

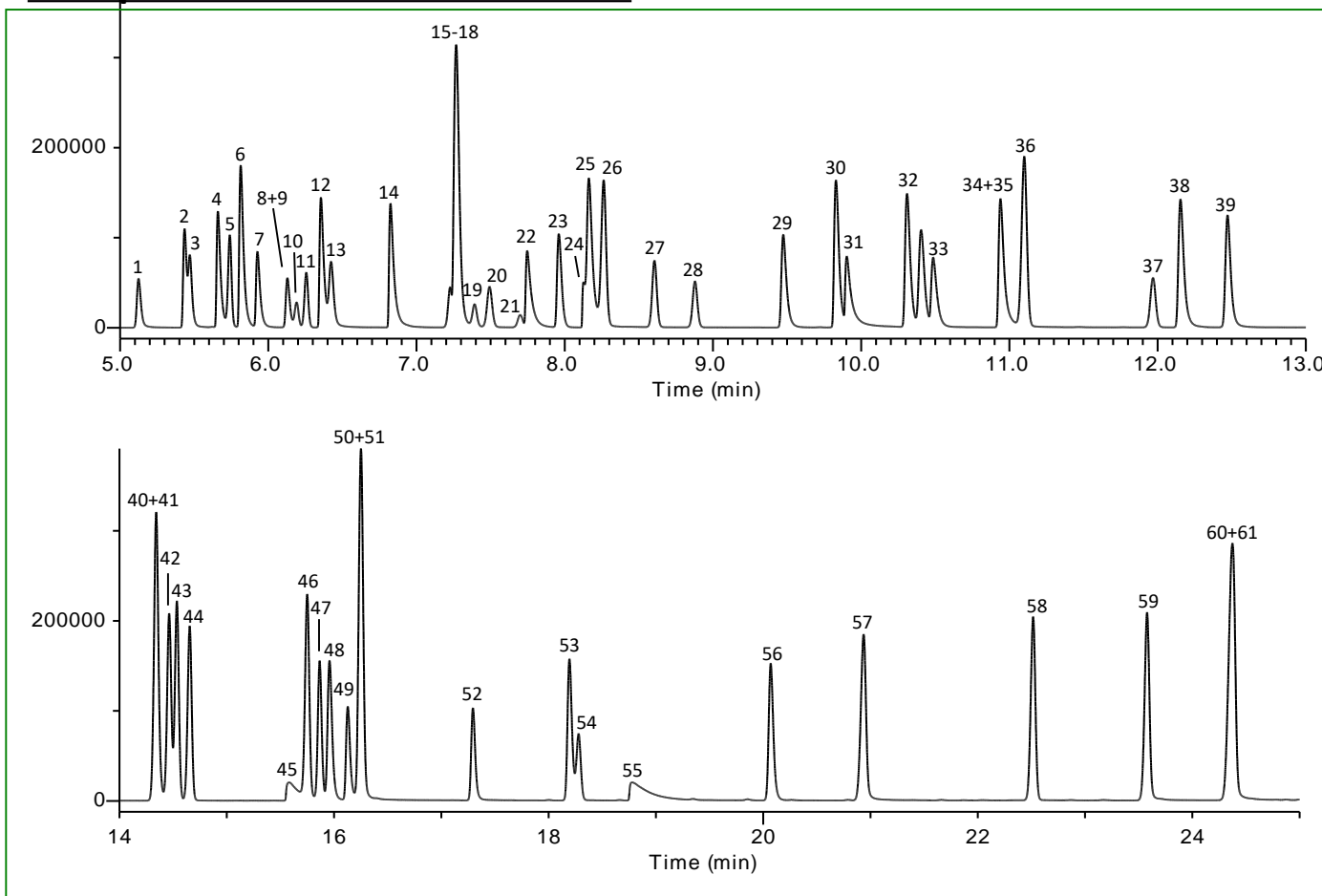
Analysis and Retention Index of 61 Components of Organic Solvents - Using InertCap 17

The retention index is a relatively representative index of the retention ratio of straight-chain alkanes and is used to study constituents based on the number of carbons in the molecule. It is one of the most useful pieces of information for qualitative analysis.

