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GAS–LIQUID CHROMATOGRAPHIC ANALYSES

XLVIII*. BENZYL, (±)-1-PHENYLETHYL AND 2-PHENYLETHYL ALCOHOLS AND THE CORRESPONDING ESTERS OF BENZOIC ACID AND ITS 2-, 3- AND 4-CHLORO, PENTAFLUORO, 4-NITRO AND 3,5-DINITRO DERIVATIVES ON SE-30 AND OV-351 CAPILLARY COLUMNS

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SUMMARY

The gas chromatographic retention behaviour of a mixture of benzyl, (±)-1-phenylethyl and 2-phenylethyl alcohols and their benzoyl, 2-, 3- and 4-chlorobenzoyl, pentafluorobenzoyl, 4-nitrobenzoyl and 3,5-dinitrobenzoyl esters was studied on low-polarity (SE-30) and highly polar (OV-351) capillary columns under temperature-programmed and isothermal conditions. The relative retention data, the Kováts retention indices and the retention index increments due to conversion of alcohols into esters, for methylene units and chloro, fluoro and nitro substituents were determined and the separation of a mixture of 24 compounds is discussed. The results are compared with those reported earlier for the corresponding aliphatic esters.

INTRODUCTION

The gas chromatography (GC) of various groups of aliphatic alcohols, *i.e.*, saturated normal-chain[1–6], saturated branched-chain[7–10], unsaturated[9–12] and chloro alcohols[13], has been extensively studied, as has that of the corresponding esters of series of aliphatic[14,15] and aromatic[16] acids.

In contrast to aliphatic alcohols and their esters, the GC retention behaviour of aromatic alcohols has not been investigated and studies of their esters are limited, constituting exclusively benzyl[17–23], pentafluorobenzyl[24–27] and some *p*-substituted benzyl[28] esters of aliphatic carboxylic acids. The purpose of these studies most frequently was the quantitative derivatization of organic acids of biological interest prior to separation and analysis by GC, rather than a systematic study of the related esters. Packed columns coated with SE-30[17,23], EGSS-X[17,19], E-30[18], OV-1[21], OV-17[20,22,24–26,28], OV-25[23], Silar-10C[22,23], QF-1[23], Carbowax terephthalic acid[27] or

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OV-225[27] stationary phases have been used, but retention data have been reported only in a few papers[18,21,23]. A systematic study of the GC retention behaviour of aromatic esters including some lower benzyl esters has been carried out only by Haken *et al.*[23] who demonstrated the influence of the stationary phase polarity on the retention index increments.

Previous GC studies from this laboratory on aromatic esters involved the retention behaviour of benzoyl[16,29–36], 2-, 3- and 4-chlorobenzoyl[29–32], pentafluorobenzoyl[33,34] and 4-nitro- and 3,5-dinitrobenzoyl[16,35,36] esters of the following aliphatic alcohols: saturated C_1–C_{12} *n*-alcohols[29,33,35], saturated C_3–C_5 branched-chain alcohols[16,30,34,36], unsaturated C_3–C_6 alcohols[16,31,34,36] and ethanol, 2-chloroethanol, 2,2-dichloroethanol and 2,2,2-trichloroethanol[16,32,36]. All data were obtained on a low-polarity SE-30 and a highly polar OV-351 capillary column under various operating conditions. The separations of the esters, the Kováts retention indices and the relative incremental effects of the various alkyl and/or acyl chain parameters, *i.e.*, length, branching, unsaturation and particularly substitution, were variously examined and discussed.

This paper describes the isothermal and temperature-programmed capillary GC of benzyl, (±)-1-phenylethyl and 2-phenylethyl alcohols and their benzoyl, 2-, 3- and 4-chlorobenzoyl, pentafluorobenzoyl, 4-nitrobenzoyl and 3,5-dinitrobenzoyl esters on SE-30 and OV-351. The relative retention data, the retention indices and the retention index increments upon conversion of alcohols into esters, for methylene units and chloro, pentafluoro, nitro and dinitro substituents were determined and the separation of a mixture of 24 compounds on both columns is discussed. The results are compared with those reported previously for the aliphatic esters of the corresponding aromatic acids.

EXPERIMENTAL

Materials

Benzyl and (±)-1-phenylethyl alcohols were obtained from Fluka (Buchs, Switzerland) and 2-phenylethyl alcohol from BDH Chemicals (Poole, U.K.).

Esters listed in Table I were synthesized from the redistilled alcohols and acid chlorides as described earlier[37]. Benzoyl, 4-nitrobenzoyl and 3,5-dinitrobenzoyl chlorides were obtained from Merck-Schuchardt (Darmstadt, F.R.G.), pentafluorobenzoyl chloride from Fluka; 2-, 3- and 4-chlorobenzoyl chlorides were synthetic products[29].

Mixtures of *n*-alkanes were obtained from different commercial sources.

