Petroleum fractions	87, 383, 421
Phenols	39a, 422
Phenoxypropanoic acid derivatives	412
Phenylacetic acid derivatives	204
Phenylpropionic acid derivatives	204
Polyaromatic hydrocarbons	38, 72, 303
Polychlorinated biphenyls	197
Poly(ether alcohols)	109
Pristane and other isoprenoids	6
Pyrazines	288, 363
Pyridines	372
p-Quinones	361
Sedative hypnotic drugs	134
Simulants	158
Steroidal alkaloids	410
Steroids	46, 95
Sterols	45

(*Continued on p. 74*)

TABLE 105 (*continued*)

Compound type	*References*
Substituted salicylic acids	402
Sulphides	206
Sulphur compounds	228
Sulphur(II)-containing compounds	174a
Sulphur vesicants	398
Thianes	415
Thiols	94, 206
Thiophenes	415
Toxic compounds	151
Trichothecene toxins	97, 147
Vesicants	158

17. LIST OF STATIONARY PHASES

Retention indices measured on different stationary phases are listed in Table 106.

TABLE 106

REFERENCES TO RETENTION INDICES MEASURED ON DIFFERENT STATIONARY PHASES

Stationary phase	*References*
Acetyltributyl citrate	23, 42, 285
Apiezon K	387
Apiezon L	19, 19a, 58, 78, 88, 105, 141, 246, 257
Apiezon M	58, 167, 211
Apolane-87	53, 198, 271, 341
BP-1	327
Cation exchanger	17, 96, 183
Cyanopropylsilicone	4, 406
CHOB	35b
Citroflex-A4	418
Carbowax: see PEG	
DB-1	45, 48, 75, 91, 127, 134, 135, 158, 175, 197, 201, 318, 398, 418
DB-5	45, 75, 127, 134, 152, 158, 243, 304, 318, 372, 398
DB-1701	318
DC-550	206
Dexsil-300	36, 232, 376
Dexsil-400	232
Dexsil-410	232
Di-2-ethylhexyl sebacate	2
Dioctyl phthalate	166, 296, 324, 375
DEGS	49, 50, 79, 163, 248, 355, 361, 374
Emulphor-ON-870	19
FFAP	125, 185
Fluorinated	369
HP-1	319
Hallcomid M-18	149
JXR	421
Liquid alkylammonium sulphonates	345, 368, 423, 424a
Liquid crystalline	85, 86, 117, 286

TABLE 106 (*continued*)

Stationary phase	*References*
Mixed	71, 86, 176, 218, 306, 337, 379
Methylpolysiloxane	421
N-Lauroyl-(*R*)-α-(1-naphthyl)ethylamine	236
NPP	35b
OBO	35b
Oronite NIW	166, 324
OV-101	25, 44, 54, 72, 73, 93a, 111, 130, 131, 144, 167, 169, 170, 182, 200, 204, 209, 219, 249, 253, 255, 258, 288, 289, 291, 297, 306, 327, 329, 330, 332, 363, 367, 373, 379, 379a, 392, 394, 413, 418
OV-1	36, 37a, 46, 58a, 84, 118, 129, 137, 160, 163, 248, 331, 339, 340, 404, 417
OV-3	55, 118, 258, 413
OV-7	55, 72, 118, 258, 413
OV-11	55, 118, 258, 413
OV-17	37a, 55, 72, 73, 118, 144, 163, 169, 170, 200, 204, 248, 258, 355, 361, 374, 376, 379a, 387, 417, 430
OV-22	55, 118, 258
OV-25	55, 65, 118, 123, 124, 163, 258, 306, 359, 379a, 413
OV-61	413
OV-105	375
OV-210	167, 248, 327
OV-215	4, 93, 327, 373
OV-225	25, 76, 77, 144, 159, 163, 248, 295, 354, 355, 366, 367, 373, 379
OV-275	79, 354, 355
OV-351	60, 61, 63, 119–121, 177–180, 185, 186, 188–196, 269, 270, 282–284
OV-1701	158, 327, 398, 409
PEG-400	23, 285
PEG-1000	58, 65, 79, 166, 248, 324
PEG-1540	2, 23, 51, 52, 104, 218, 285, 343
PEG-4000	27
PEG-20M	5, 6, 23, 27, 42, 49, 50, 58, 62, 78, 87, 88, 101, 103, 105, 112–115, 136, 137, 149, 159, 161, 167, 185, 206, 208, 212, 212a, 214, 243, 248, 256, 257, 271, 285, 288, 291, 297, 298, 329, 332, 340, 354, 355, 361, 374, 379, 381, 392
Pluronic-F88	166, 324
Porapak S, PS, Q, R	90
PPG-425	323
QF-1	65, 79, 355, 387
SE-30	4, 7, 23, 36, 40a, 58, 58a, 60, 61–63, 65, 72, 87, 90, 93, 95, 103, 109, 112, 113, 119–125, 136, 148, 149, 151, 161, 166, 177–180, 186–196, 210, 213, 214, 260, 269, 270, 282–284, 285, 292, 295, 296, 324, 359, 361, 364, 374, 387, 414, 418
SE-52	1, 4, 12, 41, 72, 92, 97, 147
SE-54	46, 182, 241, 247, 256, 366, 374
Sil-5	238, 298, 410
Silar-10C	4, 65, 76, 77
Siponate DS-10	93
SP-255	409

