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Temperature dependence of the retention index for perfumery compounds on a SE-30 glass capillary column I. Linear equations

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Abstract

The temperature dependence of the retention index was studied for about 340 perfumery compounds on an SE-30 glass capillary column within usual temperature ranges. Two linear equations, with column temperature and its reciprocal as variables, were comparatively reported. The first shows a slightly better precision and is more convenient for different applications, particularly for correlation with structure. © 1997 Elsevier Science B.V.

Keywords: Retention indices; Perfumery compounds

1. Introduction

Perfumes and essential oils are currently analysed on dimethylsilicone and Carbowax-20M capillary columns, under temperature-programmed conditions. Thus, the published specific [1–4] and more general [5] retention data libraries or software products, contain mainly temperature-programmed indices. According to Davies [3], Budahegyi and coworkers [6,7] and Evans and Haken [8], there are few sources of isothermal retention indices and studies on their temperature dependence for large groups of perfumery compounds; there are several studies for small groups, e.g., dimethylsilicones [9–13]. Recently the interest in this field has increased, in tandem with the development of methods for the precalculation of programmed temperature retention indices from isothermal data [14,15]. The importance of the temperature increment of the retention index in qualitative analysis is well known [6–8,16,17].

The linear equations for the dependence of the retention index against column temperature t, °C or $1/T$, K^{-1}:

$$I = a + bt \quad (1)$$

$$I = A + B/T \quad (2)$$

are valid for more or less extended temperature ranges and varieties of solutes and stationary phases [6,7,16]. Because $b = dI/dT$, Eq. (1) corresponds (as $10 \cdot dI/dT$) to the initially introduced Kováts [17] retention index increment per 10°C obtained by finite differences, $\delta I/10°C$. The comparative evaluation of the Eqs. (1) and (2) was only graphically considered in Ref. [16], concluding that the second equation is less linear than the first for larger temperature ranges. The complete equations with statistics, are seldom reported [18–23], with most authors only indicating the $\delta I/10°C$ or $10 \cdot dI/dT$ value. The above equations approximate narrower temperature range

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sections of a more general hyperbolic curve, which can be deduced theoretically [24].

This work tries to provide substantial experimental information as a support for future discussion on: the theory of the temperature dependence of the retention index; classification of the solutes for qualitative analysis; quantitative retention–structure relationships.

2. Experimental

An Erba Science Fractovap 4160 equipped with a flame ionisation detector (FID) and Minigrator integrator was used, with hydrogen (delivered by an Elhygen Milton Roy hydrogen generator) as carrier gas. The injector and detector temperatures were 250°C. The sampling was carried out in the split mode with 0.1 μl injections of 0.05–0.1% solutions, with 1:20 split ratio.

A glass capillary column of 40 m×0.35 mm I.D. with a film thickness of 0.35 μm, operated at gas linear velocity 50 cm/s, was used. The column was prepared from a soft glass capillary tube obtained with a Hewlett-Packard 1045A glass capillary drawing machine, acid leached, dried, HMDS-silylated [25,26] and coated using 0.4% SE-30 in *n*-pentane by the static method [26–28]. The column was tested with Grob test mixture at 120°C and in standardised temperature-programmed conditions [29]. The retention factors, retention indices, film thickness, 2,6-dimethyl aniline/2,6-dimethyl phenol ratio (DMA/DMP=1.1) were stable in time. At the end of measurements, there appeared to be a slight decrease in column efficiency from 2900 to 2500 theoretical plates per meter (methyl-undecanoate, $k=8.4$), and of TZ (Trennzahl) measured with methyl-alkanoates, from 36 to 31.

The *n*-alkanes C_6–C_{24} and many of the investigated compounds were from Fluka (Buchs, Switzerland). The other solutes were commercial samples from the main perfumery companies, with over 95% purity. Some of the reagents were well known [1,30] mixtures of isomers, indicated with numbers in the elution order, in Table 1.

Determination of the retention indices was done with a repeatability of 0.2–0.5 index units (i.u.), occasionally to 1 i.u. The logarithmic Kováts equation [17] was used, for the interpolation of the adjusted retention times of the solutes between those of the appropriate *n*-alkane pairs with z and $(z+1)$ carbon atoms. The dead time was calculated from the *n*-alkane retention times using a program [31] with a Hewlett-Packard 97 desk computer; over 140°C it was identical with the methane retention time. The regressions were calculated on a personal computer.

3. Results and discussion

Table 1 lists the parameters of Eqs. (1) and (2) and statistical data; they are respectively: r, R correlation coefficients; s, S standard deviations against the regression with $(n-2)$ degrees of freedom where n is the number of experimental points. The results are presented in the experimental retention index order at several temperature levels, to follow the volatility of solutes. Because of some non-uniformity of the temperature ranges, several retention indices are extrapolated values, generally using the hyperbolic equation (see Part 2). However, a number of compounds investigated in the 180–200°C range, but with the retention sequence in the 150°C group of solutes, can be found in the 180°C group.

No particular advantage of Eq. (2) results from the examination of correlation coefficients and standard deviations for the two linear equations. So, the mean standard deviations for the 339 solutes are: $s=1.01\pm0.75$ and $S=1.06\pm0.81$, compatible with the values from Refs. [16,18,21,32]. The standard deviation contains, in addition to the experimental errors, a systematic component due to the departure from the true hyperbolic curve. Most solutes were studied with only three points on a 20–40°C interval. However, the hyperbola can be applied for a part of the compound having more measured points, larger temperature range and the necessary precision (see Part 2). The use of hyperbola emphasises the contribution of systematic error. For instance, methyl salicylate, methyl acetate, vanillin and nerolidols show a drastically reduced standard deviation with the hyperbolic equation. Nevertheless, for many solutes, the precision of the three equations is practically the same on the investigated ranges. In contrast to Eq. (1), the numerical values of the

Table 1
The parameters: a, b; A, B, correlation coefficients: r, R and standard deviations with $(n-2)$ degrees of freedom: s, S, for the linear regressions, respectively by the Eq. (1) and Eq. (2)