Methods

GC analyses were carried out on a Perkin-Elmer Sigma 3 instrument under the following operating conditions: injection and flame-ionization detection (FID) temperatures, 275°C; nitrogen carrier gas velocities for methane at 160°C, 29.6 (SE-30) and 61.3 cm s^{-1} (OV-351); splitting ratio, 1:30; and chart speed, 10 mm min^{-1}. The columns used were a vitreous silica SE-30 wall-coated open-tubular (WCOT) column (25 m × 0.33 mm I.D.), supplied by SGE (North Melbourne, Australia), and a fused silica OV-351 WCOT column (25 m × 0.32 mm I.D.), supplied by Nordion Instruments Oy (Helsinki, Finland). The operating temperatures used are shown in Tables III–V.

The chromatographic data were recorded with a Hewlett-Packard Model 3390A reporting integrator with suitable programs. The retention times were measured from the time of sample injection and the Kováts retention indices were calculated off-line as described earlier[38]. The dead volumes were determined by the injection of methane.

RESULTS AND DISCUSSION

Table II shows the relative retention data for aromatic alcohols and their esters (Table I), obtained with temperature programming under the conditions shown in Figs. 1 (SE-30) and 2 (OV-351). The retention indices for alcohols are presented in Table III and those for the esters in Tables IV (SE-30) and V (OV-351). Fig. 3 illustrates the retentions of compounds, together with the retention enhancements on a highly polar stationary phase, *viz.*, $I_{OV\text{-}351} - I_{SE\text{-}30}$.

The alcohols and their esters are eluted on SE-30 in the order 1 < 2 < 3, corresponding to that of their boiling points (Figs. 1 and 3). On OV-351 the order is changed, *i.e.*, 2 < 1 < 3, the branched-chain components being eluted first (Figs.

TABLE I

LIST AND NOTATION OF AROMATIC ALCOHOLS AND ESTERS INVESTIGATED

Compound	*Notation*	*Peak No.**
Benzyl alcohol	1	1
(±)-1-Phenylethanol	2	2
2-Phenylethanol	3	3
Benzyl benzoate	B1	4
(±)-1-Phenylethyl benzoate	B2	5
2-Phenylethyl benzoate	B3	6
Benzyl 2-chlorobenzoate	2ClB1	7
(±)-1-Phenylethyl 2-chlorobenzoate	2ClB2	8
2-Phenylethyl 2-chlorobenzoate	2ClB3	9
Benzyl 3-chlorobenzoate	3ClB1	10
(±)-1-Phenylethyl 3-chlorobenzoate	3ClB2	11
2-Phenylethyl 3-chlorobenzoate	3ClB3	12
Benzyl 4-chlorobenzoate	4ClB1	13
(±)-1-Phenylethyl 4-chlorobenzoate	4ClB2	14
2-Phenylethyl 4-chlorobenzoate	4ClB3	15
Benzyl pentafluorobenzoate	F_5B1	16
(±)-1-Phenylethyl pentafluorobenzoate	F_5B2	17
2-Phenylethyl pentafluorobenzoate	F_5B3	18
Benzyl 4-nitrobenzoate	$4NO_2B1$	19
(±)-1-Phenylethyl 4-nitrobenzoate	$4NO_2B2$	20
2-Phenylethyl 4-nitrobenzoate	$4NO_2B3$	21
Benzyl 3,5-dinitrobenzoate	$35NO_2B1$	22
(±)-1-Phenylethyl 3,5-dinitrobenzoate	$35NO_2B2$	23
2-Phenylethyl 3,5-dinitrobenzoate	$35NO_2B3$	24

* In Figs. 1 and 2.

TABLE II

RETENTION DATA FOR AROMATIC ALCOHOLS AND THEIR BENZOYL, HALOBENZOYL AND NITROBENZOYL DERIVATIVES, DETERMINED ON SE-30 AND OV-351 CAPILLARY COLUMNS WITH TEMPERATURE PROGRAMMING

Conditions as in Figs. 1 and 2.