The retention index can be determined because in isothermal analysis the logarithm of the retention ratio for straight-chain alkanes is linearly related to the number of carbons, and the retention ratio is also linear to the number of carbons in thermal rise analysis.

In this report, InertCap 17 was used to determine the retention index of 61 components of organic solvents by isothermal and temperature rise analysis..

Example: Measurement of standard



Conditions

System	: GC - FID
Column	: InertCap 17 0.25 mm I.D. x 60 m df = 0.25 μ m
Col. Temp.	: 40 $^{\circ}$ C - 5 $^{\circ}$ C/min - 220 $^{\circ}$ C
Carrier Gas	: He 160 kPa
Injection	: Split flow 150 mL/min 240 $^{\circ}$ C
Detection	: FID Range 10 ⁰ 240 $^{\circ}$ C
Sample Size	: Mixed evenly 0.2 μ L

Chromatographic conditions described above.

For isothermal analysis, adjust the pressure so that the linear velocity is constant.

Retention index in the temperature rise analysis

Peak No.	Component	Retention index	Retention time	Peak No.	Component	Retention index	Retention time
1	Methanol	466	5.108	31	2-Ethoxyethanol (Cellosolve)	835	9.898
2	Ethanol	541	5.415				
3	Ethyl ether	550	5.511	32	4-Methyl-2-pentanone (MIBK)	849	10.302
4	2-Propanol (Isopropyl alcohol)	585	5.704				
5	<i>n</i> -Hexane	600	5.787	33	1,4-Dioxane	855	10.478
6	Tert-Butanol	607	5.829	34	1-Pentanol(Amyl alcohol)	871	10.941
7	Acetone	617	5.941	35	Isobutyl acetate	870	10.967
8	Carbon disulfide	633	6.118	36	Toluene	877	11.099
9	Methyl acetate	634	6.128	37	Tetrachloroethylene	906	11.967
10	Dichloromethane	635	6.193	38	2-Hexanone(MBK)	912	12.149
11	<i>trans</i> -1,2-Dichloroethylene	644	6.249	39	<i>n</i> -Butyl acetate	919	12.471
12	1-Propanol	655	6.374	41	Isopentyl acetate (Isoamyl acetate)	978	14.353
13	Acetonitrile	658	6.408				
14	2-Butanol	693	6.858	42	<i>p</i> -Xylene	981	14.466
15	Ethyl acetate	719	7.274	43	<i>m</i> -Xylene	983	14.539
16	2-Methyl-1-propanol (Isobutyl alcohol)	719	7.274	44	Chlorobenzene	987	14.649
				45	<i>N,N</i> -Dimethylformamide	1012	15.502
17	<i>cis</i> -1,2-Dichloroethylene	717	7.280	46	<i>o</i> -Xylene	1019	15.757
18	Methyl ethyl ketone	720	7.281	47	<i>n</i> -Pentyl acetate	1022	15.865
19	Chloroform	725	7.382	48	1-Methylcyclohexanol	1025	15.969
20	1,1,1-Trichloroethane	730	7.487	49	2-Butoxyethanol (Butyl cellosolve)	1030	16.127
21	Carbon tetrachloride	740	7.697				
22	Tetrahydrofuran	742	7.741	50	Cyclohexanol	1033	16.247
23	Isopropyl acetate	753	7.960	51	Styrene	1034	16.260
24	2-Methoxyethanol (Methyl cellosolve)	762	8.127	52	2-Ethoxyethyl acetate (Cellosolve acetate)	1063	17.297
26	Benzene	768	8.259	53	Cyclohexanone	1089	18.200
27	1,2-Dichloroethane	785	8.599	54	1,1,2,2-Tetrachloroethane	1092	18.281
28	Trichloroethylene	799	8.875	55	<i>N,N</i> -Dimethylacetamide	1100	18.581
29	<i>n</i> -Propyl acetate	820	9.468	56	4-Methylcyclohexanone	1143	20.091
30	3-Methyl-1-butanol (Isoamyl alcohol)	832	9.822	57	Phenol	1167	20.928
				58	1,2-Dichlorobenzene	1216	22.546
				59	<i>o</i> -Cresol	1252	23.627
				60	<i>p</i> -Cresol	1276	24.380
				61	<i>m</i> -Cresol	1277	24.410

In the case of temperature programming...