(*Continued on p. 76*)

TABLE 106 (*continued*)

Stationary phase	*References*
SP-400	281
SP-1000	10, 182, 212, 212a, 404
SP-2100	54, 227, 248, 298
SP-2250	248
SP-2330	248
SP-2340	379
Siloxane/silarylene	322
Squalane	2, 8, 23, 49, 50, 64, 79, 90, 101, 102, 104, 138, 155, 173, 218, 246, 247, 285, 297, 316, 327, 339, 343, 354, 355, 358, 365, 382, 385, 418, 421
TCEP	23, 42, 163, 285, 355
Tetrakis(2-cyanoethoxy)butane	271, 341
Tricresyl phosphate	257
Triton X-305	58, 65
TXP	167, 247
UCON 50-HB-280X	42
UCON 50-HB-250	285
UCON LB-550X	2, 23, 42, 167, 182, 247, 285, 300, 332, 340, 361, 418
XE-60	211, 361
Wax-51	93, 350

18. LIST OF IMPORTANT RETENTION INDEX RESEARCH ESTABLISHMENTS

To help with communication between researchers in this field, the addresses of some important retention index establishments are presented in Table 107.

TABLE 107

LIST OF IMPORTANT RETENTION INDEX RESEARCH ESTABLISHMENT

Country	*Establishment*
Algeria	Institute de Chimie, Laboratoire de Chromatographie, B.P. 32, El-Alia, Bab-Ezzour, Algiers
Saudia Arabia	University of Petroleum and Minerals, Dhahran
Australia	Department of Polymer Science, University of New South Wales, P.O. Box 1, Kensington, N.S.W., Australia 2033
Belgium	Service de Chimie Génerale et Chabochimie, Faculté des Sciences Appliquées (CP 165), Université Libre de Bruxelles, Avenue Franklin Roosevelt 50, B-1050 Bruxelles
	Research Institute for Chromatography, P.O.B. 91, B-8610 Wevelgem
	Laboratory of Organic Chemistry, University of Ghent, Kriigshan 281(S4), B-9000 Gent
Bulgaria	Institute of Chemical Technology, 8010 Burgas
	Chemical Pharmaceutical Institute, 1156 Sofia
	University of Sofia, Faculty of Chemistry, Bulv. Anton Ivanov 1, 1126 Sofia
	Petrochemical Research Institute, Economic Combine "Neftochim", 8104 Burgas

TABLE 107 (*continued*)