No	Name	eI 100°C	Range °C	n	b	a	r^2	s	$-B$	A	R^2	S
1	2,3-Butandione	572.0	80–100	3	0.345	536.7	0.866	1.9	45170	692.2	0.855	2.0
2	2,3-Pentandione	662.0	80–100	3	−0.305	694.8		2.7	−39465	558.6		3.0
3	2,3-Hexandione	757.7	80–100	3	−0.080	766.2		1.1	−10371	730.4		1.2
4	3,4-Hexandione	773.4	80–100	3	−0.090	780.9	0.751	0.7	−11748	740.4	0.742	0.8
5	Ethyl n-butyrate	780.2	80–150	4	−0.018	783.5		1.2	−2900	773.9		1.2
6	3-Hexanol	780.2	80–100	3	0.010	779.1		0.3	1269	783.5		0.3
7	2-Hexanol	780.3	80–100	3	0.015	779.7		2.2	2297	787.4		2.2
8	trans-2-Hexenal	830.6	90–150	4	0.161	814.9	0.989	0.6	24888	897.7	0.980	0.7
9	cis-3-Hexen-1-ol	839.3	80–100	3	0.040	835.4	0.752	0.3	5318	853.7	0.760	0.3
10	n-Hexanol	848.2	80–150	6	−0.262	873.5	0.967	1.4	−38852	742.9	0.948	1.7
11	Isoamyl acetate	857.8	80–150	4	−0.215	877.6	0.969	1.5	−32239	769.4	0.951	1.8
12	Anisole	901.9	80–100	3	0.185	883.8	0.876	1.0	24525	968.0	0.878	1.0
13	Ethyl acetoacetate	903.0	80–100	3	−0.070	910.1	0.942	0.2	−9186	878.5	0.935	0.3
14	Benzaldehyde	939.3	90–150	6	0.347	904.1	0.992	0.8	53353	1081.9	0.992	0.8
15	α-Pinene	940.9	80–110	4	0.339	907.8	0.938	1.4	45702	1064.3	0.924	1.5
16	n-Heptanol	951.6	90–150	6	−0.053	956.4	0.820	1.6	−8062	929.5	0.811	1.8
17	Camphene	957.1	70–140	5	0.479	909.8	0.990	1.5	67561	1139.6	0.983	2.0
18	1-Octene-3-ol	963.2	80–120	5	−0.050	967.5	0.630	0.7	−6799	944.3	0.604	0.7
19	6-Methyl-5-heptene-2-one	963.9	80–130	4	0.094	954.9	0.934	0.6	13402	1000.4	0.917	0.7
20	cis-3-Hexenyl acetate	976.4	90–160	4	0.208	956.3	0.991	0.8	32692	1064.8	0.991	0.8
21	2-Octanol	976.7	100–130	4	0.350	941.6	0.993	0.5	52632	1117.5	0.992	0.5
22	β-Pinene	980.3	90–110	3	0.390	942.2	0.959	1.1	54081	1126.2	0.952	1.2
23	n-Octanal	981.8	90–150	3	0.010	980.8	0.998	0.0	1549	986.0	0.999	0.0
24	Diethylene glycol monoethyl ether	982.9	140–150	2	−0.020	985.6			−3497	947.3		
25	β-Myrcene	983.2	90–110	3	−0.055	988.9	0.881	0.3	−7695	962.8	0.891	0.3
26	p-Cresol methyl ether	986.6	80–110	3	0.376	949.0	0.998	0.3	51072	1123.6	0.996	0.5
27	Dipropylene glycol 1	989.7	90–140	3	−0.019	993.6	0.812	0.4	−2922	983.9	0.800	0.4
28	trans-2-Hexenyl acetate	991.4	80–150	7	−0.164	1007.6	0.985	0.5	−24245	926.1	0.970	0.8
29	n-Hexyl acetate	993.1	80–150	5	−0.089	1001.9	0.994	0.2	−13419	956.9	0.996	0.2
30	2,6-Dimethyl-hepten-1-ol-6	995.7	90–140	4	0.177	978.3	0.895	1.7	26248	1066.4	0.873	1.8
31	α-Phellandrene	1001.4	70–110	4	0.181	982.9	0.941	1.0	23822	1064.9	0.953	0.8
32	2-Carene	1001.6	70–150	5	0.346	967.8	0.996	0.6	50557	1138.6	0.987	0.8
33	Benzyl alcohol	1006.8	100–150	5	0.286	977.3	0.969	1.2	44975	1126.2	0.957	1.4
34	Δ-3-Carene	1011.0	90–110	3	0.215	989.9	0.979	0.5	29842	1091.4	0.974	0.5
35	2,6-Dimethyl-hepten-5-ol-1	1011.8	120–150	3	0.121	997.0	0.702	1.7	19891	1062.1	0.685	1.8
36	Phenylacetaldehyde	1014.1	100–130	3	0.271	986.7	0.945	1.4	40380	1121.9	0.936	1.5
37	Dipropylene glycol 2	1014.3	90–140	3	−0.034	1016.2		2.4	−5372	998.4		2.3
38	α-Terpinene	1015.5	90–110	3	0.180	997.0	0.952	0.6	25128	1082.4	0.958	0.5
39	p-Cymene	1017.0	90–150	4	0.247	992.2	0.994	0.6	38259	1119.6	0.990	0.8
40	1,4-Cineole	1018.9	120–150	3	0.186	998.5	0.990	0.4	30844	1099.3	0.986	0.5
41	1,8-Cineole	1025.5	110–150	4	0.455	979.4	0.997	0.6	73798	1221.8	0.997	0.6
42	Limonene	1027.1	90–150	6	0.311	996.3	0.995	0.6	47448	1154.6	0.990	0.8
43	Diethyl malonate	1033.3	80–150	4	−0.224	1055.1	0.991	0.8	−33291	943.2	0.980	1.2
44	n-Amyl isobutyrate	1038.1	80–140	4	−0.056	1043.6	0.986	0.2	−8142	1016.1	0.974	0.3
45	Acetophenone	1038.4	80–100	3	0.275	1010.9	0.999	0.1	36214	1135.4	0.998	0.2
46	Isoamyl n-butyrate	1039.4	80–140	4	−0.111	1050.9	0.931	1.0	−16376	995.7	0.938	0.9
47	γ-Terpinene	1052.4	90–110	3	0.290	1023.6	0.996	0.2	40306	1160.7	0.994	0.3
48	Dihydromyrcenol	1053.3	120–150	3	0.248	1027.3	0.998	0.2	41047	1161.4	0.996	0.3
49	n-Octanol	1053.9 120°	110–130	3	−0.070	1060.5	0.993	0.1	−10824	1024.5	0.995	0.1
50	Guaiacol	1066.8	120–150	3	0.474	1010.0	1.000	0.0	79037	1267.7	1.000	0.2
51	Linalool oxide 1	1067.5	110–150	5	0.323	1028.8	0.959	1.2	52254	1200.6	0.955	1.3
52	Dehydrolinalool	1068.4	120–150	3	0.156	1049.8	0.994	0.3	25845	1134.2	0.996	0.2