Peak No.	*Compound**	*SE-30*				*OV-351*				
		*ART***	*RRT****	*RRT*§	*RRT*§§	*ART***	*RRT****	*RRT*§	*RRT*§§	*RRT*§§§
1	1	2.70	0.34	1.00	0.19	6.72	3.75	1.00	0.38	2.49
2	2	2.91	0.37	1.00	0.20	5.84	3.26	1.00	0.34	2.01
3	3	3.44	0.43	1.00	0.22	7.23	4.04	1.00	0.38	2.10
4	B1	14.00	1.77	5.19	1.00	17.70	9.89	2.63	1.00	1.26
5	B2	14.39	1.81	4.95	1.00	17.00	9.50	2.91	1.00	1.18
6	B3	15.62	1.97	4.54	1.00	18.81	10.51	2.60	1.00	1.20
7	2ClB1	16.99	2.14	6.29	1.21	21.82	12.19	3.25	1.23	1.28
8	2ClB2	17.21	2.17	5.91	1.20	20.79	11.61	3.56	1.22	1.21
9	2ClB3	18.58	2.34	5.40	1.19	23.71	13.25	3.28	1.26	1.28
10	3ClB1	16.94	2.14	6.27	1.21	20.57	11.49	3.06	1.16	1.21
11	3ClB2	17.19	2.17	5.91	1.19	19.72	11.02	3.38	1.16	1.15
12	3ClB3	18.41	2.32	5.35	1.18	21.88	12.22	3.03	1.16	1.19
13	4ClB1	16.98	2.14	6.29	1.21	20.59	11.50	3.06	1.16	1.21
14	4ClB2	17.20	2.17	5.91	1.20	19.74	11.03	3.38	1.16	1.15
15	4ClB3	18.51	2.33	5.38	1.19	21.92	12.25	3.03	1.17	1.18

16	F_5B1	11.19	1.41	4.14	0.80	11.91	6.65	1.77	0.67	1.06
17	F_5B2	11.59	1.46	3.98	0.81	11.13	6.22	1.91	0.65	0.96
18	F_5B3	12.95	1.63	3.76	0.83	13.26	7.41	1.83	0.70	1.02
19	$4NO_2B1$	20.35	2.57	7.54	1.45	–	–	–	–	–
20	$4NO_2B2$	20.59	2.60	7.08	1.43	–	–	–	–	–
21	$4NO_2B3$	21.76	2.74	6.33	1.39	–	–	–	–	–
22	$35NO_2B1$	24.22	3.05	8.97	1.73	–	–	–	–	–
23	$35NO_2B2$	24.28	3.06	8.34	1.69	–	–	–	–	–
24	$35NO_2B3$	25.41	3.20	7.39	1.63	–	–	–	–	–
C_{14}	*n*-Tetradecane	7.93	1.00	–	–	1.79	1.00	–	–	0.23

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* Compounds are listed in Table I.

** Absolute retention times (min) were measured from the time of sample injection (Figs. 1 and 2).

*** Relative retention time for *n*-tetradecane (C_{14}) taken as 1.00.

§ Relative retention time for the corresponding alcohol (1–3) taken as 1.00.

§§ Relative retention time for the corresponding ester of benzoic acid (B1–B3) taken as 1.00.

§§§ Relative retention time for the corresponding compound on SE-30 taken as 1.00.

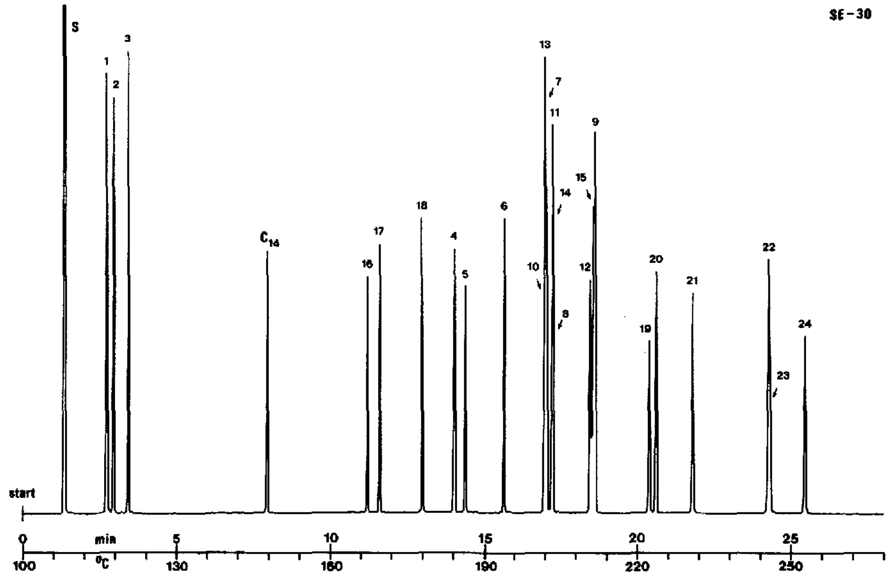

Fig. 1. Chromatogram of a mixture of aromatic alcohols and their aromatic esters, separated on an SE-30 quartz capillary column with temperature programming from 100°C at 6°C min^{-1} until elution of peaks had ceased. S = Solvent; C_{14} = *n*-tetradecane; peaks as in Table I.

