GT078

GL Sciences Inc.

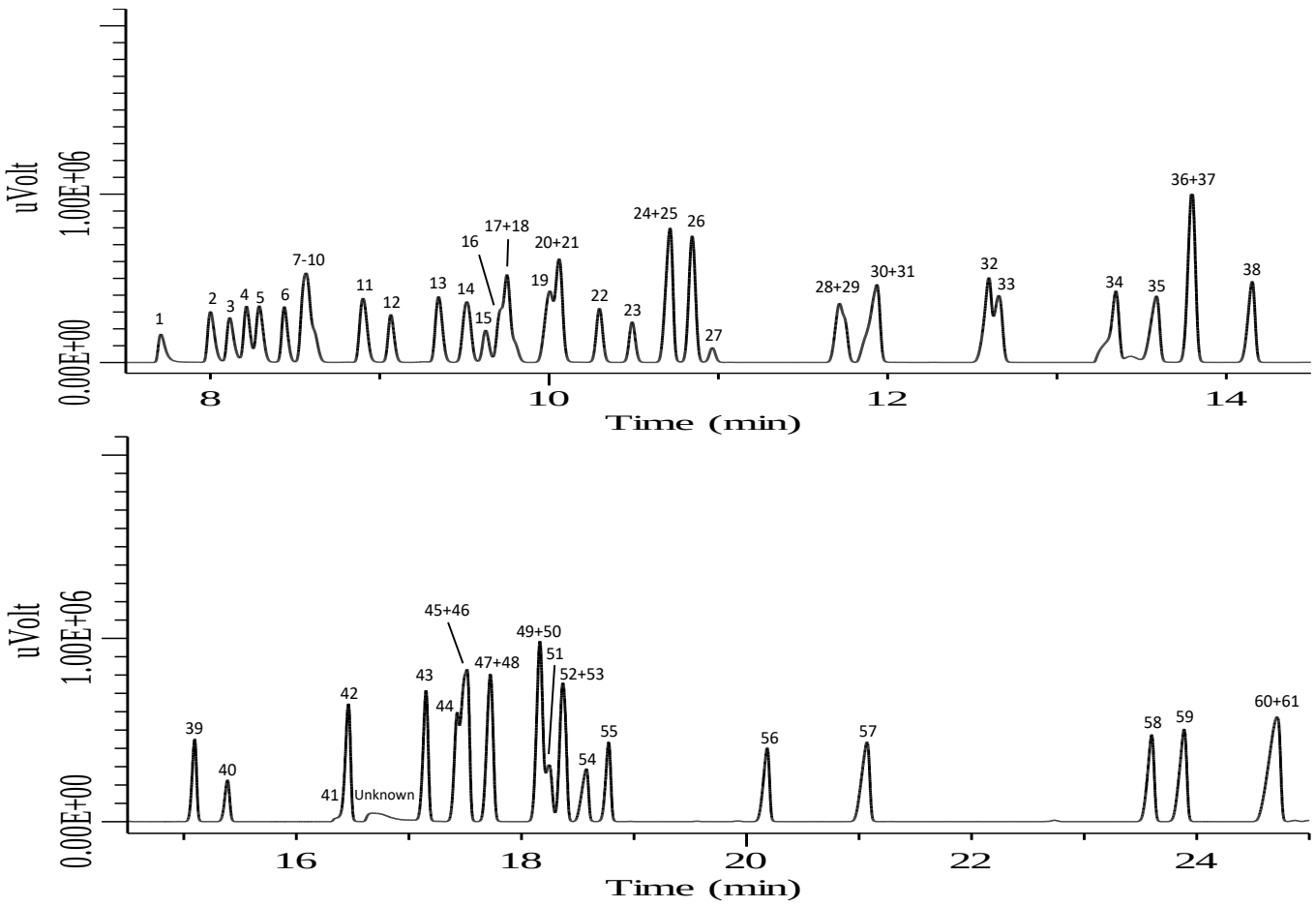
Analysis and Retention Index of 61 Components of Organic Solvents using Nitrogen Carrier Gas - Using InertCap 1

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 1 was used to determine the isothermal and temperature-rise retention indices of 61 organic solvents using nitrogen as the carrier gas.

Example: Measurement of standards



Conditions

System	: GC - FID
Column	: InertCap 1 0.25 mm I.D. x 60 m df = 0.25 µm
Col. Temp.	: 40 ˚C - 5 ˚C/min - 220 ˚C
Carrier Gas	: N_2 90 kPa
Injection	: Split 1:50 240 ˚C
Detection	: FID Range 10^0 240 ˚C
Sample Size	: Mixed evenly 0.2 µL

Chromatographic conditions described above.

