

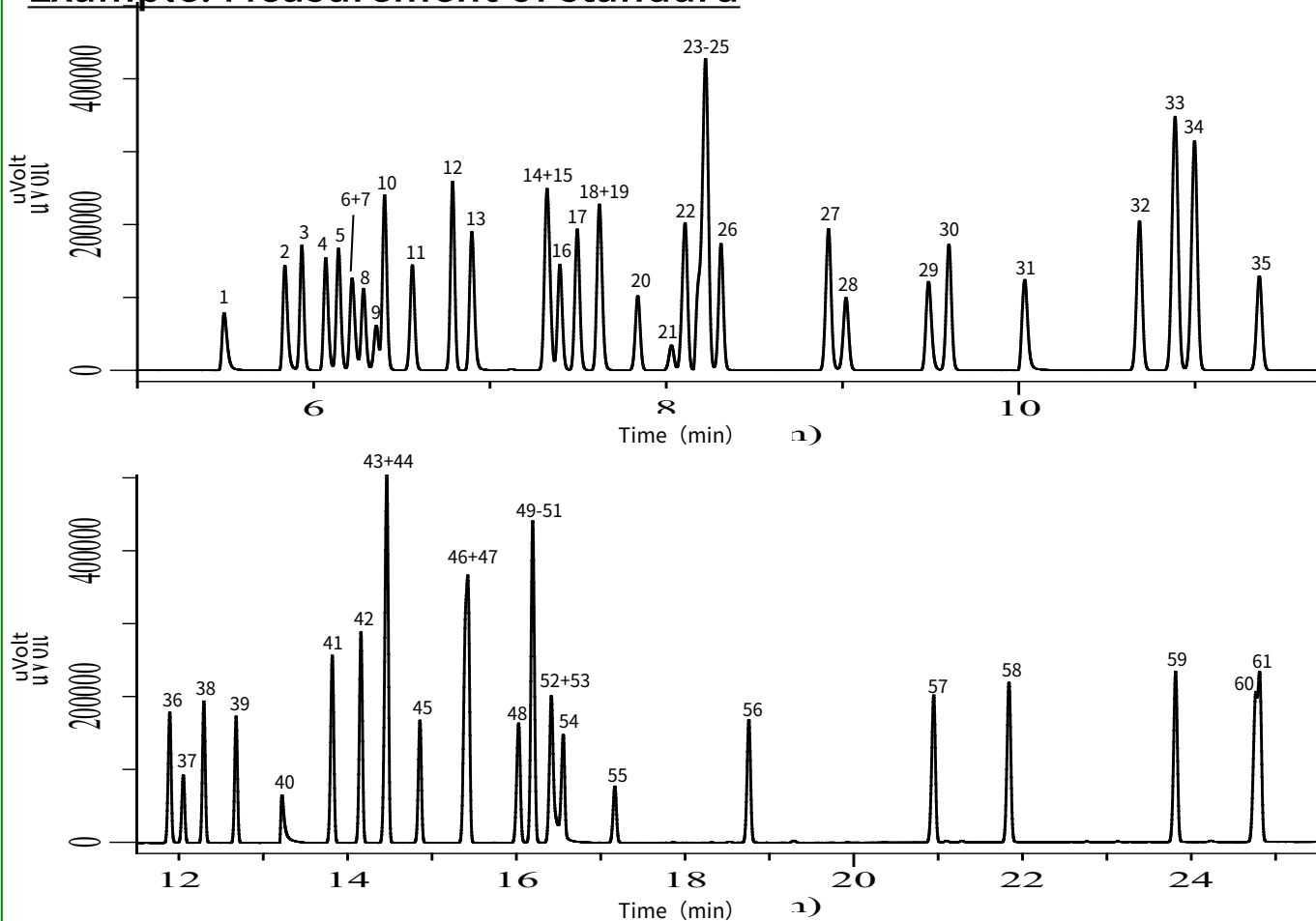
Analysis and Retention Index for 61 Components of Organic Solvents - Using InertCap 1301

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 application note, InertCap 1301 was used to determine the retention index of 61 components in organic solvents by isothermal and temperature-rise analysis.