Country	*Establishment*
Canada	Defence Research Establishment Suffield, Ralston, Alberta TOJ 2NO
	Science and Technology Advisory Group, "L" Directorate, R.C.M. Police, Ottawa, Ontario
China	Department of Chemistry, Peking University, Beijing
	Beijing Institute of Labour Hygiene and Occupational Diseases, Dong Da Qiao, Beijing
Czechoslovakia	Research Institute for Pharmacy and Biochemistry, 130 60 Prague 3
	Pharmaceutical Faculty, Charles University, Hradec Kralové
	Research Institute for Rheumatology, Na Slupi 4, 128 50 Prague
	Department of Analytical Chemistry, Charles University, Hlavova 2030, Prague
	Chemical Institute, Comenius University, 842 15 Bratislava
	Department of Analytical Chemistry, Institute of Chemistry, Institute of Chemical Technology, 532 10 Pardubice
	Institute of Chemical Technology, Suchbatarova 5, Prague 6
	Research Institute for Cruide Oil and Hydrocarbon Gases, Vlcie Hrdlo, 824 17 Bratislava
	Institute of Analytical Chemistry, Chechoslovak Academy of Sciences, Leninova 82, 611 42 Brno
	Institute of Experimental Pharmacology, Centre of Physiological Sciences, Slovak Academy of Sciences, 842 16 Bratislava
	Department of Analytical Chemistry, Faculty of Chemical Technology, Slovak Technical University, 812 37 Bratislava
F.R.G.	Bundesanstalt für Materialprüfung, Unter den Eichen 87, D-1000 Berlin 45
	Abteilung Analytische Chemie, Universität Ulm, D-7900 Ulm
	Laboratorium für Organische Chemie der Universität Bayreuth, Postfach 3008, D-8580 Bayreuth
	Medizinische Klinik und Poliklinik der Universität Göttingen, Robert Koch Strasse 40, D-3400 Göttingen
	Institute of Forensic Medicine, Karl-Ruprecht-University, Vossstr. 2, D-6900 Heidelberg
	Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, Mülheim/Ruhr
Finland	Department of Chemistry, University of Jyväskylä, Kyllikinkatu 1–3, SF-40100 Jyväskylä 10
France	Université de Recherche Scientifique, Avenue Phillipon, 64000 Pau
	Ministère des Universités, École Centrale des Arts et Manufactures, Laboratoire de Chimie Organique, Grande Voie des Vignes, 92290 Chatenay-Malabry

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TABLE 107 (*continued*)

Country	*Establishment*
	Laboratoire de Biochimie des Intéractions Cellulaires, Faculté des Sciences-Mirande, B.P. 138, 21004 Dijon Cédex
G.D.R.	Akademie der Wissenschaften der D.D.R., Zentralinstitut für Organische Chemie, Rudower Chaussee 5, 1199 Berlin-Adlershof
	Department of Chemistry, Karl-Marx Universität, Liebigstrasse 18, 7010 Leipzig
	Institut für Gerichtliche Medizin des Bereiches Medizin der Wilhelm-Pieck Universität Rostock, Runge Strasse 13, 2500 Rostock
	Karl-Marx Universität Leipzig, Sektion Chemie, Tallstrasse 35, 7010 Leipzig
Hungary	Department of Chemical Technology, L. Eötvös University, H-1088 Budapest
	Technical University, Institute of Chemical Technology, Budafoki ut 9/11, 1111 Budapest
	MÁFKI, H-8200 Veszprém
	Veszprémi Vegyipari Egyetem, Analitikai Kémiai Tanszék, Schönherz Z., u. 2, H-8200 Veszprém
	Institute for Drug Research, P.O.B. 82, H-1325 Budapest
	Budapesti Müszaki Egyetem, Biokémia és Élelmiszertechnológiai Tanszék, Müegyetem rkp 3–9, 1111 Budapest
	Research Institute for the Plastics Industry, H-1950 Budapest
	Research Laboratory for Inorganic Chemistry, Hungarian Academy of Sciences, Budaörsi ut 45, H-1112 Budapest
India	Indian Institute of Petroleum, Dehradun-248005
Iraq	Petroleum Research Centre, Council of Scientific Research, Baghdad
Israel	Department of Organic Chemistry, Weizmann Institute of Science, Rehovot
Italy	Istituto di Chimica Industriale, Università di Genova, Corso Europa 30, 16132 Genova
	Dipartimento di Chimica, Università "La Sapienza", Piazzale Aldo Moro 5, 00185 Rome
	Dipartimento di Scienca Chimiche, Università di Catania, Viale Andrea Doria 6, 95125 Catania
	Istituto di Medicina Legale e delle Assicuarizioni, Università di Catania, Via Biblioteca 4, 95124 Catania
	Dipartimento di Chimica, Università di Perugia, Via Elce di Scotto 10, 06100 Perugia
Japan	Department of Industrial Chemistry Faculty of Engineering, Kyoto University Yoshida-Honmachi, Sakyo-Ku, Kyoto-Shi, Kyoto 606
Nigeria	Chemistry Department, Bendel State University, Ekpoma, Bendel State
Poland	Department of Chemistry, Warsaw University, Pasteura 1, 02-93 Warsaw
	Technical University of Poznan, Institute of Chemical Technology and Engineering, Pl. Skłodowskiej-Curie, Poznan

TABLE 107 (*continued*)