Table 1. Continued

No	Name	eI 100°C	Range °C	n	b	a	r^2	s	−B	A	R^2	S
53	Methyl benzoate	1077.8	110–130	3	0.325	1038.5	0.994	0.4	50252	1205.4	0.996	0.3
54	Methyl nor-bornenyl cetone	1078.0	100–130	3	0.426	1026.7	0.956	2.0	64530	1242.1	0.963	1.8
55	Linalool oxide 2	1080.6	110–150	5	0.321	1041.9	0.942	1.3	50602	1209.2	0.934	1.5
56	2-Phenylpropanal	1083.9	120–150	4	0.327	1044.5	0.897	1.8	54385	1222.0	0.896	1.8
57	Fenchone	1084.1	110–150	4	0.463	1028.0	0.993	0.8	74896	1274.2	0.997	0.5
58	Thujone 1	1085.1	110–150	5	0.840	984.7	0.977	2.3	135765	1431.1	0.970	2.5
59	n-Nonanal	1085.4	100–150	6	0.164	1065.7	0.651	2.5	25835	1151.2	0.650	2.5
60	Linalool	1085.8	110–150	5	0.161	1066.5	0.906	1.0	26329	1152.8	0.922	0.9
61	Tetrahydromyrcenol	1088.6	90–150	4	0.124	1074.3	0.932	1.1	18777	1137.1	0.915	1.2
62	Tetrahydrolinalool	1088.9	90–150	4	0.143	1071.8	0.993	0.4	21902	1144.9	0.993	0.4
63	Isoamyl 2-methyl butyrate	1089.3	110–150	5	0.093	1078.4		1.6	14733	1127.0		1.6
64	1-Octene-3-yl-acetate	1089.5	90–120	4	−0.174	1110.3	0.995	0.2	−24833	1026.3	0.995	0.2
65	Isoamyl isovalerate	1090.7	110–150	5	0.060	1083.1		1.7	9359	1114.1		1.7
66	Phenylethyl alcohol	1092.0	80–150	6	0.328	1053.4	0.989	1.1	48815	1217.5	0.982	1.4
67	Maltol	1092.2	130–150	3	0.145	1074.8	0.875	0.8	24602	1154.7	0.865	0.8
68	Benzyl cyanide	1097.5	120–150	3	0.350	1056.5	0.942	1.9	58684	1247.7	0.951	1.7
69	Thujone 2	1100.2	110–150	5	0.691	1017.7	0.971	2.2	111670	1384.8	0.965	2.4
70	α-Fenchyl alcohol	1111.9	110–140	4	0.548	1046.3	0.958	1.8	86776	1332.9	0.958	1.8
71	Dihydrolinalool	1119.9	120–150	3	0.224	1093.0	0.995	0.3	37008	1213.9	0.992	0.4
72	Isocyclocitral 1	1119.9	120–150	3	0.364	1076.5	0.976	1.2	60547	1274.2	0.981	1.1
73	p-Tolylacetaldehyde	1119.9	120–150	3	0.306	1084.3	0.895	2.3	51469	1251.9	0.906	2.1
74	trans,trans-Alloocimene	1121.0	120–150	3	0.112	1107.6	0.995	0.2	18620	1168.4	0.994	0.2
75	Ethyl-2-methyl-1,3-dioxolane-2-acetate	1123.1	120–150	3	0.209	1097.7	0.996	0.3	34889	1211.5	0.993	0.4
76	Guethol	1127.8	120–150	3	0.331	1088.5	0.991	0.7	55293	1268.7	0.994	0.5
77	3-Phenylpropanal	1132.0	120–150	4	0.330	1094.2	0.788	2.7	55500	1274.8	0.798	2.6
78	Benzyl acetate	1135.1	120–180	5	0.326	1095.6	0.987	1.0	57506	1280.7	0.981	1.2
79	Neoalloocimene	1135.0	120–150	3	0.131	1119.1	0.959	0.6	21703	1190.0	0.960	0.7
80	Camphor	1135.1	110–150	5	0.671	1054.8	0.998	0.6	108665	1411.9	0.996	0.8
81	Citronellal	1135.2	100–150	5	0.091	1124.9		1.8	15211	1174.5		1.5
82	Ethynyl cyclohexyl acetate	1136.7	120–160	4	0.214	1110.3	0.919	1.3	36426	1228.5	0.913	1.4
83	Dimethyl benzyl carbinol	1140.9	120–150	3	0.301	1105.2	0.979	1.0	50447	1269.7	0.984	0.8
84	Isocyclocitral 2	1141.8	120–150	3	0.331	1102.3	0.984	0.9	55057	1282.0	0.988	0.8
85	p-Cresyl acetate	1142.4	120–170	4	0.525	1077.4	0.946	3.2	90482	1370.3	0.926	3.7
86	Menthone	1142.7	120–150	4	0.469	1088.4	0.893	2.5	78580	1344.3	0.906	2.4
87	1,4-Dimethoxybenzene	1143.4	130–150	3	0.105	1128.2	0.714	0.9	18068	1186.7	0.727	0.9
88	Tetrahydrolavandulol	1145.9	120–150	4	0.165	1126.5	0.828	1.2	27625	1216.5	0.838	1.2
89	Ethyl benzoate	1148.7	110–150	3	0.463	1094.3	0.951	3.0	74438	1339.4	0.938	3.4
90	Neomenthol	1152.8	110–150	5	0.526	1090.0	0.978	1.4	85399	1370.4	0.974	1.6
91	Isomenthone	1152.9	120–150	4	0.424	1103.2	0.950	1.5	70844	1334.1	0.958	1.4
92	n-Nonanol	1153.6	120–150	4	0.088	1143.1		2.6	14904	1191.5		2.6
93	Isoborneol	1154.6	110–150	5	0.536	1089.9	0.980	1.4	87016	1375.6	0.982	1.3
94	3,7-Dimethyl octanal	1156.0										
95	Menthofuran	1157.9	120–150	3	0.393	1110.5	0.991	0.8	65003	1323.0	0.987	1.0
96	p-Methyl acetophenone	1161.0	120–150	3	0.455	1106.8	0.997	0.6	76022	1354.7	0.999	0.4
97	3,5,5-Trimethyl hexyl acetate	1161.7	120–180	5	0.185	1139.0	0.982	0.7	32701	1244.3	0.977	0.9
98	Borneol	1162.6	110–150	5	0.474	1104.8	0.992	0.6	77166	1358.1	0.993	0.5
99	n-Octanal dimethyl acetal	1162.8	100–130	4	−0.056	1170.7		1.0	−8605	1142.1		1.0
100	Menthol	1166.6	110–150	4	0.356	1122.4	0.956	1.6	58203	1313.2	0.966	1.4
101	Methyl heptyn carbonate	1166.6	130–180	3	0.215	1139.9	0.965	1.5	38912	1264.4	0.952	1.7
102	Styrallyl acetate	1166.7	120–160	4	0.110	1154.3	0.883	0.9	18868	1215.4	0.895	0.8