Example: Measurement of standard



Conditions

System	: GC - FID
Column	: InertCap 1301 0.25 mm I.D. x 60 m df = 0.25 μ m
Col. Temp.	: 40 °C - 5 °C/min - 220 °C
Carrier Gas	: He 160 kPa
Injection	: Split flow 150 mL/min 240 °C
Detection	: FID Range 10 ⁴ 240 °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	421	5.473	32	4-Methyl-2-pentanone (MIBK)	775	10.672
2	Ethanol	500	5.819	33	3-Methyl-1-butanol (Isoamyl alcohol)	783	10.897
3	Ethyl ether	511	5.918	34	Toluene	786	10.982
4	Acetone	525	6.052	35	Isobutyl acetate	799	11.353
5	2-Propanol (Isopropyl alcohol)	532	6.125	36	1-Pentanol (Amyl alcohol)	815	11.897
6	Acetonitrile	540	6.202	37	Tetrachloroethylene	819	12.037
7	Carbon disulfide	542	6.215	38	2-Hexanone (MBK)	827	12.291
8	Methyl acetate	547	6.268	39	<i>N-Butyl acetate</i>	838	12.669
9	Dichloromethane	555	6.339	40	<i>N,N-Dimethylformamide</i>	853	13.196
10	Tert-Butanol	560	6.388	41	Chlorobenzene	871	13.830
11	<i>Trans-1,2-Dichloroethylene</i>	576	6.544	42	Ethylbenzene	882	14.173
12	<i>N-Hexane</i>	600	6.773	43	<i>m-Xylene</i>	890	14.467
13	1-Propanol	606	6.886	44	<i>P-Xylene</i>	891	14.481
14	Methyl ethyl ketone	629	7.302	45	Isopentyl acetate (Isoamyl acetate)	902	14.871
15	<i>cis-1,2-Dichloroethylene</i>	630	7.316	46	<i>o-Xylene</i>	917	15.407
16	Ethyl acetate	633	7.378	47	Styrene	918	15.442
17	2-Butanol	639	7.483	48	Cyclohexanol	934	16.047
18	Tetrahydrofuran	645	7.598	49	1-Methylcyclohexanol	939	16.201
19	Chloroform	646	7.603	50	<i>n-Pentyl acetate</i>	939	16.207
20	1,1,1-Trichloroethane	658	7.825	51	2-Ethoxyethyl acetate (Cellosolve acetate)	939	16.226
21	Carbon tetrachloride	668	8.017	52	<i>N,N-Dimethylacetamide</i>	944	16.372
22	2-Methyl-1-propanol (Isobutyl alcohol)	672	8.090	53	Cyclohexanone	945	16.429
23	2-Methoxyethanol (Methyl cellosolve)	676	8.164	54	2-Butoxyethanol (Butyl cellosolve)	949	16.577
24	1,2-Dichloroethane	678	8.193	55	1,1,2,2-Tetrachloroethane	966	17.165
25	Benzene	679	8.210	56	4-Methylcyclohexanone	1010	18.782
26	Isopropyl acetate	684	8.297	57	1,2-Dichlorobenzene	1072	20.966
27	1-Butanol	712	8.924	58	Phenol	1098	21.885
28	Trichloroethylene	715	9.017	59	<i>o-Cresol</i>	1156	23.844
29	1,4-Dioxane	732	9.474	60	<i>p-Cresol</i>	1184	24.789
30	<i>n-Propyl acetate</i>	736	9.586	61	<i>m-Cresol</i>	1186	24.838
31	2-Ethoxyethanol (Cellosolve)	752	10.032				

※Retention time in minutes

In the case of temperature programming...

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

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

T R = retention time of the target component

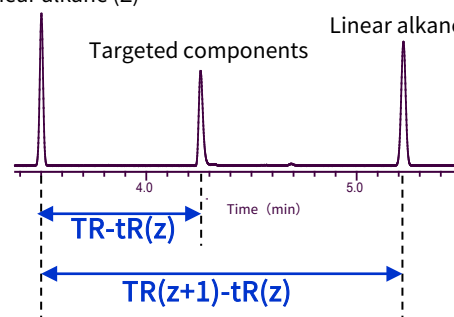
T R(Z) = retention time of straight-chain alkanes that precede the components of interest

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

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

Linear alkane (Z)

Linear alkane (Z+1)