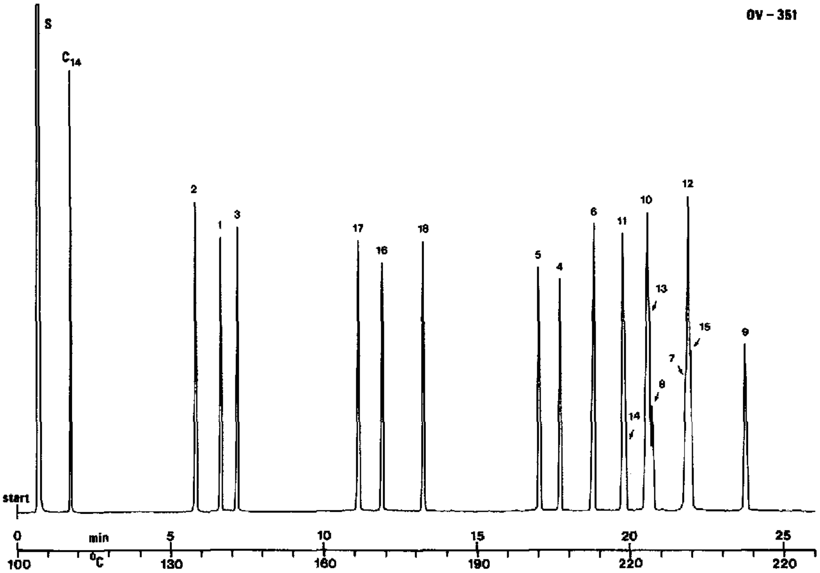

Fig. 2. Chromatogram of the same mixture as in Fig. 1, separated on an OV-351 quartz capillary column with temperature programming from 100 to 220°C at 6°C min^{-1} and held at 220°C until elution of peaks had ceased. Peaks as in Fig. 1.

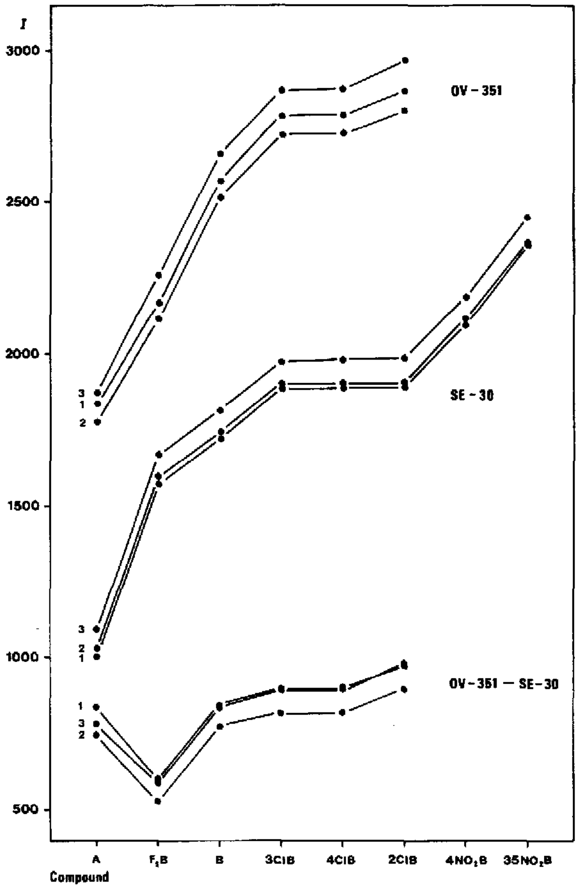

Fig. 3. Plot showing retentions of aromatic alcohols (A) and their benzoyl (B), 2-chlorobenzoyl (2ClB), 3-chlorobenzoyl (3ClB), 4-chlorobenzoyl (4ClB), pentafluorobenzoyl (F_5B), 4-nitrobenzoyl ($4NO_2B$) and 3,5-dinitrobenzoyl ($35NO_2B$) esters, obtained on SE-30 and OV-351 with temperature programming under the conditions shown in Figs. 1 and 2. The retention enhancements on a highly polar column are also shown. Curves: 1, benzyl alcohol and related esters; 2, (±)-1-phenylethyl alcohol and its esters; 3, 2-phenylethyl alcohol and its esters. I = Retention index units.

2 and 3). The mutual retention behaviour of benzoyl and substituted benzoyl esters of aromatic alcohols is as reported previously for the corresponding aliphatic esters[16,29–36], *viz.*, (i) the esters appear in order $F_5B < B < 3ClB \leqslant 4ClB < 2ClB < 4NO_2B < 35NO_2B$, (ii) all monochlorobenzoates are eluted close together on SE-30, as also are the 3- and 4-chloro esters on OV-351, (iii) the retention of the 2-chloro esters on OV-351 is markedly increased[29–32], (iv) a highly polar column is unsuitable for the higher nitrobenzoyl esters[16,35,36], especially for the aromatic esters studied in the present work (results omitted due to their very low FID response, broadened and tailing peak shapes and relatively higher retention times compared with the other esters).

