SELECTIVITY OF A PHENYL-BONDED SILICA GEL*

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SUMMARY

The selectivity of a phenyl-bonded silica gel was examined as the difference between the capacity ratios of five groups of compounds in acetonitrile– and tetrahydrofuran–water mixtures, in pure tetrahydrofuran and in *n*-hexane. The five groups were polyaromatic hydrocarbons, alkylbenzenes, halogenated benzenes, aliphatic alcohols and alkanes. In the reversed-phase mode, the polyaromatic hydrocarbons were retained more than the other groups, as expected, but selectivity was clearly observed in the chromatographic behavior of the chlorobenzenes. The use of the π energy effect obtained from the Van der Waals volume and the delocalization energy of solutes was tested for the optimization of reversed-phase liquid chromatography.

INTRODUCTION

Octadecyl-bonded silica gels are commonly used in liquid chromatography. The prediction of retention times on these gels in the reversed-phase mode has been discussed previously[1]. A difficult separation on octadecyl-bonded silica gels can be achieved by changing the eluent or the column. In particular, π–π interactions on phenyl-bonded silica gels are expected, as was previously observed on organic porous polymer gels[2]. However, the nature of the interactions on phenyl-bonded silica gels was hardly discussed. Therefore, in this work the chromatographic behaviour of five types of compounds, namely alkanes, alkylbenzenes, aliphatic alcohols, halogenated benzenes and polyaromatic hydrocarbons, was examined on phenyl- and octadecyl-bonded silica gels. Their capacity ratios were related to their Van der Waals volumes, molecular connectivity, partition coefficient between octanol and water (log *P*) and π energy. The Van der Waals volume was calculated by the Bondi method[3], the molecular connectivity was evaluated according to Kier and Hall's method[4] and the log *P* values were obtained by Rekker's method[5]. The π energy effect was related to delocalization energies taken from the literature[6–8]. The chromatographic behavior of the different compounds on both packings was examined in tetrahydrofuran–water mixtures and *n*-hexane.

TABLE I

PHYSICAL PARAMETERS AND LOGARITHM OF CAPACITY RATIOS OF STANDARD COMPOUNDS

No.	Compound	V_{wv}*	x**	$\log P$***	Dle§	YMC phenyl§§	
						ACN conc. (%)	
						80	70
1	Benzene	48.36	2.000	2.280	2.000	−0.3707	−0.1252
2	Naphthalene	73.96	3.405	3.208	3.683	−0.2308	0.0373
3	Biphenyl	90.08	4.017	3.772	4.383	−0.1684	0.1211
4	Fluorene	93.22	4.611	3.906	4.75	−0.1402	0.1525
5	Phenanthrene	99.56	4.815	4.378	5.448	−0.1069	0.1850
6	Anthracene	99.56	4.809	4.378	5.314	−0.0950	0.1988
7	Pyrene	109.04	5.559	5.030	6.506	−0.0296	0.2675
8	Chrysene	125.16	6.226	5.545	7.190	0.0214	0.3419
9	Tetrasene	125.16	6.214	5.790	6.932	0.0465	0.3713
10	Benzopyrene	134.64	6.970	6.200	—	0.1055	0.4290
11	Pentacene	150.76	7.619	6.960	—	—	—
12	Toluene	59.51	2.411	2.588	2.15	−0.3113	−0.0545
13	Ethylbenzene	69.74	2.971	3.118	—	−0.2531	−0.0218
14	Isopropylbenzene	77.02	3.354	3.525	—	−0.2070	0.0860
15	Propylbenzene	79.97	3.471	3.648	—	−0.1908	0.0998
16	Butylbenzene	90.20	3.971	4.178	—	−0.1335	0.1758
17	Hexylbenzene	110.66	4.971	5.238	—	−0.0128	0.3290
18	Heptylbenzene	120.89	5.471	5.768	—	0.0454	0.4055
19	Octylbenzene	131.12	5.971	6.297	—	0.1045	0.4829
20	Nonylbenzene	141.35	6.471	6.828	—	0.1625	0.5563
21	Decylbenzene	151.58	6.971	7.358	—	0.2204	0.6333
22	Chlorobenzene	57.84	2.513	2.808	2.05	−0.3113	−0.0516
23	1,2-Dichlorobenzene	67.32	3.031	3.523	—	−0.2531	0.0164
24	1,3-Dichlorobenzene	67.32	3.025	3.532	—	−0.2523	0.0288
25	1,4-Dichlorobenzene	67.32	3.025	3.532	—	−0.2479	0.0288
26	1,2,4-Trichlorobenzene	76.80	3.544	4.197	—	−0.1870	0.1018
27	1,3,5-Trichlorobenzene	76.80	3.538	4.197	—	−0.1739	0.1161
28	1,2,3,4-Tetrachlorobenzene	86.28	4.068	4.944	—	−0.1154	0.1776
29	1,2,3,5-Tetrachlorobenzene	86.28	4.062	4.944	—	−0.1170	0.1853
30	1,2,4,5-Tetrachlorobenzene	86.28	4.062	4.944	—	−0.1165	0.1819
31	Pentachlorobenzene	95.76	4.587	5.691	—	−0.0403	0.2675
32	Hexachlorobenzene	105.24	5.105	6.438	—	0.0465	0.3651
33	Bromobenzene	60.96	2.492	3.017	—	−0.2915	−0.0245
34	Iodobenzene	65.48	3.215	3.334	—	−0.2436	0.0288
35	Butyl alcohol	52.40	2.023	0.801	—	−0.7406	−0.5214
36	Pentyl alcohol	62.63	2.523	1.331	—	−0.6603	−0.4386
37	Hexyl alcohol	72.86	3.023	1.861	—	−0.5877	−0.3541
38	Heptyl alcohol	83.09	3.525	2.391	—	−0.5134	−0.2566
39	Octyl alcohol	93.32	4.023	2.921	—	−0.4499	−0.1849
40	Decyl alcohol	113.78	5.024	3.981	—	−0.3138	−0.0235
41	Dodecyl alcohol	134.24	6.024	5.041	—	−0.1889	0.1318
42	Tetradecyl alcohol	154.70	7.024	6.071	—	−0.0620	0.2857
43	Hexadecyl alcohol	175.16	8.024	7.101	—	0.0617	0.4449
44	Pentane	58.03	2.414	2.994	—	−0.2191	0.0866
45	Hexane	68.26	2.914	3.524	—	−0.1684	0.1495
46	Heptane	78.49	3.414	4.054	—	−0.1059	0.2131
47	Octane	88.72	3.914	4.584	—	−0.0457	0.2981
48	Decane	109.18	4.914	5.644	—	0.0816	0.4511
49	Dodecane	129.64	5.914	6.704	—	0.1944	0.6136
	Void volume (ml)††					1.850	1.750