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

Retention index in the temperature-rise analysis

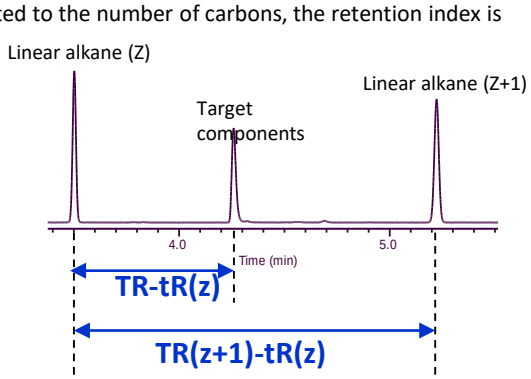
Peak No.	Component	Retention index	Retention time	Peak No.	Component	Retention index	Retention time
1	Methanol	397	7.674	32	3-Methyl-1-butanol (Isoamyl alcohol)	717	12.567
2	Ethanol	405	7.965				
3	Acetonitrile	428	8.084	33	4-Methyl-2-pentanone (MIBK)	719	12.634
4	Acetone	448	8.183				
5	2-Propanol (Isopropyl alcohol)	462	8.257	34	*N,N-Dimethylformamide*	739	13.268
				35	1-Pentanol(Amyl alcohol)	747	13.546
6	Ethyl ether	492	8.409	36	Isobutyl acetate	754	13.761
7	Carbon disulfide	509	8.568	37	Toluene	755	13.782
8	*Tert-Butanol*	506	8.528	38	2-Hexanone(MBK)	766	14.134
9	Methyl acetate	508	8.554	39	*N-Butyl acetate*	795	15.071
10	Dichloromethane	511	8.596	40	Tetrachloroethylene	803	15.359
11	1-Propanol	533	8.878	41	*N,N-Dimethylacetamide*	829	16.308
12	*Trans-1,2-Dichloroethylene*	546	9.045	42	Chlorobenzene	832	16.441
13	Methyl ethyl ketone	568	9.327	43	Ethylbenzene	851	17.128
14	2-Butanol	580	9.491	44	Isopentyl acetate (Isoamyl acetate)	858	17.381
15	*cis-1,2-Dichloroethylene*	589	9.602				
16	Ethyl acetate	596	9.697	45	*M-Xylene*	859	17.448
17	*n-Hexane*	600	9.746	46	*P-Xylene*	860	17.488
18	Chloroform	602	9.786	47	Cyclohexanone	866	17.682
19	2-Methyl-1-propanol (Isobutyl alcohol)	610	9.975	48	Cyclohexanol	866	17.682
				49	2-Ethoxyethyl acetate (Cellosolve acetate)	877	18.12
20	Tetrahydrofuran	613	10.037				
21	2-Methoxyethanol (Methyl cellosolve)	614	10.060	50	Styrene	878	18.125
				51	1-Methylcyclohexanol	879	18.177
22	1,2-Dichloroethane	623	10.281	52	1,1,2,2-Tetrachloroethane	881	18.269
23	1,1,1-Trichloroethane	632	10.478	53	*O-Xylene*	883	18.332
24	Isopropyl acetate	641	10.683	54	2-Butoxyethanol (Butyl cellosolve)	888	18.528
25	1-Butanol	642	10.705				
26	Benzene	654	10.975	55	*N-Pentyl acetate*	894	18.742
27	Carbon tetrachloride	653	10.948	56	4-Methylcyclohexanone	931	20.171
28	1,4-Dioxane	685	11.684	57	Phenol	953	21.037
29	Trichloroethylene	687	11.723	58	1,2-Dichlorobenzene	1018	23.582
30	2-Ethoxyethanol (Cellosolve)	693	11.877	59	*O-Cresol*	1025	23.868
				60	*P-Cresol*	1048	24.752
31	*n-Propyl acetate*	695	11.915	61	*M-Cresol*	1049	24.791

* Retention time in minutes
* Components with a symmetry factor of 1.5 or higher are highlighted in red.

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.

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



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)