The incremental effects for methylene and for the conversion of the alcohols

TABLE III

RETENTION INDICES FOR AROMATIC ALCOHOLS, DETERMINED ON SE-30 AND OV-351 AT A VARIETY OF TEMPERATURES

Column temperature	*SE-30*			*OV-351*		
	*1**	*2*	*3*	*1*	*2*	*3*
Programmed						
(A)**	1022	1050	1100	1835	1776	1875
(B)***	1005	1029	1092	1837	1777	1873
Isothermal						
60°C	1009	1035	1084			
80°C	1009	1037	1086			
100°C	1009	1038	1092	1834	1780	1865
120°C	1014	1042	1099	1846	1785	1874
140°C				1857	1796	1892
160°C				1870	1812	1904
180°C				1875	1813	1906
200°C				1887	1817	1914
Ratio: OV-351/SE-30						
(B)***				1.83	1.73	1.72
Subtraction: OV-351–SE-30						
(B)***				832	748	781

* Alcohols are listed in Table I.

** (A) SE-30, from 50°C at 10°C min^{-1} until elution of peaks had ceased; OV-351, from 50 to 220°C at 10°C min^{-1} and held at 220°C until elution of peaks had ceased.

*** (B) SE-30, from 100°C at 6°C min^{-1} until elution of peaks had ceased; OV-351, from 100 to 220°C at 6°C min^{-1} and held at 220°C until elution of peaks had ceased.

into the benzoate and substituted benzoate esters are shown in Tables VI (SE-30) and VII (OV-351).

The methylene increments for series 1 to 3 on SE-30 are quite constant for all eight groups of the compounds, *i.e.*, in the range 85–94 retention index units (i.u.), obtained with temperature programming (Table VI). These values are on the average 7 i.u. lower than reported earlier for the corresponding aliphatic ester pairs[29,33,35], *viz.*, ethyl ester, *n*-propyl ester, where the values were in the range 95–100 i.u. On OV-351 the increments between different groups of the compounds vary from 36 (alcohols) to 103 i.u. (2-chlorobenzoates). The former is markedly lower than for the pair ethanol, 1-propanol[5] (close to 100 i.u.), whereas the latter is considerable higher than for the pair ethyl, *n*-propyl ester[29] (77 i.u.). The methylene increments for the other compounds, presented in Table VII, are in the same ranges as for the aliphatic esters, however.

The methylene increments obtained from series 1 to 2 on SE-30 and OV-351 are in the ranges 4–24 and from −64 to −50 i.u., respectively (Tables VI and VII), all values being markedly lower as found earlier for the series ethanol[5] to 2-propanol[9] and ethyl[29,33,35] to methylethyl[16,30,34] esters. Thus, the α-methyl substitution into benzyl alcohol and its esters leads to a reduction in the retention and a reverse in the retention order of the compounds on a highly polar OV-351 column as compared

TABLE IV

RETENTION INDICES FOR BENZOYL, HALOBENZOYL AND NITROBENZOYL ESTERS OF AROMATIC ALCOHOLS, DETERMINED ON AN SE-30 CAPILLARY COLUMN AT A VARIETY OF TEMPERATURES

*Compound**	*Programmed*		*Isothermal (°C)*					
	*(A)***	*(B)***	*140*	*160*	*180*	*200*	*220*	*240*
B1	1736	1724	1712	1725	1741	1756	1771	1789
B2	1757	1745	1733	1744	1760	1771	1784	1796
B3	1828	1815	1796	1809	1825	1836	1849	1863
2ClB1	1904	1893	1867	1883	1900	1914	1929	1944
2ClB2	1917	1905	1882	1897	1912	1924	1937	1949
2ClB3	2001	1987	1953	1969	1989	2006	2020	2037
3ClB1	1901	1890	1866	1880	1897	1912	1926	1942
3ClB2	1915	1904	1880	1894	1910	1923	1936	1949
3ClB3	1990	1977	1945	1962	1978	1993	2007	2024
4ClB1	1903	1892	1866	1881	1899	1914	1928	1944
4ClB2	1916	1905	1881	1895	1911	1925	1938	1952
4ClB3	1994	1983	1950	1966	1985	2000	2017	2034
F$_5$B1	1581	1572	1573	1578	1583	1589		
F$_5$B2	1603	1593	1594	1597	1601	1605		
F$_5$B3	1675	1666	1662	1667	1674	1680		
4NO$_2$B1	2106	2097		2071	2087	2106	2121	2141
4NO$_2$B2	2123	2112		2084	2103	2119	2137	2155
4NO$_2$B3	2201	2189		2156	2169	2189	2211	2230
35NO$_2$B1	2368	2358		2309	2325	2342	2357	2377
35NO$_2$B2	2370	2362		2310	2327	2344	2358	2377
35NO$_2$B3	2460	2443		2383	2399	2420	2439	2460

* Compounds are listed in Table I.