 * Van der Waals volume (cm^3/mole) calculated by the Bondi method[3].
 ** Molecular connectivity[4].
 *** Partition coefficient between octanol-water calculated by Rekker's method[5].
 § Delocalization energy (kcal) from refs. 6 8.
 §§ ACN = acetonitrile; THF = tetrahydrofuran.

60	50	THF conc. (%) 60	50	π_I[§§§]	ACN conc. (%) 90	70	THF conc. (%) 70	60	π_{II}[§§§]
0.0852	0.2953	0.1662	0.2931	2.185	−0.2626	0.2203	0.1735	0.3801	1.875
0.2864	0.5616	0.2322	0.4144	3.399	−0.0723	0.4741	0.1916	0.4255	3.865
0.4014	0.7173	0.2903	0.5125	5.130	0.0013	0.6085	0.2266	0.4886	5.556
0.4319	0.7489	0.2970	0.5208	4.830	0.0768	0.6768	0.2331	0.5002	5.264
0.4705	0.7960	0.2788	0.5026	5.448	0.1292	0.7322	0.1930	0.4564	5.743
0.4906	0.8258	0.2927	0.5204	4.687	0.1598	0.7709	0.2090	0.4695	5.353
0.5589	0.9038	0.2829	0.5129	4.855	0.2956	0.9097	0.1943	0.4569	5.401
0.6604	1.043	0.3239	0.5825	7.209	0.3536	1.024	0.2090	0.4966	7.305
0.7019	1.094	0.3473	0.6166	5.688	0.4185	1.107	0.2642	0.5338	6.467
0.7576	1.156	0.3278	0.5910	6.288	0.5456	1.231	0.2167	0.5015	6.566
—	—	—	—	—	—	—	—	—	—
0.1740	0.4168	0.2142	0.3786	2.698	−0.1341	0.3772	0.2331	0.4569	2.254
0.2729	0.5461	0.2669	0.4634	2.728	−0.0308	0.5183	0.2770	0.5307	2.661
0.3540	0.6517	0.3070	0.5343	2.478	0.0552	0.6447	0.3142	0.5792	2.747
0.3733	0.6770	0.3216	0.5458	2.691	0.0926	0.6886	0.3303	0.6006	2.816
0.4701	0.8072	0.3701	0.6219	2.838	0.2154	0.8564	0.3771	0.6713	2.975
0.662	1.066	0.4568	0.7627	2.892	0.4644	1.200	0.4677	0.7972	3.244
0.7635	1.194	0.4974	0.8276	2.990	0.5925	1.378	0.5080	0.8646	3.292
0.8624	1.325	0.5374	0.8938	3.025	0.7223	—	0.5525	0.9221	3.353
0.9586	1.449	0.5748	0.9517	3.179	0.8514	—	0.5936	1.017	3.433
1.055	1.556	0.6112	1.011	3.395	0.9825	—	0.6370	1.112	3.566
0.1833	0.4250	0.2021	0.3640	1.988	−0.1484	0.3651	0.1889	0.4109	2.118
0.2642	0.5288	0.2161	0.3960	2.269	−0.0324	0.5024	0.1889	0.4199	2.410
0.2815	0.5530	0.2635	0.4648	1.682	0.0311	0.5787	0.2619	0.5121	1.679
0.2807	0.5560	0.2837	0.4899	1.672	−0.0122	0.5405	0.2630	0.5160	2.076
0.3708	0.6654	0.3178	0.5481	1.653	0.1578	0.7356	0.3162	0.5881	1.778
0.3855	0.6860	0.3701	0.6113	n[†]	0.2566	0.8461	0.4129	0.7007	0.785
