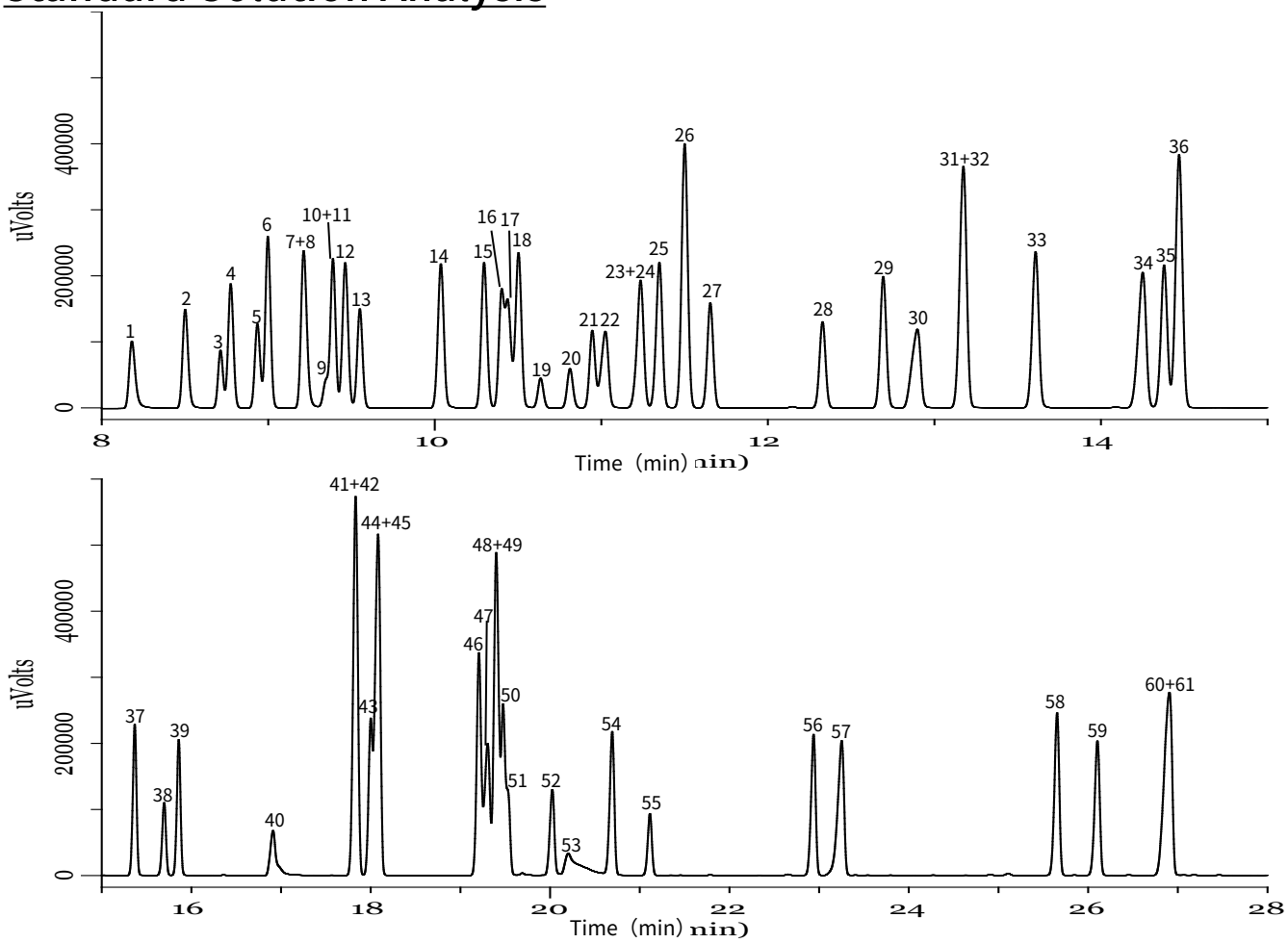
GT126

GL Sciences Inc.