Table 1. Continued

No	Name	*eI* 100°C	Range °C	*n*	*b*	*a*	r^2	*s*	$-B$	*A*	R^2	*S*
103	Ethyl linalool 1	1168.9	120–150	3	0.202	1144.6	0.999	0.1	33485	1254.0	0.998	0.2
104	Terpinene-4-ol	1169.6	110–150	4	0.434	1118.2	0.984	1.3	70171	1348.9	0.978	1.5
105	Methyl salicylate	1176.5	120–180	4	0.517	1113.1	0.980	2.2	90865	1406.0	0.966	3.0
106	Carvomenthone 1	1178.0	110–150	4	0.346	1137.0	0.996	0.5	56068	1321.3	0.992	0.7
107	α-Terpineol	1179.3	110–140	4	0.411	1130.3	0.990	0.7	64950	1344.9	0.987	0.8
108	Estragole	1180.7	110–150	5	0.341	1139.4	0.993	0.7	55372	1321.2	0.995	0.5
109	Tetrahydrogeraniol	1180.7	100–150	5	0.103	1168.9	0.682	1.6	15926	1221.8	0.659	1.6
110	Myrtenal	1181.3	110–150	5	0.532	1117.7	0.981	1.4	86049	1400.5	0.976	1.5
111	Dihydrocarveol	1181.5	110–150	4	0.434	1129.5	0.968	1.8	70394	1360.8	0.968	1.8
112	Ethyl linalool 2	1181.8	120–150	3	0.181	1160.0	0.997	0.1	30041	1258.1	0.995	0.2
113	γ-Terpineol	1185.4	110–150	5	0.349	1143.7	0.994	0.5	56495	1329.3	0.991	0.6
114	n-Decanal	1185.8	80–150	8	0.083	1175.8	0.779	1.2	12440	1217.5	0.788	1.1
115	Myrtenol	1185.8	110–160	4	0.482	1127.9	0.994	1.1	79971	1389.4	0.991	1.3
116	Carvomenthone 2	1185.9	110–150	4	0.293	1150.3	0.954	1.3	47860	1307.2	0.963	1.2
117	Verbenone	1190.9	100–160	5	0.516	1131.3	0.951	3.5	83180	1405.4	0.936	4.0
118	n-Octyl acetate	1191.9	120–160	5	−0.100	1204.0	0.985	0.2	−16973	1148.9	0.979	0.3
119	Bromstyrene	1194.5	120–150	3	0.532	1130.5	1.000	0.2	88783	1420.1	0.998	0.5
120	2-Geranonitrile 1	1196.4	120–150	3	0.253	1166.5	0.979	0.8	42317	1304.4	0.984	0.7
121	Phenylacetaldehyde dimethyl acetal	1197.5	120–150	3	0.296	1161.7	0.997	0.4	49426	1323.0	0.995	0.5
122	Linalyl formate	1201.7	120–180	3	0.271	1169.0	0.993	1.0	47726	1322.8	0.985	1.4
123	trans-Carveol	1202.6	110–150	4	0.405	1153.8	0.983	1.1	65902	1370.1	0.984	1.1
124	3-Phenylpropyl alcohol	1203.0	110–150	4	0.333	1162.7	0.994	0.4	55291	1343.2	0.990	0.5
125	β-Citronellol	1209.8	110–150	5	0.041	1204.8	0.858	0.3	6631	1226.6	0.850	0.3
126	Nerol	1211.6	110–150	5	0.142	1194.6	0.755	1.5	23214	1270.7	0.768	1.4
127	Allyl amyl glycolate	1212.8	120–180	4	0.082	1199.9		3.3	13961	1245.3		3.4
128	cis-Carveol	1213.5	110–150	4	0.424	1162.4	0.975	1.4	69057	1389.1	0.976	1.4
129	Cuminaldehyde	1218.0	110–150	5	0.475	1161.1	0.981	1.2	76990	1414.1	0.981	1.4
130	Pulegone	1220.1	120–150	3	0.543	1154.8	0.999	0.4	89916	1448.6	0.997	0.6
131	p-Anisaldehyde	1220.4	120–150	4	0.460	1165.3	0.990	0.7	76582	1415.1	0.992	0.7
132	Neral	1220.4	110–150	4	0.138	1204.1	0.977	0.4	22335	1277.5	0.985	0.4
133	Tetrahydrolinalyl acetate	1221.1	120–180	3	0.114	1207.2	0.988	0.5	20130	1272.1	0.989	0.7
134	Carvone	1225.8	130–150	3	0.280	1191.3	0.996	0.2	47718	1346.0	0.994	0.3
135	β-Phenylethyl acetate	1228.2	120–160	3	0.225	1200.9	0.947	1.6	37862	1324.2	0.938	1.7
136	2-Geranonitrile 2	1228.3	120–150	3	0.222	1202.3	0.936	1.3	37256	1323.7	0.945	1.2
137	Benzyl n-propionate	1230.4	130–180	3	0.358	1183.6	0.948	3.0	65018	1391.2	0.933	3.4
138	Geraniol	1233.2	110–150	3	0.143	1216.7	0.963	0.8	23232	1293.0	0.955	0.9
139	Piperitone	1233.3	110–150	5	0.481	1175.2	0.982	1.2	78133	1431.8	0.986	1.1
140	trans-Cinnamic aldehyde	1235.1	120–150	4	0.495	1175.9	0.953	1.7	82521	1445.0	0.957	1.7
141	Carvenone	1236.2	110–150	4	0.605	1163.9	0.996	0.8	98175	1486.4	0.992	1.2
142	Methyl benzyl acetate 1	1237.2	120–180	5	0.300	1200.2	0.971	1.4	52837	1370.3	0.956	1.8
143	Linalyl acetate	1239.7	110–150	5	0.030	1236.3		1.3	4845	1252.3		1.3
144	Methyl benzyl acetate 2	1240.1	120–180	5	0.247	1209.4	0.948	1.6	43416	1349.3	0.928	1.9
145	Myrtenyl acetate	1243.0	130–150	3	0.145	1224.9	0.918	0.6	24629	1304.8	0.910	0.6
146	9-Decen-1-ol	1243.9	110–150	4	−0.045	1250.0		2.1	−7199	1226.2		2.0
147	Geranial	1246.8	110–150	4	0.100	1234.9	0.988	0.2	16144	1288.1	0.981	0.3
148	Anis alcohol	1246.8	110–150	3	0.352	1204.4	0.996	0.3	58295	1394.9	0.993	0.4
149	Ethyl salicylate	1249.1	120–180	4	0.458	1193.7	0.979	2.0	80986	1454.3	0.976	2.2
150	Tetrahydrolavandulyl acetate	1254.3	120–160	4	0.020	1252.0		0.8	3527	1263.3		0.8
151	Hydroxycitronellal	1255.2	120–150	3	0.134	1239.1	0.999	0.1	22272	1311.9	1.000	0.1
152	Citronellyl formate	1255.6	120–180	3	0.206	1232.0	0.983	1.2	36356	1349.2	0.977	1.4

Table 1. Continued

No	Name	eI 100°C	Range °C	n	b	a	r^2	s	−B	A	R^2	S
153	n-Decanol	1255.7	120–150	4	−0.010	1256.8		0.5	−1374	1253.3		0.5
154	Indole	1255.9	110–150	3	0.285	1222.2	0.971	1.4	45944	1373.4	0.961	1.6
155	Safrole	1264.5	120–150	3	0.489	1205.8	1.000	0.2	81514	1471.6	0.999	0.4
156	Thymol	1265.1	120–150	4	0.053	1259.2		0.8	8875	1288.1		0.8
157	trans-Anethole	1265.2	120–150	4	0.377	1218.9	0.840	2.6	62554	1423.1	0.836	2.6
158	β-Terpinyl acetate	1267.2	120–150	4	0.256	1237.7	0.866	1.6	42935	1377.5	0.880	1.5
159	Menthanyl acetate 1	1268.3	120–150	3	0.343	1227.8	0.975	1.2	57392	1414.8	0.981	1.0
160	Dimethyl phenylethyl carbinol	1270.5	120–150	3	0.345	1228.6	0.984	0.9	57449	1416.1	0.980	1.1
161	trans-Cinnamyl alcohol	1271.8	120–150	4	0.366	1227.8	0.982	0.8	60817	1426.3	0.980	0.8
162	Carvacrol	1273.8	110–150	4	0.115	1260.6	0.940	0.8	18663	1321.8	0.929	1.0
163	2-Methyl decanal	1274.0										
164	Bornyl acetate	1275.2	110–150	5	0.460	1219.6	0.943	2.1	74804	1465.2	0.948	2.0
165	Isobornyl acetate	1275.2	120–150	4	0.448	1221.9	0.983	0.9	74640	1465.4	0.986	0.8
166	Phenylacetaldehyde ethylene glycol acetal	1276.9	130–150	3	0.460	1221.7	0.992	0.6	78558	1476.3	0.995	0.5
167	Dihydrocuminalcohol	1277.0	120–150	3	0.399	1228.8	0.978	1.3	65884	1444.2	0.973	1.4
168	10-Undecen-1-al	1277.2	140–160	3	0.265	1241.2	0.950	0.9	47269	1392.6	0.944	0.9
169	n-Undecanal	1278.5	120–150	4	0.104	1265.5		2.1	17354	1322.0		2.1
170	Terpinhydrate	1279.0	130–150	3	0.450	1224.7	0.992	0.6	76852	1473.8	0.994	0.5
171	Menthyl acetate	1279.2	110–150	4	0.219	1253.2	0.966	0.9	35432	1369.7	0.955	1.0
172	Geranyl formate	1281.6	120–180	4	0.186	1258.3	0.799	3.0	32479	1363.3	0.779	3.2
173	2-tert-Butylcyclohexyl acetate 1	1281.6	120–160	4	0.390	1234.6	0.960	1.8	66095	1449.4	0.950	2.0
174	p-Cresyl isobutyrate	1289.1	120–180	4	0.239	1259.3	0.938	1.6	41741	1394.0	0.916	1.9
175	Menthanyl acetate 2	1289.3	120–150	4	0.351	1246.5	0.958	1.2	58174	1436.5	0.951	1.2
176	n-Nonyl acetate	1291.7	120–180	6	0.014	1289.6		1.6	2343	1297.3		1.6
177	Heliotropine	1292.2	120–150	3	0.578	1223.1	0.995	0.9	95897	1536.3	0.997	0.7
178	Dimethyl benzyl carbinyl acetate	1297.5	130–180	5	0.402	1247.1	0.994	0.7	73258	1480.8	0.991	0.8
179	Neral dimethyl acetal	1300.4	120–150	3	0.076	1291.2	1.000	0.0	12761	1332.9	1.000	0.0
180	Menthanyl acetate 3	1304.0	120–150	4	0.378	1257.2	0.872	2.3	62447	1461.3	0.860	2.4
181	2-tert-Butylcyclohexyl acetate 2	1305.5	120–160	4	0.139	1288.8	0.826	1.8	24621	1367.9	0.826	1.8
182	Methyl anthranilate	1306.3	120–180	4	0.489	1247.2	0.997	0.8	86383	1525.3	0.990	1.5
183	Tetrahydrogeranyl acetate	1313.7	120–150	3	−0.070	1321.9	0.942	0.4	−11737	1283.7	0.951	0.4
184	Benzyl n-butyrate	1315.8	120–180	4	0.297	1279.3	0.971	1.6	52174	1447.5	0.954	2.0
185	4-tert-Butylcyclohexyl acetate 1	1315.8	130–180	5	0.420	1265.4	0.956	2.0	76656	1509.8	0.959	1.9
186	Menthanyl acetate 4	1316.4	120–150	4	0.421	1265.7	0.998	0.5	70154	1494.5	0.995	0.6
187	Ethyl linalyl acetate 1	1316.5	120–180	5	0.021	1313.7		0.8	3891	1325.8		0.8
188	γ-Nonalactone	1320.3	120–150	3	0.433	1267.9	0.973	1.6	71530	1501.8	0.967	1.7
189	p-Methyl quinoline	1320.9	120–150	3	0.684	1238.7	0.999	0.4	114034	1610.6	0.998	0.7
190	Linalyl n-propionate	1321.4	120–170	4	0.068	1312.8	0.785	0.9	11549	1350.3	0.760	1.0
191	Benzylidene acetate	1322.3	130–170	4	0.506	1257.8	0.958	2.2	89565	1545.7	0.946	2.5
192	Geranial dimethyl acetal	1322.6	120–150	3	0.094	1311.4	0.997	0.1	15721	1362.5	0.995	0.1
193	Eugenol	1327.7	110–150	5	0.340	1286.9	0.992	0.6	55236	1468.3	0.996	0.4
194	Hydroxycitronellol	1329.5	120–150	3	0.147	1311.6	0.898	1.1	24241	1390.9	0.887	1.1
195	p-tert-Amyl cyclohexanone	1331.5	140–170	4	0.878	1213.3	0.956	3.0	160114	1723.6	0.948	3.2
196	Dihydrogeranyl acetate	1332.2	120–160	4	−0.043	1337.6	0.678	0.7	−73741	313.7	0.687	0.7
197	α-Terpinyl acetate	1332.3	120–150	4	0.233	1305.4	0.885	1.3	39038	1432.5	0.897	1.3
198	Ethyl linalyl acetate 2	1333.9	120–180	5	−0.009	1335.7		1.6	−1316	1331.2		1.6
199	Citronellyl acetate	1335.0	120–150	4	−0.028	1338.1		0.4	−4723	1322.7		0.4
200	Neryl acetate	1342.2	120–160	5	0.019	1340.1		2.2	3707	1351.7		2.3
201	Skatole	1343.0	120–150	3	0.542	1277.8	1.000	0.2	90452	1572.8	0.998	0.5
202	10-Undecen-1-ol	1345.2	120–150	4	0.051	1338.7		0.7	8918	1367.5		0.8