** Conditions (A) and (B) are given in Table III.

with that on SE-30. Such a trend occurs only rarely with the ethyl and methylethyl esters of a wide range of aliphatic and aromatic acids investigated earlier.

The incremental effects due to conversion of the aromatic alcohols into their esters shown in Tables VI and VII are to some extent higher than in the case of an aliphatic alcohol series, ethanol, 2-propanol and 1-propanol[5,9,16,29,30,33–35]. The increment ratio between two different columns is lowest with pentafluorobenzoates (0.58–0.67), increasing to 1.16–1.22 with 2-chlorobenzoates (Table VII). It seems, however, that nitrobenzoates would have shown still increased ratios, if analysed on a polar column.

Tables VIII (SE-30) and IX (OV-351) show the retention increments of the various substituents on the aromatic acyl chain. As expected, the effect of the different alkyl groups on the increments is negligible, the values being in the same ranges as previously reported for the aliphatic esters of benzoic acid and its derivatives[16,29–36]. The higher retention increment ratios between OV-351 and SE-30 shown in Table IX

TABLE V

RETENTION INDICES FOR BENZOYL AND HALOBENZOYL ESTERS OF AROMATIC ALCOHOLS, DETERMINED ON AN OV-351 CAPILLARY COLUMN AT A VARIETY OF TEMPERATURES

*Compound**	*Programmed*		*Isothermal (°C)*				$I_{OV\text{-}351}/I_{SE\text{-}30}$*** *(Programmed B**)*	$I_{OV\text{-}351}-I_{SE\text{-}30}$*** *(Programmed B**)*
	*(A)***	*(B)***	*160*	*180*	*200*	*220*		
B1	2583	2570	2547	2576	2607	2636	1.49	846
B2	2530	2518	2504	2530	2558	2583	1.44	773
B3	2668	2654	2621	2652	2682	2712	1.46	839
2ClB1	2877	2865	2799	2833	2869	2905	1.51	972
2ClB2	2807	2802	2760	2786	2814	2839	1.47	897
2ClB3	2979	2968	2894	2927	2959	2994	1.49	981
3ClB1	2799	2786	2737	2768	2797	2831	1.47	896
3ClB2	2739	2722	2692	2717	2745	2771	1.43	818
3ClB3	2888	2869	2810	2841	2873	2905	1.45	892
4ClB1	2801	2787	2740	2772	2801	2832	1.47	895
4ClB2	2741	2723	2699	2723	2749	2773	1.43	818
4ClB3	2887	2872	2814	2844	2875	2906	1.45	889
F$_5$B1	2165	2168	2172	2180	2191	2200	1.38	596
F$_5$B2	2118	2118	2130	2149	2170	2190	1.33	525
F$_5$B3	2252	2255	2259	2265	2271	2276	1.35	589

* Compounds are listed in Table I.

** Conditions (A) and (B) are given in Table III.

*** For the retention indices on SE-30, see Table IV.

would indicate an increase in the polar effects with the aromatic alcohol derivatives, however.

It has been previously reported[23] that the index increase effected by stationary phase polarity is much larger for aromatic than for aliphatic esters. The same trend is shown in Table X, where a comparison of the retention indices of aliphatic and aromatic alcohols and their aromatic esters having the same total carbon number is presented. On SE-30 the retention of benzyl alcohol derivatives is increased by 64–81 i.u. from that of the 1-heptanol derivatives, the difference between 2-phenylethanol and 1-octanol derivatives being lower, *i.e.*, in the range 50–64 i.u. On OV-351 the disparity between the retentions of the aromatic and aliphatic alcohol derivatives is increased, being in the ranges 381–419 and 346–377 i.u., respectively. These values are lower as previously shown[23] with the pair *n*-butyl hexanoate and *n*-propyl benzoate analysed on SE-30 and Silar-10C, due to the different character of the polar OV-351 and Silar-10C stationary phases.

The results given in the present paper are in accordance with those obtained previously for the other aromatic esters[16,23,29–36]. A further study of the higher aromatic alcohol esters would be of interest for extending the data and explaining the effects, but their analysis on polar columns causes difficulties as shown with the nitrobenzoyl esters in the present work.

TABLE VI

RETENTION INCREMENTS FOR METHYLENE AND FOR CONVERSION OF ALCOHOLS INTO ESTERS, DETERMINED ON SE-30

*Compound**	*Programmed***			*Isothermal (160°C)*	
	ΔI***	ΔI_{CH_2}§	$\Delta I_{\alpha\text{-}CH_2}$§§	ΔI_{CH_2}§	$\Delta I_{\alpha\text{-}CH_2}$§§
1		–	–		
2			24		
3		87			
B1	719	–	–	–	–
B2	716		21		19
B3	723	91		84	
2ClB1	888	–	–	–	–
2ClB2	876		12		14
2ClB3	895	94		86	
3ClB1	885	–	–	–	–
3ClB2	875		14		14
3ClB3	885	87		82	
4ClB1	887	–	–	–	–
4ClB2	876		13		14
4ClB3	891	91		85	
F_5B1	567	–	–	–	–
F_5B2	564		21		19
F_5B3	574	94		89	
4NO_2B1	1092	–	–	–	–
4NO_2B2	1083		15		13
4NO_2B3	1097	92		85	
35NO_2B1	1353	–	–	–	–
35NO_2B2	1333		4		1
35NO_2B3	1351	85		74	

* Compounds are listed in Table I.