Analysis and Retention Indices of 61 Organic Solvent Components by Nitrogen Carriers

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

Standard Solution Analysis



Conditions

System	: GC-FID
Column	: InertCap 25 0.25 mm I.D. × 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 Auto Range 240 °C
Sample Size	: Mixed evenly 0.2 µL

The above chromatographic conditions.

Constant-temperature analytical conditions regulate the pressure so that the linear velocity is constant.

Retention Index in the Warming Analysis

Peak No.	Peak name	Retention index	Retention time	Peak No.	Peak name	Retention index	Retention time
1	Methanol	424	8.185	32	1,4-Dioxane	781	13.158
2	Ethanol	497	8.498	33	4-Methyl-2-pentanone (MIBK)	798	13.598
3	Ethyl ether	522	8.827				
4	2-Propanol (Isopropyl alcohol)	529	8.708	34	1-Pentanol (Amyl alcohol)	817	14.227
5	Acetone	548	8.930	35	Isobutyl acetate	821	14.362
6	Tert-Butanol	555	8.993	36	Toluene	824	14.460
7	Methyl acetate	580	9.205	37	2-Hexanone (MBK)	851	15.353
8	Acetonitrile	580	9.213				
9	Dichloromethane	595	9.342	38	Tetrachloroethylene	861	15.685
10	Carbon disulfide	598	9.368	39	*n-Butyl acetate*	865	15.847
11	*n-Hexane*	600	9.383	40	*N,N-Dimethylformamide*	897	16.892
12	1-Propanol	605	9.458	41	Chlorobenzene	922	17.802
13	*Trans-1,2-Dichloroethylene*	610	9.552	42	Ethylbenzene	922	17.822
14	2-Butanol	639	10.030	43	Isopentyl acetate (Isoamyl acetate)	927	17.977
15	Methyl ethyl ketone	654	10.285				
16	Ethyl acetate	661	10.390	44	*p-Xylene*	928	18.032
17	*Cis-1,2-Dichloroethylene*	664	10.437	45	*m-Xylene*	929	18.060
18	2-Methyl-1-propanol (Isobutyl alcohol)	667	10.497	46	*o-Xylene*	960	19.188
				47	Cyclohexanol	961	19.255
19	Chloroform	675	10.628	48	1-Methylcyclohexanol	964	19.338
20	Tetrahydrofuran	686	10.800	49	Styrene	965	19.382
21	1,1,1-Trichloroethane	694	10.937	50	*n-Pentyl acetate*	967	19.442
22	2-Methoxyethanol (Methyl cellosolve)	698	11.010	51	2-Butoxyethanol (Butyl cellosolve)	967	19.473
23	Carbon tetrachloride	706	11.202	52	2-Ethoxyethyl acetate (Cellosolve acetate)	982	19.990
24	Isopropyl acetate	707	11.225				
25	1-Butanol	711	11.330	53	*N,N-Dimethylacetamide*	982	20.015
26	Benzene	717	11.488	54	Cyclohexanone	1000	20.663
27	1,2-Dichloroethane	723	11.643	55	1,1,2,2-Tetrachloroethane	1011	21.077
28	Trichloroethylene	749	12.318	56	4-Methylcyclohexanone	1062	22.915
29	*n-Propyl acetate*	763	12.683	57	Phenol	1069	23.173
30	2-Ethoxyethanol (Cellosolve)	770	12.872	58	1,2-Dichlorobenzene	1119	25.637
				59	*o-Cresol*	1126	26.082
31	3-Methyl-1-butanol (Isoamyl alcohol)	781	13.148	60	*p-Cresol*	1136	26.818
				61	*m-Cresol*	1137	26.868