Table 1. Continued

No	Name	eI 100°C	Range °C	n	b	a	r^2	s	−B	A	R^2	S
203	Vanillin	1347.9	120–200	4	0.521	1285.0	0.996	1.5	95409	1590.0	0.990	2.3
204	2-Methylundecanal	1349.8	120–150	4	0.107	1335.9	0.916	0.5	17883	1394.2	0.925	0.5
205	4-tert-Butylcyclohexyl acetate 2	1352.0 150°	130–180	5	0.442	1297.0	0.980	1.5	80781	1554.5	0.973	1.8
206	n-Undecanol	1356.4	120–150	3	0.008	1355.0		0.9	1185	1359.0		0.9
207	Geranyl acetate	1359.7	120–150	4	−0.043	1365.9	0.779	0.4	−7225	1342.4	0.794	0.4
208	Linalyl isobutyrate	1361.7	120–150	4	0.122	1345.2	0.881	0.7	20127	1411.0	0.866	0.8
209	Dihydrojasmone	1362.4	120–150	3	0.324	1314.1	0.997	0.4	53685	1489.4	0.998	0.3
210	trans-Jasmone	1363.9	120–150	3	0.324	1315.5	0.979	1.0	54270	1492.4	0.984	0.9
211	Phenylethyl isobutyrate	1375.3	120–180	5	0.358	1322.6	0.950	2.2	63047	1525.8	0.937	2.5
212	cis-Jasmone	1376.3	120–150	3	0.426	1312.4	0.998	0.4	71230	1544.7	0.999	0.2
213	9-Decen-1-yl acetate	1378.6	150–180	3	−0.059	1387.4		1.9	−9428	1563.5		1.9
214	Anisyl acetate	1382.5	150–180	4	0.368	1327.2	0.996	0.3	70751	1549.5	0.996	0.3
215	Isoamyl phenylethyl ether	1382.8	120–150	3	0.307	1336.7	1.000	0.1	51256	1503.9	0.999	0.2
216	Diphenyl oxide	1389.9	140–160	3	1.030	1236.0	0.996	0.9	184144	1825.9	0.994	1.1
217	Hexahydropseudo-ionone	1389.8	140–160	3	0.165	1365.2	0.997	0.1	29502	1459.6	0.996	0.2
218	n-Dodecanal	1390.1	140–170	3	0.165	1366.1	0.881	0.9	29376	1460.2	0.872	0.9
219	n-Decyl acetate	1391.3	130–190	6	−0.030	1396.0		0.7	−5461	1378.5		0.7
220	Longicyclene	1399.1	140–160	3	1.050	1241.0	0.999	0.5	187962	1843.0	1.000	0.1
221	β-Terpinyl isobutyrate	1402.4	120–150	4	0.322	1354.4	0.993	0.4	53632	1529.4	0.995	0.4
222	Coumarin	1404.9	120–150	4	0.766	1289.8	0.977	1.9	127386	1705.5	0.976	1.9
223	Tetrahydro-para-methylquinoline	1405.7	120–150	3	0.662	1306.3	1.000	0.1	109727	1664.8	0.999	0.4
224	Dihydro-nor-dicyclopentadienyl acetate	1406.7	150–180	4	0.705	1300.2	0.988	1.2	134897	1724.5	0.984	1.4
225	Allyl-3-cyclohexyl propionate	1406.7	150–190	5	0.394	1347.4	0.994	0.6	77170	1588.7	0.992	0.6
226	Linalyl n-butyrate	1408.2	120–150	4	0.119	1390.4	0.988	0.2	19831	1455.1	0.991	0.2
227	Geranylacetone 1	1412.0	130–160	3	0.140	1391.9	0.879	1.1	24201	1470.1	0.867	1.2
228	Ethyl methylphenyl glycidate 1	1412.9	120–140	3	0.550	1330.4	0.996	0.5	89403	1623.8	0.998	0.4
229	Nopyl acetate	1413.1	130–180	4	0.575	1327.8	0.990	1.5	104583	1661.7	0.981	2.0
230	Cinnamyl acetate	1413.2	150–190	5	0.236	1377.6	0.957	0.9	46195	1522.1	0.955	0.9
231	Hydroxycitronellal dimethyl acetal	1413.7	120–190	4	0.145	1395.0	0.824	2.4	25995	1478.4	0.792	2.8
232	Diphenyl methane	1414.6	160–220	4	0.597	1326.1	0.999	0.4	122020	1703.1	1.000	0.1
233	α-Ionone	1414.9	120–150	3	0.379	1357.8	0.997	0.5	62801	1563.0	0.995	0.6
234	Isoamyl benzoate	1418.2	150–190	4	0.543	1335.7	0.988	1.3	106499	1668.7	0.982	1.6
235	cis-Methylisoeugenol	1422.0	130–160	3	0.149	1400.0	0.981	0.5	25911	1483.6	0.975	0.5
236	Dimethyl phenylethyl carbinyl acetate	1423.7	150–180	4	0.493	1349.6	0.994	0.6	94360	1646.4	0.990	0.8
237	Tetrahydroionol 1	1424.0	140–160	3	0.550	1341.1	1.000	0.1	91503	1639.8	1.000	0.1
238	Citronellyl propionate	1424.7	150–180	4	0.112	1407.3	0.684	1.2	21405	1474.6	0.680	1.2
239	Longifolene	1427.0	110–160	4	0.896	1292.2	0.999	0.9	148772	1778.6	1.000	0.1
240	Tetrahydroionone	1427.1	140–160	3	0.570	1342.3	0.988	0.9	101836	1668.6	0.985	1.0
241	Dihydro-β-ionone	1427.8	140–160	3	0.475	1356.8	0.998	0.3	84943	1628.8	0.997	0.4
242	Geranyl acetone 2	1430.0	130–160	3	0.161	1406.6	0.929	1.0	27952	1496.9	0.920	1.0
243	2-n-Heptyl-cyclopentanone	1430.7	130–160	3	0.352	1378.3	0.996	0.5	61198	1575.8	0.993	0.6
244	γ-Decalactone	1431.4	140–190	3	0.481	1359.3	1.000	0.1	92701	1650.9	0.999	0.5
245	trans-β-Cariophyllene	1432.6	120–150	4	0.688	1329.6	0.996	0.7	114440	1703.1	0.996	0.7
246	Tetrahydroionol 2	1432.8	140–160	3	0.590	1344.8	0.995	0.6	105472	1682.6	0.993	0.7
247	Methyl-β-naphtyl ether	1433.2	130–180	4	0.715	1325.5	0.999	0.7	131173	1743.6	1.000	0.1
248	α-Cedrene	1433.4	130–160	4	1.013	1282.0	0.994	1.2	176550	1851.4	0.990	1.4
249	trans-Isoeugenol	1436.4	170–200	3	0.449	1360.4	0.936	2.5	94075	1649.0	0.928	2.7
250	p-Isopropyl-α-methyl hydrocinnamic aldehyde	1436.5	130–150	3	0.435	1371.5	0.990	0.6	74300	1612.3	0.993	0.5
251	Ethyl cinnamate	1437.2	150–190	5	0.525	1358.2	0.997	0.5	102981	1680.1	0.999	0.3
252	Thujopsene	1446.8	140–160	3	0.810	1325.0	0.999	0.4	145005	1789.3	1.000	0.1