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	440	5.472	429	4.903	414	4.681	400	4.418
2	Ethanol	506	5.918	494	5.029	485	4.731	470	4.443
3	Ethyl ether	517	6.021	514	5.082	510	4.754	496	4.456
4	Acetone	534	6.209	534	5.138	532	4.778	522	4.468
5	2-Propanol (Isopropyl alcohol)	545	6.344	534	5.138	525	4.770	512	4.463
6	Acetonitrile	551	6.424	551	5.195	551	4.800	543	4.478
7	Carbon disulfide	548	6.383	563	5.240	575	4.843	594	4.509
8	Methyl acetate	558	6.527	554	5.208	551	4.801	541	4.477
9	Dichloromethane	564	6.610	566	5.252	569	4.825	569	4.493
10	Tert-Butanol	572	6.738	562	5.235	555	4.806	550	4.482
11	<i>Trans</i> -1,2-Dichloroethylene	581	6.911	585	5.333	589	4.855	588	4.505
12	<i>n</i> -Hexane	600	7.288	600	5.408	599	4.873	596	4.510
13	1-Propanol	612	7.554	599	5.402	591	4.858	582	4.501
14	Methyl ethyl ketone	636	8.215	635	5.611	635	4.940	633	4.538
15	<i>cis</i> -1,2-Dichloroethylene	636	8.198	639	5.639	645	4.960	648	4.550
16	Ethyl acetate	642	8.397	636	5.618	632	4.933	625	4.531
17	2-Butanol	650	8.653	639	5.637	633	4.936	627	4.533
18	Tetrahydrofuran	651	8.688	656	5.763	664	5.005	668	4.569
19	Chloroform	653	8.751	654	5.744	658	4.991	660	4.561
20	1,1,1-Trichloroethane	662	9.088	670	5.870	679	5.044	686	4.587
21	Carbon tetrachloride	671	9.446	680	5.963	691	5.077	700	4.602
22	2-Methyl-1-propanol (Isobutyl alcohol)	682	9.945	669	5.868	663	5.002	657	4.558
23	2-Methoxyethanol (Methyl cellosolve)	681	9.914	680	5.960	682	5.051	682	4.583
24	1,2-Dichloroethane	680	9.853	686	6.022	694	5.088	700	4.602
25	Benzene	680	9.848	689	6.048	698	5.108	710	4.613
26	Isopropyl acetate	689	10.298	683	5.989	678	5.041	672	4.572
27	1-Butanol	719	11.978	706	6.229	699	5.102	694	4.595
28	Trichloroethylene	714	11.701	722	6.412	730	5.205	738	4.648
29	1,4-Dioxane	733	13.005	738	6.627	745	5.260	751	4.666
30	<i>n</i> -Propyl acetate	742	13.710	737	6.613	733	5.216	729	4.636
31	2-Ethoxyethanol (Cellosolve)	757	14.947	755	6.873	755	5.302	756	4.673

In the 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, the retention index is given by the following equation.

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

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 components of interest

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

$t'R$ = 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 order during heating	Peak name	40°C		80°C		120°C		160°C	
		Retention index	Retention time	Retention index	Retention time	Retention index	Retention time	Retention index	Retention time
32	4-Methyl-2-pentanone (MIBK)	778	17.087	778	7.276	780	5.416	782	4.714
33	3-Methyl-1-butanol (Isoamyl alcohol)	791	18.697	780	7.306	773	5.384	772	4.697
34	Toluene	783	17.695	792	7.555	802	5.538	813	4.769
35	Isobutyl acetate	802	20.205	798	7.676	794	5.489	791	4.729
36	1-Pentanol (Amyl alcohol)	824	23.509	812	7.994	805	5.547	802	4.748
37	Tetrachloroethylene	813	21.793	825	8.338	839	5.755	851	4.848
38	2-Hexanone (MBK)	828	24.313	828	8.418	830	5.698	833	4.808
39	<i>N</i> -Butyl acetate	843	27.103	838	8.690	835	5.727	831	4.804
40	<i>N,N</i> -Dimethylformamide	854	29.554	856	9.231	860	5.912	867	4.885
41	Chlorobenzene	862	31.410	876	9.945	891	6.172	907	4.992
42	Ethylbenzene	874	34.490	884	10.288	895	6.223	907	4.993
43	<i>m</i> -Xylene	882	36.857	892	10.617	902	6.291	913	5.011
44	<i>p</i> -Xylene	883	36.970	893	10.633	903	6.297	914	5.013
45	Isopentyl acetate (Isoamyl acetate)	905	44.145	901	11.019	899	6.249	908	4.995
46	<i>o</i> -Xylene	906	44.623	918	11.824	931	6.588	945	5.112
47	Styrene	908	45.313	919	11.867	931	6.586	943	5.108
48	Cyclohexanol	933	55.886	934	12.692	940	6.693	951	5.134
49	1-Methylcyclohexanol	934	56.509	938	12.954	947	6.781	959	5.164
50	<i>n</i> -Pentyl acetate	943	60.782	939	12.992	936	6.644	933	5.074
51	2-Ethoxyethyl acetate (Cellosolve acetate)	949	63.843	939	13.012	932	6.594	927	5.052
52	<i>N,N</i> -Dimethylacetamide	943	60.634	943	13.278	948	6.790	954	5.145
53	Cyclohexanone	931	54.974	945	13.365	961	6.968	979	5.244
54	2-Butoxyethanol (Butyl cellosolve)	949	63.703	949	13.613	951	6.834	955	5.149
55	1,1,2,2-Tetrachloroethane	961	70.865	965	14.701	972	7.129	983	5.259
56	4-Methylcyclohexanone	992	92.138	1006	18.215	1023	8.018	1044	5.547
57	1,2-Dichlorobenzene	—	—	1062	25.019	1082	9.430	1106	5.943
58	Phenol	—	—	1107	32.758	1088	9.636	1082	5.777
59	<i>o</i> -Cresol	—	—	1164	46.904	1152	11.811	1149	6.288
60	<i>p</i> -Cresol	—	—	1195	57.523	1181	13.116	1176	6.535
61	<i>m</i> -Cresol	—	—	1197	58.137	1183	13.189	1177	6.548

* Retention time in minutes

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