** Condition (B) as shown in Table III.

*** $\Delta I = I$ (ester) $-$ I (alcohol).

§ Obtained from series 1 to 3.

§§ Obtained by replacement of α-hydrogen atom by a methyl group, *i.e.*, from series 1 to 2.

TABLE VII

RETENTION INCREMENTS FOR METHYLENE AND FOR CONVERSION OF ALCOHOLS INTO ESTERS, DETERMINED ON OV-351

*Compound**	*Programmed***			*Isothermal (160°C)*			$\Delta I_{OV\text{-}351}/\Delta I_{SE\text{-}30}$§§§ *(Programmed B**)*
	ΔI***	ΔI_{CH_2}§	$\Delta I_{\alpha\text{-}CH_2}$§§	ΔI***	ΔI_{CH_2}§	$\Delta I_{\alpha\text{-}CH_2}$§§	
1		–	–		–	–	
2			−60			−58	
3		36			34		
B1	733	–	–	677	–	–	1.02
B2	741		−52	692		−43	1.03
B3	781	84		717	74		1.08
2ClB1	1028	–	–	929	–	–	1.16
2ClB2	1025		−63	948		−39	1.17
2ClB3	1095	103		990	95		1.22
3ClB1	949	–	–	867	–	–	1.07
3ClB2	945		−64	880		−45	1.08
3ClB3	996	83		906	73		1.13
4ClB1	950	–	–	870	–	–	1.07
4ClB2	946		−64	887		−41	1.08
4ClB3	999	85		910	74		1.12
F_5B1	331	–	–	302	–	–	0.58
F_5B2	341		−50	318		−42	0.60
F_5B3	382	87		355	87		0.67

*,**,***,§,§§ As in Table VI.

§§§ For the retention increments on SE-30, see Table VI.

TABLE VIII

RETENTION INCREMENTS FOR CHLORO, FLUORO AND NITRO SUBSTITUTION ON SE-30 AT A VARIETY OF TEMPERATURES

*Compound**	*Retention increment* (ΔI_{Cl}, ΔI_F, ΔI_{NO_2})**						
	*Programmed****	*Isothermal (°C)*					
		140	*160*	*180*	*200*	*220*	*240*
2ClB1	169	155	158	159	158	158	155
2ClB2	160	149	153	152	153	153	153
2ClB3	172	157	160	164	170	171	174
3ClB1	166	154	155	156	156	155	153
3ClB2	159	147	150	150	152	152	153
3ClB3	162	149	153	153	157	158	161
4ClB1	168	154	156	158	158	157	155
4ClB2	160	148	151	151	154	154	156
4ClB3	168	154	157	160	164	168	171
F_5B1	−152	−139	−147	−158	−167		
F_5B2	−152	−139	−147	−159	−166		
F_5B3	−149	−134	−142	−151	−156		
$4NO_2B1$	373		346	346	350	350	352
$4NO_2B2$	367		340	343	348	353	359
$4NO_2B3$	374		347	344	353	362	367
$35NO_2B1$	634		584	584	586	586	588
$35NO_2B2$	617		566	567	573	574	581
$35NO_2B3$	628		574	574	584	590	597

* Compounds are listed in Table I.

** $\Delta I = I$ (chloro-, fluoro- and nitrobenzoate) − I (benzoate).

*** Condition (B) as shown in Table III.

TABLE IX

RETENTION INCREMENTS FOR CHLORO AND FLUORO SUBSTITUTION ON OV-351 AT A VARIETY OF TEMPERATURES

*Compound**	*Retention increment* (ΔI_{Cl}, ΔI_F)**					$\Delta I_{OV\text{-}351}/\Delta I_{OV\text{-}351}/\Delta I_{SE\text{-}30}$§	
	*Programmed****	*Isothermal (°C)*				*Programmed****	*160°C*
		160	*180*	*200*	*220*		
2ClB1	295	252	257	262	269	1.75	1.59
2ClB2	284	256	256	256	256	1.78	1.67
2ClB3	314	273	275	277	282	1.83	1.71
3ClB1	216	190	192	190	195	1.30	1.23
3ClB2	204	188	187	187	188	1.28	1.25
3ClB3	215	189	189	191	193	1.33	1.24
4ClB1	217	193	196	194	196	1.29	1.24
4ClB2	205	195	193	191	190	1.28	1.29
4ClB3	218	193	192	193	194	1.30	1.23
F_5B1	−402	−375	−396	−416	−436		
F_5B2	−400	−374	−381	−388	−393		
F_5B3	−399	−362	−387	−411	−436		

* Compounds are listed in Table I.