0.4566	0.7729	0.3328	0.5693	n	0.2765	0.8766	0.3293	0.6095	2.020
0.4708	0.7924	0.3887	0.6477	n	0.3464	0.9614	0.4266	0.7250	1.296
0.4682	0.7895	0.3938	0.6551	n	0.3238	0.9399	0.4194	0.7157	1.511
0.5679	0.9116	0.4306	0.7103	n	0.4633	1.110	0.4772	0.7886	1.495
0.6809	1.051	0.44991	0.8041	n	0.6022	1.288	0.5611	0.8883	1.282
0.2134	0.4635	0.2132	0.3837	1.816	−0.1031	0.4128	0.1930	0.4239	2.174
0.2772	0.5336	0.2377	0.4259	1.180	−0.0340	0.4970	0.2077	0.4473	2.132
−0.3942	−0.2699	−0.1876	−0.2189	—	−0.6669	−0.3570	−0.2294	−0.1340	—
−0.2676	−0.1192	−0.0956	−0.0817	—	−0.5425	−0.2021	−0.1755	−0.0267	—
−0.1618	0.0286	−0.0471	0.0289	—	−0.4142	−0.0417	−0.0947	0.0363	—
−0.0563	0.1685	0.0152	0.1305	—	−0.2773	0.1243	−0.0741	0.1229	—
0.0482	0.3021	0.0671	0.2227	—	−0.1436	0.2884	−0.0221	0.1937	—
0.2493	0.5687	0.1541	0.3734	—	0.1162	0.6283	0.0770	0.3294	—
0.4485	0.8221	0.2377	0.5116	—	−0.3786	0.9774	0.1693	0.4541	—
0.6411	1.072	0.3193	0.6390	—	0.6438	1.333	0.2607	0.5787	—
0.8353	1.326	0.3932	0.7606	—	0.8991	—	0.3401	0.7078	—
0.3328	0.6171	0.3343	0.5367	0	0.2402	0.8099	0.4269	0.6938	0
0.4243	0.7416	0.3845	0.6200	0	0.3699	1.035	0.4795	0.7648	0
0.5264	0.8668	0.4264	0.6842	0	0.5055	1.170	0.5298	0.8323	0
0.6308	1.005	0.4562	0.7596	0	0.6408	1.384	0.5810	0.8978	0
0.8322	1.272	0.5415	0.8817	0	0.9115	—	0.6473	1.011	0
1.028	—	0.6241	1.015	0	1.114	—	0.7415	—	0
1.700	1.690	1.670	1.460	—	2.295	2.040	1.672	1.665	—

[§§§] π energy effect; π_I obtained on the phenyl packing and π_{II} obtained on the ODS packing.

[†] Not available.

[††] The void volume in acetonitrile–water mixtures was obtained from the elution volume of fructose and that n tetrahydrofuran–water mixtures was obtained from that of tetrahydrofuran[9].

EXPERIMENTAL

The instrument used has been described previously[1]. The columns were a YMC phenyl (10 cm × 6.0 mm I.D.) and a YMC ODS (15 cm × 6.0 mm I.D.), kindly donated by Yamamura Chem. Lab., Kyoto, Japan. The theoretical plate number of both columns was over 74,000/m. The pore size of the silica gel was 100 Å and the particle size was 5 μm. The column temperature was 40°C. The chemicals used are listed in Table I with their related physical parameters.