Table 1. Continued

No	Name	eI 100°C	Range °C	n	b	a	r^2	s	−B	A	R^2	S
253	Geranyl n-propionate	1449.8	150–170	3	0.035	1445.3		1.8	6872	1466.7		1.8
254	Aromadendrene	1453.6	140–160	3	0.905	1318.6	0.996	0.9	161785	1836.8	0.994	1.0
255	n-Butyl salicylate	1454.8	150–180	3	0.469	1385.0	0.992	0.9	90262	1668.5	0.995	0.7
256	n-Dodecanol	1456.6	130–150	3	0.000	1456.6		0.1	13	1456.7		0.1
257	p-Ethyl-α_α-dimethyl hydrocinnamic aldehyde	1456.8	120–150	3	0.430	1392.3	1.000	0.0	71769	1626.4	1.000	0.2
258	trans-Methylisoeugenol	1461.8	130–160	3	0.179	1435.3	0.986	0.5	31130	1535.8	0.982	0.5
259	Anisyl acetone	1462.0	160–200	4	0.449	1393.1	0.973	1.6	91626	1676.4	0.969	1.7
260	α-Terpinyl isobutyrate	1462.4	120–150	4	0.279	1421.1	0.977	0.7	46555	1572.9	0.983	0.6
261	α-Humulene	1464.4	140–160	3	0.770	1348.4	0.997	0.6	137875	1789.9	0.999	0.3
262	β-Ionone	1470.1	120–150	3	0.426	1405.6	0.982	1.2	70390	1635.7	0.977	1.4
263	α-Isomethylionone	1471.8	120–150	3	0.480	1399.6	0.999	0.4	79505	1659.4	0.997	0.6
264	γ-Gurjunene	1482.1	140–160	3	0.675	1379.1	0.951	2.2	121152	1766.7	0.963	1.9
265	Phenoxyethyl isobutyrate	1482.5	150–180	4	0.415	1420.3	1.000	0.1	79546	1670.4	0.999	0.2
266	Myrac aldehyde 1	1490.8	120–150	3	0.427	1427.0	0.998	0.4	70855	1658.4	0.999	0.3
267	γ-Cadinene	1496.6	120–150	4	0.762	1381.6	0.995	0.9	126550	1794.8	0.993	1.1
268	Myrac aldehyde 2	1497.3	120–150	3	0.440	1431.9	0.986	1.1	73081	1670.5	0.990	1.0
269	Dihydro-nor-dicyclopentadienyl propionate	1498.6	150–190	5	0.597	1408.8	0.990	1.1	116921	1774.4	0.989	1.2
270	4-tert-Butyl-α-methyl hydrocinnamic aldehyde	1500.0	120–150	3	0.455	1432.3	0.991	0.9	75542	1678.9	0.994	0.8
271	Ethyl methylphenyl glycidate 2	1500.5	120–140	3	0.495	1426.2	0.990	0.7	80504	1690.3	0.993	0.6
272	Ledene	1501.0	120–160	4	0.610	1409.6	0.990	1.3	103517	1746.0	0.990	1.2
273	α-n-Methylionone	1503.2	120–150	3	0.394	1444.2	1.000	0.0	65235	1657.3	1.000	0.1
274	Pseudoionone 1	1507.9	120–150	3	0.301	1462.6	0.998	0.3	49801	1625.4	0.996	0.4
275	Isoamyl salicylate	1515.4	150–180	4	0.613	1423.3	1.000	0.2	117468	1792.7	0.999	0.4
276	cis-Nerolidol	1517.1	120–160	4	0.199	1487.9	0.929	1.2	33461	1596.8	0.913	1.3
277	γ-Undecalactone	1532.6	140–180	4	0.427	1469.0	0.982	1.2	79937	1722.1	0.974	1.4
278	trans-Nerolidol	1546.4	120–160	4	0.200	1517.0	0.924	1.2	33649	1626.6	0.909	1.3
279	cis-3-Hexenyl benzoate	1550.1	150–180	3	0.305	1504.3	0.999	0.1	54595	1679.1	1.000	0.1
280	Diethyl phtalate	1551.1	160–200	5	0.350	1498.6	0.989	0.7	71905	1720.5	0.994	0.5
281	n-Amyl salicylate	1552.0	150–180	4	0.550	1469.6	0.998	0.4	105488	1801.2	0.999	0.3
282	β-n-Methylionone	1556.8	120–150	3	0.422	1493.6	0.999	0.2	70001	1722.3	1.000	0.1
283	Pseudoionone 2	1557.6	120–150	3	0.260	1518.6	1.000	0.0	43093	1659.4	1.000	0.1
284	α-Cedrene epoxide	1568.7	150–190	4	1.015	1415.6	0.998	1.0	199289	2038.4	0.994	1.6
285	6-sec-Butylquinoline	1577.3	140–160	3	0.775	1460.9	1.000	0.2	138708	1905.0	1.000	0.1
286	Cedrol	1589.6	150–180	3	1.039	1433.9	1.000	0.2	199780	2061.6	1.000	0.2
287	Methyl dihydrogalenonate	1614.9	150–190	5	0.343	1563.3	0.993	0.5	67159	1773.3	0.991	0.6
288	α-n-Amylcinnamic aldehyde	1615.1	140–160	3	0.325	1566.1	0.994	0.4	58216	1752.4	0.996	0.3
289	Dibenzyl ether	1616.2	150–210	3	0.555	1532.9	1.000	0.3	112787	1882.7	1.000	0.2
290	Patchouli alcohol	1639.8	140–210	4	1.221	1457.1	0.997	2.5	244110	2217.8	0.994	4.0
291	n-Hexyl Salicylate	1651.5	150–180	4	0.554	1568.2	0.995	0.6	106287	1902.3	0.996	0.5
292	Bisabolol 1	1664.0	120–170	3	0.442	1597.2	0.998	0.7	76765	1845.3	1.000	0.1
293	Allyl α-ionone	1664.5	140–180	4	0.446	1597.9	0.974	1.5	83646	1862.6	0.970	1.6
294	Bisabolol 2	1666.0 180°	120–170	3	0.424	1601.5	0.994	1.1	73647	1839.5	0.998	0.7
295	p-Methoxy-acetophenone	1337.0	180–200	3	1.075	1143.4	0.999	0.4	230393	1845.2	0.999	0.6
296	Benzylideneacetone	1346.2	180–200	3	0.685	1222.3	0.976	1.5	146568	1669.0	0.972	1.6
297	Ethylvanillin	1433.0	180–200	3	0.760	1296.4	0.984	1.4	162669	1792.2	0.980	1.5
298	Ethyl-β-naphtyl ether	1520.0	180–200	3	0.840	1369.3	0.991	1.1	180298	1918.3	0.993	1.0
299	Isoeugenyl acetate 1	1534.4	180–200	3	0.120	1512.9	0.991	0.2	25757	1591.3	0.993	0.1
300	Trichloro methyl phenyl carbinyl acetate	1541.3	180–200	3	0.760	1404.3	0.998	0.5	162839	1900.4	0.997	0.6
301	Isoeugenyl acetate 2	1581.2	180–200	3	0.190	1547.4	0.900	0.9	40903	1671.8	0.907	0.9
302	β-Methyl naphtyl ketone	1598.4	180–200	3	1.320	1360.1	0.991	2.0	282601	2221.1	0.988	2.3