** $\Delta I = I$ (chloro- and fluorobenzoate) − I (benzoate).

*** Condition (B) as shown in Table III.

§ For the retention increments on SE-30, see Table VIII.

TABLE X

COMPARISON OF RETENTION INDICES OF ALIPHATIC AND AROMATIC ALCOHOLS AND THEIR AROMATIC ESTERS WITH THE SAME TOTAL CARBON NUMBER, OBTAINED ON SE-30 AND OV-351 AT 180°C

Compound	*Formula*	*SE-30*		*OV-351*		*OV-351 – SE-30*	
		I	ΔI^*	*I*	ΔI^*	*I*	ΔI^*
Heptanol**	$C_7H_{16}O$	950***		1427***		477	
Benzyl alcohol	C_7H_8O	1014***	64	1846***	419	832	355
Heptyl benzoate§	$C_{14}H_{20}O_2$	1665		2184		519	
Benzyl benzoate	$C_{14}H_{12}O_2$	1741	76	2576	392	835	316
Heptyl 2-chlorobenzoate§	$C_{14}H_{19}ClO_2$	1826		2452		626	
Benzyl 2-chlorobenzoate	$C_{14}H_{11}ClO_2$	1900	74	2833	381	933	307
Heptyl 3-chlorobenzoate§	$C_{14}H_{19}ClO_2$	1822		2365		543	
Benzyl 3-chlorobenzoate	$C_{14}H_{11}ClO_2$	1897	75	2768	403	871	328
Heptyl 4-chlorobenzoate§	$C_{14}H_{19}ClO_2$	1825		2369		544	
Benzyl 4-chlorobenzoate	$C_{14}H_{11}ClO_2$	1899	74	2772	403	873	329
Heptyl pentafluorobenzoate§§	$C_{14}H_{15}F_5O_2$	1519		1788		269	
Benzyl pentafluorobenzoate	$C_{14}H_7F_5O_2$	1583	64	2180	392	597	328
Heptyl 4-nitrobenzoate§§§	$C_{14}H_{19}NO_4$	2007		2771		764	
Benzyl 4-nitrobenzoate	$C_{14}H_{11}NO_4$	2087	80	–	–	–	–
Heptyl 3,5-dinitrobenzoate§§§	$C_{14}H_{18}N_2O_6$	2244		3164		920	
Benzyl 3,5-dinitrobenzoate	$C_{14}H_{10}N_2O_6$	2325	81	–	–	–	–

Octanol**	$C_8H_{18}O$	1049***		1528***		479	
2-Phenylethanol	$C_8H_{10}O$	1099***	50	1874***	346	775	296
Octyl benzoate§	$C_{15}H_{22}O_2$	1764		2287		523	
2-Phenylethyl benzoate	$C_{15}H_{14}O_2$	1825	61	2652	365	827	304
Octyl 2-chlorobenzoate§	$C_{15}H_{21}ClO_2$	1925		2555		630	
2-Phenylethyl 2-chlorobenzoate	$C_{15}H_{13}ClO_2$	1989	64	2927	372	938	308
Octyl 3-chlorobenzoate§	$C_{15}H_{21}ClO_2$	1920		2466		546	
2-Phenylethyl 3-chlorobenzoate	$C_{15}H_{13}ClO_2$	1978	58	2841	375	863	317
Octyl 4-chlorobenzoate§	$C_{15}H_{21}ClO_2$	1924		2470		546	
2-Phenylethyl 4-chlorobenzoate	$C_{15}H_{13}ClO_2$	1985	61	2844	374	859	313
Octyl pentafluorobenzoate§§	$C_{15}H_{17}F_5O_2$	1618		1888		270	
2-Phenylethyl pentafluorobenzoate	$C_{15}H_9F_5O_2$	1674	56	2265	377	591	321
Octyl 4-nitrobenzoate§§§	$C_{15}H_{21}NO_4$	2108		2874		766	
2-Phenylethyl 4-nitrobenzoate	$C_{15}H_{13}NO_4$	2169	61	—	—	—	—
Octyl 3,5-dinitrobenzoate§§§	$C_{15}H_{20}N_2O_6$	2343		3265		922	
2-Phenylethyl 3,5-dinitrobenzoate	$C_{15}H_{12}N_2O_6$	2399	56	—	—	—	—

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* $\Delta I = I$ (aromatic alcohol derivatives) − I (aliphatic alcohol derivatives).

** From ref. 5.

*** Obtained at 120°C.

§ From ref. 29.

§§ From ref. 33.

§§§ From ref. 35.

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