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	378	7.619	354	7.195	317	7.745	387	7.502
2	Ethanol	448	8.037	418	7.318	415	7.815	447	7.539
3	Acetonitrile	460	8.141	445	7.383	447	7.850	476	7.563
4	Acetone	480	8.333	461	7.428	457	7.862	485	7.572
5	2-Propanol (Isopropyl alcohol)	491	8.462	468	7.449	461	7.867	484	7.571
6	Ethyl ether	509	8.695	491	7.529	489	7.909	498	7.585
7	Carbon disulfide	509	8.687	491	7.529	491	7.912	493	7.580
8	*Tert-Butanol*	520	8.869	503	7.577	506	7.937	515	7.600
9	Methyl acetate	524	8.930	507	7.592	508	7.941	513	7.598
10	Dichloromethane	526	8.967	515	7.627	519	7.962	534	7.617
11	1-Propanol	552	9.496	534	7.720	527	7.977	541	7.624
12	*Trans-1,2-Dichloroethylene*	562	9.725	555	7.838	556	8.043	575	7.661
13	Methyl ethyl ketone	581	10.249	572	7.953	571	8.081	588	7.677
14	2-Butanol	592	10.585	580	8.008	582	8.112	590	7.680
15	*Cis-1,2-Dichloroethylene*	597	10.756	593	8.105	594	8.149	613	7.710
16	Ethyl acetate	604	11.021	592	8.097	587	8.128	592	7.683
17	*N-Hexane*	606	11.067	598	8.152	598	8.162	608	7.703
18	Chloroform	606	11.092	602	8.188	610	8.200	622	7.723
19	2-Methyl-1-propanol (Isobutyl alcohol)	620	11.633	606	8.220	602	8.175	613	7.711
20	Tetrahydrofuran	619	11.589	617	8.323	624	8.249	640	7.751
21	2-Methoxyethanol (Methyl cellosolve)	620	11.633	613	8.283	615	8.218	629	7.733
22	1,2-Dichloroethane	630	12.099	630	8.455	638	8.301	654	7.773
23	1,1,1-Trichloroethane	634	12.277	640	8.567	650	8.348	666	7.794
24	Isopropyl acetate	649	13.063	642	8.584	636	8.291	644	7.756
25	1-Butanol	649	13.069	642	8.580	638	8.302	645	7.759
26	Benzene	649	13.061	657	8.766	666	8.423	684	7.828
27	Carbon tetrachloride	655	13.371	662	8.838	673	8.452	690	7.840
28	1,4-Dioxane	685	15.442	689	9.233	695	8.567	711	7.883
29	Trichloroethylene	686	15.488	692	9.280	699	8.594	716	7.894
30	2-Ethoxyethanol (Cellosolve)	694	16.187	693	9.298	691	8.548	704	7.868
31	*N-Propyl acetate*	699	16.563	693	9.302	689	8.536	696	7.851

* Retention time in minutes
* Components with a symmetry factor of 1.5 or higher are highlighted in red.

In the case of isothermal analysis...

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.

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

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 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 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
32	3-Methyl-1-butanol (Isoamyl alcohol)	722	18.851	715	9.712	713	8.673	722	7.908
33	4-Methyl-2-pentanone (MIBK)	721	18.697	721	9.827	725	8.748	736	7.941
34	*N,N-Dimethylformamide*	739	20.861	742	10.301	748	8.905	765	8.019
35	1-Pentanol(Amyl alcohol)	754	22.924	747	10.423	745	8.884	752	7.983
36	Isobutyl acetate	760	23.753	755	10.623	753	8.946	758	8.000
37	Toluene	752	22.648	760	10.790	771	9.091	787	8.084
38	2-Hexanone(MBK)	768	25.064	768	10.988	769	9.077	781	8.067
39	*n-Butyl acetate*	799	31.041	794	11.813	789	9.259	795	8.111
40	Tetrachloroethylene	795	30.203	806	12.255	819	9.562	836	8.259
41	*N,N-Dimethylacetamide*	827	38.136	830	13.123	838	9.787	851	8.318
42	Chlorobenzene	823	36.940	834	13.332	849	9.931	867	8.388
43	Ethylbenzene	843	43.012	852	14.222	864	10.140	878	8.442
44	Isopentyl acetate (Isoamyl acetate)	862	49.713	858	14.520	856	10.028	859	8.352
45	*m-Xylene*	852	45.945	861	14.677	870	10.234	882	8.463
46	*p-Xylene*	853	46.363	862	14.732	871	10.242	885	8.478
47	Cyclohexanone	854	46.568	866	15.008	882	10.421	902	8.562
48	Cyclohexanol	860	49.053	866	14.958	875	10.309	890	8.501
49	2-Ethoxyethyl acetate (Cellosolve acetate)	886	60.426	878	15.695	871	10.253	871	8.408
50	Styrene	868	52.032	878	15.709	889	10.542	905	8.578
51	1-Methylcyclohexanol	870	52.877	879	15.772	890	10.559	908	8.597
52	1,1,2,2-Tetrachloroethane	873	54.268	881	15.920	892	10.589	910	8.607
53	*o-Xylene*	872	53.872	883	16.058	895	10.648	912	8.617
54	2-Butoxyethanol (Butyl cellosolve)	887	61.049	888	16.368	890	10.554	897	8.537
55	*n-Pentyl acetate*	899	66.827	894	16.809	891	10.570	891	8.504
56	4-Methylcyclohexanone	—	—	928	19.542	945	11.648	967	8.966
57	Phenol	—	—	955	22.227	946	11.681	948	8.841
58	1,2-Dichlorobenzene	—	—	1013	30.331	1031	14.255	1052	9.724
59	*o-Cresol*	—	—	1028	33.057	1024	14.001	1031	9.509
60	*p-Cresol*	—	—	1049	37.332	1044	14.762	1047	9.665
61	*m-Cresol*	—	—	1050	37.593	1045	14.808	1047	9.672

* Retention time in minutes
* Components with a symmetry factor of 1.5 or higher are highlighted in red.

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