RESULTS AND DISCUSSION

The specificity of the phenyl-bonded silica gel was examined in n-hexane. The retention of all the compounds was very weak, except for the alcohols. An increase in the number of double bonds increased the retention, and an increase in the length of the alkyl chain decreased the retention. The tendency was similar to that observed on a perfluorocarbon-modified silica gel[8]. In addition, the retention of the polyaromatic hydrocarbons on the phenyl-bonded silica gel was slightly weaker than that on the octadecyl-bonded silica gel. All the other compounds were more retained on the phenyl-bonded silica gel.

The size of the octadecyl column was 50% larger than the phenyl column, but the exclusion limits measured in 100% tetrahydrofuran were reversed (0.961 and 1.011 ml, respectively), which means that the octadecyl-bonded packing has a smaller pore volume than the phenyl-bonded packing. This may be related to the larger molecular size of the octadecyl chain which capped the small pore and channels; also, the thickness of the organic phase was different. This result also supports the unexpected elution volume obtained for these compounds in n-hexane, for which the elution volume on the phenyl column was larger than that on the octadecyl column.

Therefore, the capacity ratio measured with both columns were calculated following the same procedure. The indicators for the measurement of the void volume were fructose and tetrahydrofuran in acetonitrile–water and tetrahydrofuran–water mixtures[9]. The dead volume of the instrument was 89 μl for the UV detector and 319 μl for the differential refractometer.

As previously described, the system used for the prediction of retention time in reversed-phase liquid chromatography (log P) is limited with octadecyl-bonded silica gels. The molecular connectivity and Van der Waals volume based systems were not adequate alone and required the addition of the π energy effect for optimization. A similar result was obtained on both the YMC phenyl and ODS columns. Logarithms of the capacity ratios obtained from these columns are presented in Table I. Examples of the relationship between log k' measured in acetonitrile–water and the Van der Waals volumes are shown in Figs. 1 and 2.

When Figs. 1 and 2 are compared, the chromatographic behavior of all the compounds looked similar; however, as expected, the polyaromatic hydrocarbons were more retained on the phenyl-bonded silica gel and the alkanes were more retained on the octadecyl-bonded silica gel. This tendency can be clearly seen in Fig. 3.

The capacities of the two columns were different and therefore the selectivities of the columns could not be directly compared using the capacity ratios obtained.
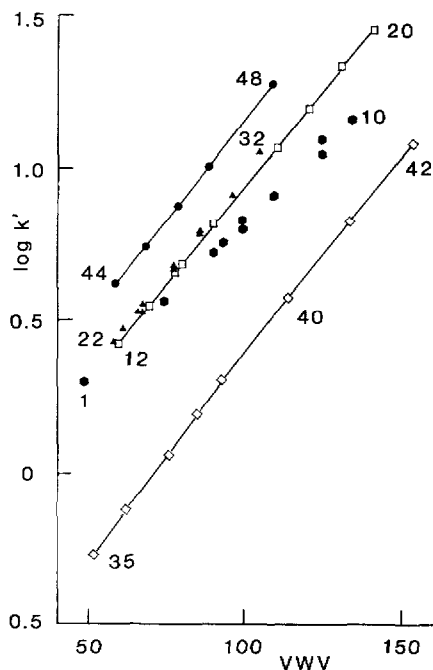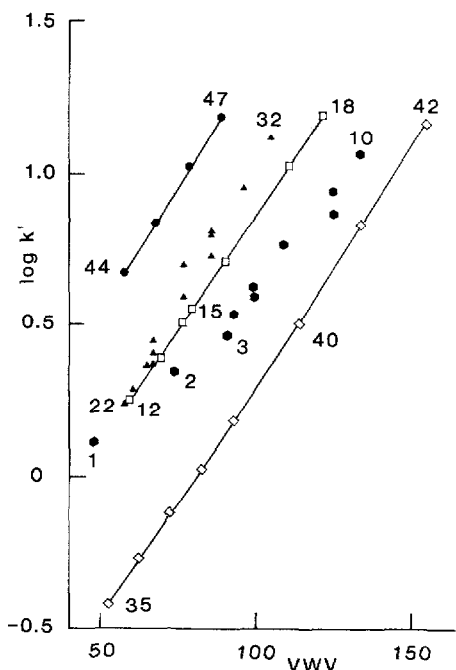
Fig. 1. Relationship between the Van der Waals volume (VWV) and log k' obtained on a YMC ODS column using 75% acetonitrile–water at 40°C. Each symbol indicates a group of compounds and the numbers are same as in Table I.