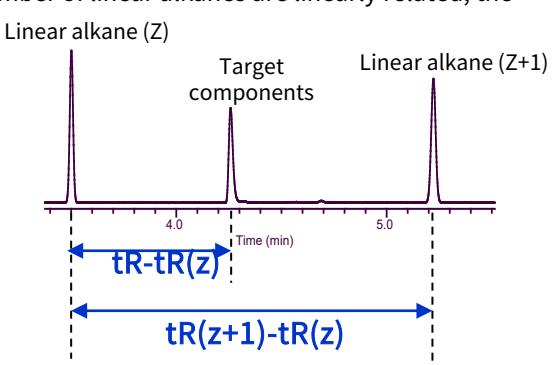
* Retention time in minutes
* Components with a symmetry factor of 1.5 or higher are in red.

In the case of warming analysis...

Since the retention ratio of linear alkanes and the carbon number of linear alkanes are linearly related, the retention index is given by the following equation:

$$\text{Retention index I} = 100 \times \frac{t_R - t_{R(Z)}}{t_{R(Z+1)} - t_{R(Z)}} + 100 \times Z$$

t_R = retention-time of the components of interest
tR(Z) = retention time of straight-chain alkanes emerging in front of the component of interest
$t_{R(Z+1)}$ = retention time of linear alkanes emerging after the components of interest
The numbers of carbons in linear alkanes with Z = retention-time $t_{R(Z)}$



Retention Index-1 in Homeothermal Analysis

During warming Peak order	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
1	Methanol	434	7.927	437	7.265	441	6.867	488	6.595
2	Ethanol	501	8.458	496	7.425	497	6.933	497	6.602
3	Ethyl ether	532	8.827	529	7.533	526	6.972	522	6.617
4	2-Propanol (Isopropyl alcohol)	541	8.953	536	7.562	531	6.978	536	6.625
5	Acetone	558	9.235	557	7.652	557	7.020	559	6.640
6	*Tert-Butanol*	566	9.380	562	7.673	562	7.027	559	6.640
7	Methyl acetate	587	9.805	583	7.783	580	7.060	583	6.657
8	Acetonitrile	586	9.785	585	7.793	589	7.078	591	6.663
9	Dichloromethane	595	10.002	599	7.875	605	7.113	614	6.683
10	Carbon disulfide	590	9.882	607	7.930	624	7.157	650	6.720
11	*n-Hexane*	600	10.128	600	7.883	600	7.102	600	6.670
12	1-Propanol	608	10.352	604	7.910	603	7.108	608	6.677
13	*Trans-1,2-Dichloroethylene*	611	10.418	615	7.982	620	7.147	626	6.695
14	2-Butanol	648	11.683	644	8.210	642	7.202	647	6.717
15	Methyl ethyl ketone	662	12.303	660	8.358	660	7.252	662	6.735
16	Ethyl acetate	670	12.690	664	8.397	660	7.252	656	6.728
17	*Cis-1,2-Dichloroethylene*	666	12.498	672	8.480	680	7.317	687	6.767
18	2-Methyl-1-propanol (Isobutyl alcohol)	675	12.913	671	8.468	668	7.278	672	6.747
19	Chloroform	677	13.032	683	8.597	689	7.348	699	6.783
20	Tetrahydrofuran	685	13.477	691	8.695	699	7.385	707	6.795
21	1,1,1-Trichloroethane	691	13.800	698	8.792	709	7.423	718	6.812
22	2-Methoxyethanol (Methyl cellosolve)	696	14.158	700	8.807	708	7.418	709	6.798
23	Carbon tetrachloride	701	14.450	712	8.980	725	7.490	737	6.842
24	Isopropyl acetate	713	15.290	706	8.892	700	7.388	693	6.775
25	1-Butanol	716	15.492	713	8.993	712	7.432	710	6.800
26	Benzene	714	15.343	724	9.158	736	7.540	749	6.862
27	1,2-Dichloroethane	723	16.035	729	9.237	737	7.545	746	6.858
28	Trichloroethylene	747	18.265	756	9.730	767	7.697	778	6.917
29	*n-Propyl acetate*	771	20.922	765	9.912	762	7.667	757	6.877
30	2-Ethoxyethanol (Cellosolve)	772	21.102	774	10.107	782	7.785	782	6.927
31	3-Methyl-1-butanol (Isoamyl alcohol)	785	22.872	783	10.320	789	7.828	783	6.928

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

In the case of homeothermal analysis....