Table 1. Continued

No	Name	eI 100°C	Range °C	n	b	a	r^2	s	−B	A	R^2	S
303	Benzophenone	1606.4	180–200	3	1.015	1424.2	0.994	1.2	217808	2087.4	0.996	0.9
304	Farnesol 1	1678.7	150–210	3	0.165	1649.9	0.976	1.1	33483	1753.7	0.963	1.4
305	Farnesol 2+3	1682.5	150–210	3	0.167	1651.5	0.971	1.2	34251	1757.3	0.982	1.0
306	Myraldyl acetate 1	1682.9	160–190	3	0.223	1643.7	0.980	0.7	44733	1782.6	0.975	0.8
307	Farnesol 4	1703.5	150–210	3	0.180	1670.9	0.999	0.2	36793	1784.7	1.000	0.1
308	Myraldyl acetate 2	1704.0	160–190	3	0.271	1655.7	0.994	0.5	54401	1824.6	0.991	0.6
309	4-Acetyl-6-tert-butyl-1,1-dimethyl indan	1705.1	180–200	3	0.705	1578.3	1.000	0.1	151164	2038.7	1.000	0.0
310	Cedroxide	1711.0	150–180	4	0.923	1544.8	1.000	0.3	177001	2101.3	1.000	0.2
311	Isoamyl+2-methyl-butan-1-yl-cinnamates	1717.6	160–190	3	0.391	1647.3	1.000	0.1	78605	1891.3	0.999	0.2
312	Hexylcinnamic aldehyde	1726.2	140–180	3	0.518	1632.4	0.988	1.6	96541	1938.4	0.982	2.0
313	Benzyl benzoate	1736.2	160–190	3	0.677	1613.1	0.989	1.6	135621	2034.4	0.992	1.3
314	Isolongifolol	1740.9	140–160	3	1.020	1545.7	0.997	0.8	182369	2129.8	0.995	1.0
315	Amyl cinnamate	1755.0	170–200	3	0.411	1679.8	0.948	2.1	83112	1937.4	0.955	1.9
316	Cedryl acetate	1768.3	160–190	4	1.059	1577.9	0.998	0.7	212226	2237.0	0.996	1.0
317	Acetyl cedrene	1770.1	190–210	3	1.050	1574.8	0.978	2.2	234509	2280.6	0.975	2.4
318	Benzyl phenylacetate	1772.4	160–190	3	0.659	1653.2	0.998	0.7	131917	2063.2	0.999	0.4
319	Ethyl n-tetradecanoate	1778.7	170–200	3	0.005	1776.9		1.1	1230	1780.5		1.1
320	Linalyl benzoate	1780.8	150–190	4	0.434	1702.7	0.998	0.4	85352	1969.3	0.998	0.4
321	Versalide	1790.6	180–200	3	0.625	1678.0	0.998	0.4	133922	2085.9	0.997	0.5
322	Farnesyl acetate 1	1794.5	180–200	3	0.065	1783.0	0.862	0.4	14004	1825.5	0.870	0.4
323	Musk ambrette	1801.5	180–200	3	0.795	1658.0	0.992	1.0	170243	2176.7	0.989	1.2
324	p-Cresyl phenylacetate	1805.0	180–200	3	0.675	1683.2	0.992	0.9	144547	2123.6	0.990	1.0
325	Isopropyl n-tetradecanoate	1812.8	160–190	4	0.053	1803.1	0.769	0.5	10746	1836.3	0.785	0.4
326	Farnesyl acetate 2	1817.6	180–200	3	0.095	1800.7	0.930	0.4	20436	1862.8	0.937	0.4
327	Styrallyl phenylacetate	1820.4 200°	160–190	4	0.439	1741.8	0.993	0.6	87932	2014.9	0.990	0.7
328	Cyclopentadecanolide	1840.6	190–210	3	1.215	1599.0	0.990	1.8	271514	2416.0	0.987	2.0
329	Musk xylol	1843.0	180–220	3	0.960	1650.6	0.995	1.0	205623	2277.1	0.993	1.2
330	Galaxolide 1+2	1846.9	190–210	3	0.500	1746.0	0.978	1.1	112077	2083.0	0.981	1.0
331	Benzyl salicylate	1850.1	190–210	3	0.790	1692.5	0.998	0.5	176665	2224.0	0.997	0.6
332	Musk moskene	1870.6	180–200	3	0.850	1700.4	0.999	0.3	182149	2255.3	0.999	0.6
333	β-Phenylethyl phenylacetate	1882.5	180–200	3	0.587	1764.5	0.997	0.8	129032	2154.8	0.999	0.5
334	3-Methyl cyclopentadecanone	1903.7	200–210	2	1.110	1681.7			253760	2440.9		
335	10-Oxahexadecanolide	1904.5	200–230	3	0.981	1707.1	0.960	4.3	232212	2394.0	0.954	4.7
336	Musk tibetene	1907.3	180–200	3	0.920	1713.1	0.980	3.5	193093	2304.8	0.982	3.3
337	Ambrettolide 1	1927.5	190–210	2	1.010	1725.5			226017	2405.7		
338	Phenylethyl salicylate	1934.0	180–210	3	0.900	1754.0	1.000	0.0	196413	2349.4	1.000	0.3
339	Ambrettolide 2	1936.0	190–210	2	1.000	1736.0			222661	2406.9		
340	Musk ketone	1942.8	180–200	3	0.870	1768.8	1.000	0.1	186529	2337.0	1.000	0.1
341	Ethylene brassylate	1988.6	180–200	3	0.920	1805.7	0.992	1.1	197449	2406.3	0.994	1.0
342	Benzyl cinnamate	2046.9	200–230	4	0.686	1908.3	0.927	3.0	162918	2389.7	0.923	3.1
343	Benzyl isoeugenol	2078.4	210–230	3	0.645	1949.4	0.998	0.5	156873	2409.5	0.999	0.3
344	Linalyl cinnamate	2082.5	190–210	3	0.410	2000.3	1.000	0.1	91721	2276.2	0.999	0.2
345	Di-(2-ethylhexyl) phtalate	2492.6	210–230	3	0.360	2420.6	0.999	0.2	87474	2677.3	0.998	0.2

parameters of Eq. (2) and of the hyperbola are extremely sensitive to the slightest variation of the experimental data. In this case, Eq. (1), already the most used in literature, shows a better precision, intuitive character and convenience for different applications.