Because the retention ratio of straight-chain alkanes is linearly related to the number of carbons in straight-chain alkanes, the retention index is given by the following equation.

$$\text{Retention index } I = 100 \times \frac{\text{TR} - tR(Z)}{\text{TR}(Z+1) - tR(Z)} + 100 \times Z$$

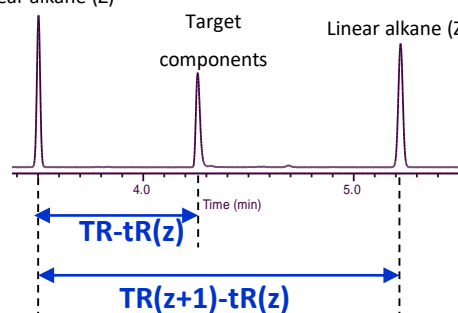
TR = retention time of the target component

TR(Z) = retention time of straight-chain alkanes that precede the components of interest

TR(Z+1) = retention time of straight-chain alkanes emerging after the components of interest

Z = number of carbons in straight-chain alkanes with a retention time tR(Z)

Linear alkane (Z)



Retention index in isothermal analysis-1

Peak No. (gradient temp.)	Component	40°C		80°C		120°C		160°C	
		Retention index	Retention time	Retention index	Retention time	Retention index	Retention time	Retention index	Retention time
1	Methanol	485	5.095	469	4.561	486	4.440	492	4.188
2	Ethanol	555	5.493	537	4.701	546	4.479	526	4.204
3	Ethyl ether	560	5.533	549	4.722	547	4.448	545	4.203
4	2-Propanol (Isopropyl alcohol)	591	5.808	577	4.785	575	4.471	576	4.214
5	<i>n</i> -Hexane	593	5.864	599	4.843	600	4.495	602	4.225
6	Tert-Butanol	611	6.041	597	4.838	595	4.490	595	4.222
7	Acetone	621	6.172	612	4.883	611	4.507	614	4.230
8	Carbon disulfide	638	6.465	665	5.056	682	4.619	716	4.291
9	Methyl acetate	643	6.498	635	4.960	634	4.533	630	4.238
10	Dichloromethane	646	6.548	650	5.019	660	4.568	670	4.260
11	<i>Trans</i> -1,2-Dichloroethylene	652	6.695	659	5.056	665	4.575	675	4.263
12	1-Propanol	664	6.921	656	5.043	658	4.598	658	4.253
13	Acetonitrile	666	6.929	664	5.080	672	4.618	675	4.263
14	2-Butanol	698	7.739	692	5.221	691	4.617	693	4.278
15	Ethyl acetate	723	8.489	720	5.426	713	4.657	709	4.289
16	2-Methyl-1-propanol (Isobutyl alcohol)	722	8.477	723	5.443	722	4.708	722	4.296
17	<i>cis</i> -1,2-Dichloroethylene	718	8.343	727	5.441	737	4.708	700	4.283
18	Methyl ethyl ketone	725	8.575	724	5.451	724	4.712	722	4.299
19	Chloroform	725	8.557	736	5.540	747	4.763	733	4.343
20	1,1,1-Trichloroethane	732	8.816	743	5.593	756	4.785	746	4.354
21	Carbon tetrachloride	742	9.171	755	5.668	771	4.791	790	4.357
22	Tetrahydrofuran	752	9.639	755	5.693	763	4.803	748	4.356
23	Isopropyl acetate	765	10.272	755	5.696	748	4.767	740	4.313
24	2-Methoxyethanol (Methyl cellosolve)	772	10.599	772	5.858	778	4.845	761	4.368
25	1-Butanol	772	10.544	769	5.830	768	4.817	747	4.355
26	Benzene	769	10.387	782	5.955	797	4.903	795	4.402
27	1,2-Dichloroethane	784	11.285	794	6.093	806	4.931	798	4.406
28	Trichloroethylene	795	11.890	807	6.252	822	4.986	820	4.431
29	<i>n</i> -Propyl acetate	826	14.377	818	6.388	816	4.967	811	4.383
30	3-Methyl-1-butanol (Isoamyl alcohol)	840	15.623	835	6.627	837	5.045	824	4.436

Case of isothermal analysis...