Country	*Establishment*
	Department of Chemistry, Pedagogical University, Czestochowa
	Department of Physical Chemistry, Medical Academy, K. Marks 107, 80-416 Gdansk
	Institute of Chemistry, A. Mickiewicz University, 60-780 Poznan
Republic of South Africa	Institute for Chromatography, University of Pretoria, Pretoria 0001
Spain	Instituto Nacional del Carbon Consejo Superior de Investigaciones Cientificas, Oviedo
	Instituto de Quimica Bio-Organica (CSIC), J. Girona Salgado 18–26, 08034-Barcelona
	Centro de Investigacion Asistencia Técnica (INSHT), Dulcet s/n, 08034-Barcelona
	Instituto de Quimica Fisica "Rocasalano", Consejo Superior de Investigationes Cientificas, Serrano 119, 28006 Madrid
	Departamento de Bioquimica, Facultad de Veterinaria, Universidad Complutense, 28040 Madrid
	Departamento de Quimica Organica, Facultad de Cienancias, Universidad de Las Islas Baleares, Palma de Malorca 07071
	Departamento de Quimica Analitica, Facultad de Ciencias, Universidad de Alcalá de Henares, Madrid
Sweden	Department of Technical Analytical Chemistry, Chemical Centre, Lund Institute of Technology, P.O. Box 740, 22007 Lund 7
	Arrhenius Laboratory, Department of Analytical Chemistry, University of Stockholm, 10691 Stockholm
Switzerland	Institut de Chimie, Université de Neuchâtel, 2000 Neuchâtel
	Department of Pharmacy, ETH Zürich, Zürich
	Institute of Physical Chemistry, ETH Lausanne, Lausanne
The Netherlands	Department of Toxycology, State University, Deusinglaan 2, 9713 AW Groningen
	Department of Chemistry and Chemical Engineering Organic Geochemistry Unit, Delft University of Technology, De Vries van Heystplantsoen 2, 2628 RZ Delft
	Department of Instrumental Analysis, Eindhoven University of Technology, Eindhoven
United Kingdom	Department of Chemistry and Applied Chemistry, University of Salford, Salford, Lancs M5 4WT
	DAFS, Freshwater Fisheries Laboratory, Pitlochry, Scotland
	Department of Chemistry, University of Stirling, Stirling, Scotland
	Department of Chemistry, University of Technology, Loughborough, Leics LE11 3TU
	Chemistry Department, University of Glasgow, Glasgow G12 8QQ
	Division of Chemical Sciences, Hatfield Polytechnic, Hatfield, Herts
	Central Research Establishment, Home Office Forensic Science Service, Aldermaston, Reading, Berks. RG7 4PN

(*Continued on p. 80*)

TABLE 107 (*continued*)

Country	*Establishment*
	Department of Chemistry, University College of Swansea, Singleton Park, Swansea, Wales SA2 8PP
U.S.A.	Sadtler Research Laboratories, Division of Bio-Rad Laboratories, 3316 Spring Garden Street, Philadelphia, PA 19104
	Department of Environmental Toxicology, University of California, Davis, CA 95616
	Department of Chemistry, Indiana University, Bloomington, IN 47405
	University of Arkansas, Fayetteville, AR 72701
	Department of Chemistry, Wayne State University, Detroit, MI 48202
	Department of Chemistry, Oregon State University, Corvallis, OR 97331
	Mesa Police Department Crime Laboratory, 130 North Robson, Mesa, AZ 85201-6697
	Perkin-Elmer Corporation, Norwalk, CT 06856
	Department of Chemistry, State University of New York at Buffalo, Buffalo, NY 14214
	Institute for Lipid Research, Baylor College of Medicine, Hollston, TX 77025
	Chemical Research Department, Hoffmann La Roche Inc., Nutley, NJ 07110
	Merck Sharp & Dohme Research Laboratories, Rahway, NJ 07065
	Chemistry Department, University of Houston, Houston, TX 77004
U.S.S.R.	Chemical Institute, U.S.S.R. Academy of Sciences, A. N. Nesmeyanov Institute of Organo-Element Chemistry of the U.S.S.R. Academy of Sciences, Vavilov St. 28, Moscow
	Institute of Chemical Technology, Dnepropetrovsk 5, Moscow
	N. D. Zelinsky Institute of Organic Chemistry, Academy of Sciences of the U.S.S.R., Moscow
	Institute of Organic Synthesis, Latvian S.S.R. Academy of Sciences, Riga
	Kuibyshev State University Chemical Department, Kuibyshev-86

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20. SUMMARY

GC retention data measured in various laboratories are given in many different forms and therefore their usefulness is limited. The retention index system according to Kováts solves the problem of the uniform expression of retention data.

In this review, the main theoretical and practical results relating to retention index systems published in the past 5 years are summarized.

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