Since the logarithm of the retention ratio of the linear alkanes and the number of carbons of the linear alkanes are in a linear relationship, the retention index is given by the following equation:

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

tR = retention time of the components of interest.
tR(Z) = retention time of straight-chain alkanes emerging in front of the component of interest
$t_{R(Z+1)}$ = retention time of linear alkanes emerging after the components of interest

The numbers of carbons in linear alkanes with Z = 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-retained components)

Retention Index-2 in Homeothermal Analysis

During warming Peak order	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	1,4-Dioxane	780	22.113	785	10.362	795	7.867	802	6.970
33	4-Methyl-2-pentanone (MIBK)	798	24.905	798	10.708	802	7.908	801	6.967
34	1-Pentanol (Amyl alcohol)	821	28.912	818	11.275	837	8.057	818	7.008
35	Isobutyl acetate	872	41.963	822	11.402	837	8.057	814	6.997
36	Toluene	816	28.002	828	11.590	869	8.215	855	7.107
37	2-Hexanone(MBK)	853	36.477	853	12.515	896	8.357	855	7.107
38	Tetrachloroethylene	848	35.273	864	12.970	915	8.603	895	7.240
39	*n-Butyl acetate*	812	27.313	867	13.108	905	8.445	858	7.118
40	*N,N-Dimethylformamide*	893	49.567	897	14.610	931	8.865	910	7.293
41	Chlorobenzene	904	54.200	921	16.053	957	9.377	958	7.498
42	Ethylbenzene	909	56.165	922	16.113	955	9.322	950	7.460
43	Isopentyl acetate (Isoamyl acetate)	931	67.440	927	16.508	948	9.177	920	7.335
44	*p-Xylene*	914	58.833	927	16.492	959	9.408	954	7.482
45	*m-Xylene*	915	59.048	928	16.540	959	9.422	955	7.483
46	*o-Xylene*	942	73.517	957	18.787	982	9.962	990	7.663
47	Cyclohexanol	950	78.497	959	18.977	981	9.940	987	7.645
48	1-Methylcyclohexanol	950	79.087	961	19.175	983	10.003	990	7.663
49	Styrene	948	77.608	962	19.253	984	10.033	993	7.680
50	*n-Pentyl acetate*	973	95.490	968	19.788	976	9.807	960	7.507
51	2-Butoxyethanol (Butyl cellosolve)	963	87.628	966	19.647	981	9.948	977	7.593
52	2-Ethoxyethyl acetate (Cellosolve acetate)	995	115.833	984	21.383	983	10.003	974	7.578
53	*N,N-Dimethylacetamide*	977	99.103	981	21.067	992	10.245	1002	7.730
54	Cyclohexanone	980	101.488	994	22.508	1012	10.770	1036	7.945
55	1,1,2,2-Tetrachloroethane	999	119.040	1007	23.987	1020	10.947	1038	7.963
56	4-Methylcyclohexanone	1037	166.425	1052	30.552	1070	12.380	1092	8.392
57	Phenol	1061	206.025	1063	32.628	1072	12.438	1087	8.345
58	1,2-Dichlorobenzene	1092	271.508	1108	44.442	1121	15.310	1136	9.248
59	*o-Cresol*	-	-	1120	51.382	1125	15.738	1134	9.195
60	*p-Cresol*	-	-	1130	58.872	1135	16.843	1143	9.440
61	*m-Cresol*	-	-	1131	59.400	1136	16.923	1144	9.460

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

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