*Retention time in minutes

Because the logarithm of the retention ratio of straight-chain alkanes is linearly related to the number of carbons of straight-chain alkanes, the retention index is given by the following equation.

$$\text{Retention index } I = 100 \times \frac{\text{Log } t'R - \text{log } t'R(Z)}{\text{Log } t'R(Z+1) - \text{log } t'R(Z)} + 100 \times Z$$

t_R = retention time of the target component

$t_R(Z)$ = retention time of straight-chain alkanes that precede the components of interest

$t_R(Z+1)$ = retention time of straight-chain alkanes emerging after the component of interest

Z = number of carbons in straight-chain alkanes with a retention time t_R

$t'R$ = corrected retention time $t'R = t_R - t_0$

t_0 = hold-up time (elution time of non-retentive components)

Retention index in isothermal analysis-2

Peak No. (gradient temp.)	Component	40°C		80°C		120°C		160°C	
		Retention index	Retention time	Retention index	Retention time	Retention index	Retention time	Retention index	Retention time
31	2-Ethoxyethanol (Cellosolve)	840	15.567	840	6.695	847	5.086	839	4.455
32	4-Methyl-2-pentanone (MIBK)	855	17.188	852	6.913	854	5.118	842	4.459
33	1,4-Dioxane	859	17.707	863	7.142	873	5.204	871	4.501
34	1-Pentanol(Amyl alcohol)	880	20.404	874	7.328	875	5.213	866	4.493
35	Isobutyl acetate	877	20.051	871	7.242	866	5.153	907	4.560
36	Toluene	870	19.121	885	7.563	902	5.359	911	4.568
37	Tetrachloroethylene	894	22.560	913	8.260	934	5.563	948	4.644
38	2-Hexanone(MBK)	915	26.239	913	8.260	914	5.434	908	4.563
39	<i>n</i> -Butyl acetate	927	28.717	921	8.459	917	5.431	833	4.447
40	Ethylbenzene	964	38.328	980	10.601	998	6.099	1018	4.783
41	Isopentyl acetate (Isoamyl acetate)	983	44.553	978	10.534	976	5.891	973	4.702
42	<i>p</i> -Xylene	968	39.443	983	10.759	1001	6.133	1021	4.792
43	<i>m</i> -Xylene	970	39.928	985	10.851	1003	6.156	1023	4.798
44	Chlorobenzene	969	39.648	989	11.026	1013	6.258	1040	4.850
45	<i>N,N</i> -Dimethylformamide	1024	62.048	1020	12.614	1024	6.383	1029	4.858
46	<i>o</i> -Xylene	1001	51.487	1019	12.593	1040	6.583	1064	4.937
47	<i>n</i> -Pentyl acetate	1028	64.789	1023	12.813	1019	6.329	1018	4.824
48	1-Methylcyclohexanol	1016	58.325	1026	13.012	1042	6.598	1062	4.928
49	2-Butoxyethanol (Butyl cellosolve)	1030	65.385	1031	13.333	1038	6.557	1048	4.877
50	Cyclohexanol	1024	62.620	1034	13.511	1050	6.707	1070	4.959
51	Styrene	1016	58.413	1033	13.422	1053	6.744	1076	4.979
52	2-Ethoxyethyl acetate (Cellosolve acetate)	1079	100.294	1066	15.832	1057	6.800	1049	4.927
53	Cyclohexanone	1069	91.908	1087	17.634	1107	7.633	1133	5.234
54	1,1,2,2-Tetrachloroethane	1075	96.316	1088	17.763	1105	7.582	1126	5.202
55	<i>N,N</i> -Dimethylacetamide	1156	147.858	1119	20.350	1112	7.728	1120	5.223
56	4-Methylcyclohexanone	1148	144.450	1155	23.493	1155	8.752	1184	5.528
57	Phenol	—	—	1190	27.059	1174	9.280	1198	5.688
58	1,2-Dichlorobenzene	—	—	—	—	1225	10.955	1265	6.222
59	<i>o</i> -Cresol	—	—	—	—	1255	12.084	1283	6.402
60	<i>p</i> -Cresol	—	—	—	—	1278	13.076	1301	6.593
61	<i>m</i> -Cresol	—	—	—	—	1279	13.122	1303	6.606

*Retention time in minutes

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