Most of the solutes fit well to Eqs. (1) and (2), with high correlation coefficients.

Leaving aside about 10 cases with $dI/dT = 0.2–0.4$, having $r^2 = 0.8–0.9$ and a higher standard deviation of 2.1 ± 0.5, a group of 59 solutes, mostly aliphatic, is considered for the following discussion.

They represent a half of all situations with $dI/dT < 0.2$. The linear correlation is not very good for this group: 28 solutes with retention indices almost independent of temperature, are characterised by $r^2 < 0.6$ (not registered in Table 1), $dI/dT = 0.008 \pm 0.045$, $s = 1.3 \pm 0.7$ and the other 31 solutes, by $r^2 = 0.6–0.9$, $dI/dT = 0.08 \pm 0.08$, $s = 1.1 \pm 0.7$. The situation can be explained by a higher ratio between the variance of residuals around the regression line described by the calculated $\hat{I}_i$ values, and the total variance of the observed retention index values I_i, against their mean $\bar{I}$. This ratio comes into one of the definitions of the correlation coefficient [33]:

$$r^2 = 1 - \frac{\sum_{i=1}^{n} (I_i - \hat{I}_i)^2}{\sum_{i=1}^{n} (I_i - \bar{I})^2} \quad (3)$$

The level of the variance of residuals is almost the same for all solutes, as it can be seen from the standard deviations. The extension of range of the observed retention indices, connected with the total variance, is for these poor correlated solutes, only up to several index units, comparatively with 10–80 i.u. for well correlated solutes. The systematic error due to the hyperbolic behaviour cannot be totally ignored for the discussed group, but is difficult to evaluate. The adsorption at gas–liquid interface can also have an influence, especially for aliphatic alcohols. The problems connected with limitations due to the precision of the data in the case of solutes with low temperature dependence of the retention index, were also noticed or can be recognised in the data from Refs. [9,18,21,32,34]. More precautions would be necessary for an accurate study of such compounds [23]. Nevertheless, the trends designated in our results for the solutes with $dI/dT < 0.2$, are rather meaningful, as will be shown in our future work on retention–structure relationship.

It is known [35,36], that the retention index on dimethylsilicone glass capillary columns has only a slight dependence on film thickness over 0.3 μm. Therefore it may be expected that our data are rather representative for usual situations, regardless of the type of capillary column and commercial name of dimethylsilicone. Indeed, the comparison for some of common solutes with literature retention indices and derived dI/dT values, is quite satisfactory for capillary columns [9,12] and even for packed columns [10,11,13].

4. Conclusions

A comprehensive set of perfumery solutes was studied for the temperature dependence of the retention index on a SE-30 glass capillary column. A good linearity with column temperature and its reciprocal, was noticed for narrow temperature intervals.

This work will be continued with the hyperbolic fitting in Part 2, comparative evaluation and correlation between the parameters of the three equations, quantitative structure–retention index relationships and structural effects on dI/dT.

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References

[1] W. Jennings and T. Shibamoto, Qualitative Analysis of Flavor and Fragrance volatiles by Glass Capillary Column Gas Chromatography, Academic Press, New York, 1980.
[2] T. Shibamoto, in P. Sandra and C. Bicchi (Editors), Capillary Gas Chromatography in Essential Oil Analysis, Huetig Verlag, Heidelberg, 1987, Ch. 8, p. 259.
[3] N.W. Davies, J. Chromatogr. 503 (1990) 1.
[4] H. Van den Dool, Thesis, Rijksuniversiteit te Groningen, 1974.
[5] The Sadtler Standard Gas Chromatography Retention Index Library, Vols. 1–4, Sadtler Research Libraries, Division of Bio-Rad Laboratories, Philadelphia, PA, 1986.
[6] M.V. Budahegyi, E.R. Lombosi, T.S. Lombosi, S.Y. Mészaros, Sz. Nyiredy, G. Tarján, I. Timár, J.M. Takács, J. Chromatogr. 271 (1983) 213.
[7] G. Tarján, Sz. Nyiredy, M. Györ, E.R. Lombosi, T.S. Lombosi, M.V. Budahegyi, S.Y. Mészaros, J.M. Takács, J. Chromatogr. 472 (1989) 1.
[8] M.B. Evans, J.K. Haken, J. Chromatogr. 472 (1989) 93.
[9] T. Saeed, G. Redant, P. Sandra, J. High Resolut. Chromatogr., Chromatogr. Commun. 2 (1979) 75.

[10] N.A. Andersen, M.S. Falcone, J. Chromatogr. 44 (1969) 52.
[11] R. Benecke, H. Thieme, Sz. Nyiredy, J. Chromatogr. 238 (1982) 175.
[12] S. Boneva, Chromatographia 23 (1987) 50.
[13] B.A. Bierl, M. Beroza, M.H. Aldridge, J. Chromatogr. Sci. 10 (1972) 712.
[14] Y. Sun, R. Zhang, Q. Wang, J. Chromatogr. A 657 (1993) 1.
[15] J.A. Garcia Dominguez, J.M. Santiuste, J. Chromatogr. 627 (1992) 203.
[16] G.D. Mitra, N.C. Saha, Chromatographia 6 (1973) 93.
[17] E.Sz. Kováts, in J.C. Giddings and R.A. Keller (Editors), Advances in Chromatography, Vol. 1, Arnold and Dekker, London, 1965, p. 229.
[18] F. Riedo, D. Fritz, G. Tarján, E.Sz. Kováts, J. Chromatogr. 126 (1976) 63.
[19] N.G. Johansen, L.S. Ettre, Chromatographia 15 (1982) 625.
[20] F. Vernon, D.B. Suratman, Chromatographia 17 (1983) 600.
[21] J. Krupčic, D. Repka, E. Benicka, T. Hevesi, J. Nolte, B. Paschold, H. Mayer, J. Chromatogr. 448 (1988) 203.
[22] J.M. Santiuste, Chromatographia 34 (1992) 636.
[23] K. Kuningas, S. Rang, T. Kailas, J. Chromatogr. 520 (1990) 137.
[24] J. Takács, M. Rockenbauer, I. Olacsi, J. Chromatogr. 42 (1969) 19.
[25] K. Grob, G. Grob, K. Grob Jr., J. High Resolut. Chromatogr., Chromatogr. Commun. 2 (1979) 31.
[26] K. Grob, Jr., Carlo Erba Practical Seminary on Glass Capillary Column Preparation, Bucharest, 1978.
[27] K. Grob, J. High Resolut. Chromatogr., Chromatogr. Commun. 3 (1980) 525.
[28] K. Grob, J. High Resolut. Chromatogr., Chromatogr. Commun. 1 (1978) 93.
[29] K. Grob Jr., G. Grob, K. Grob, J. Chromatogr. 156 (1978) 1.
[30] S. Arctander, Perfumery and Flavor Chemicals (Aroma Chemicals), S. Arctander, Montclair, NJ, 1969.
[31] S. Ebel, R.E. Kaiser, Chromatographia 7 (1974) 696.
[32] J. Kušmierz, E. Malinski, W. Czerwiek, J. Safranek, J. Chromatogr. 331 (1985) 219.
[33] K. Héberger, Chromatographia 29 (1990) 375.
[34] J.K. Haken, I.O.O. Korhonen, J. Chromatogr. 324 (1985) 343.
[35] E. Matisova, J. Krupčik, J. Garaj, Chromatographia 16 (1982) 169.
[36] P. Farkás, L. Soják, M. Kováč, J. Janak, J. Chromatogr. 471 (1989) 251.