Fig. 2. Relationship between the Van der Waals volume (VWV) and log k' obtained on a YMC phenyl column using 50% acetonitrile–water at 40°C. Symbols and numbers as in Fig. 1.
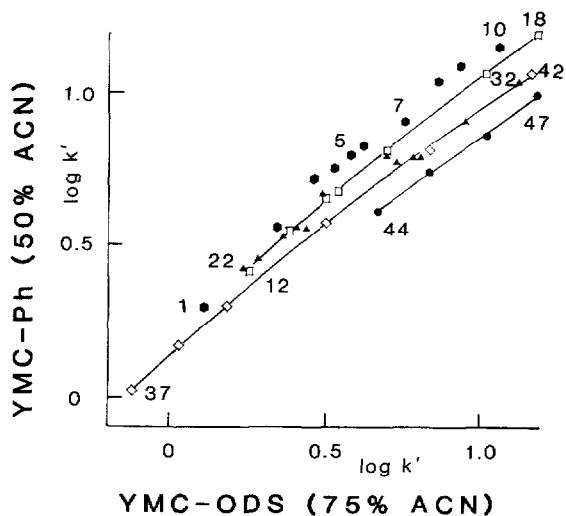
Fig. 3. Selectivity between YMC phenyl and ODS columns. For details, see Figs. 1 and 2.

Therefore, as an example, the capacity ratios obtained for each group of compounds in acetonitrile–water (50:50) on the phenyl-bonded silica gel and in acetonitrile–water (75:25) on the octadecyl-bonded silica gel were correlated.

Assuming a linear relationship between the capacity ratios on each column, the correlation coefficient found for polyaromatic hydrocarbons was 0.987 (n = 10), and they were retained 1.5 times more than on the phenyl-bonded silica gel. The retention of biphenyl was larger and that of pyrene was smaller on the phenyl-bonded silica gel than on the octadecyl-bonded silica gel. The correlation coefficient for alkylbenzenes was 0.998 (n = 7) and these compounds were retained 1.3 times more on the phenyl-bonded silica gel. For halogenated benzenes the correlation coefficient was 0.970 (n = 13) and these compounds were retained 1.2 times more on the phenyl-bonded silica gel. Good selectivity was observed within this group. Monohalogenated benzenes were relatively more retained and 1,3,5-tri-, 1,2,3,4- and 1,2,3,5-tetra-, penta- and hexachlorobenzenes were less retained on the phenyl-bonded silica gel. For alcohols the correlation coefficient was 0.995 (n = 8) and the retention was 1.2 times more on the phenyl-bonded silica gel. Finally, the correlation coefficient for alkanes was 0.9997 (n = 4) and the retention on the phenyl-bonded packing was 20% times smaller. The selectivity of alkylbenzenes, alcohols, and alkanes between both packings decreased with increase in their retention times.

Examples of the chromatographic behavior on both packings in tetrahydrofuran–water mixtures are shown in Figs. 4 and 5. It can be seen that the specific selectivity on the phenyl-bonded silica gel was not clear with the tetrahydrofuran–water mixture. Therefore, the retention ratios of each group on both packings were calculated. The correlation coefficients for polyaromatic hydrocarbons, alkylbenzenes, halogenared benzenes, alcohols and alkanes were 0.948 (n =
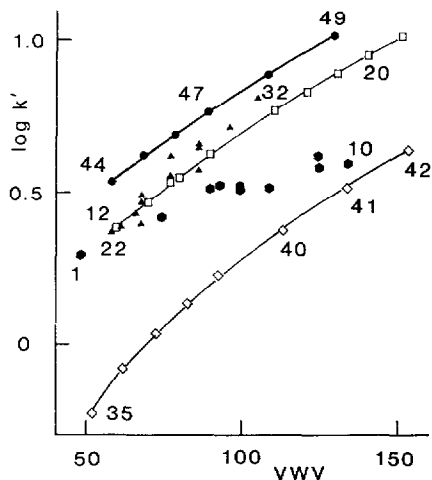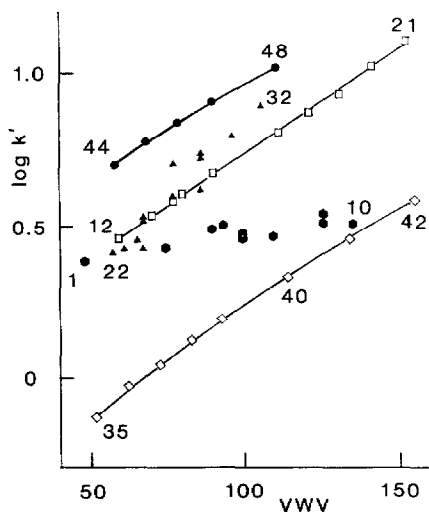

Fig. 4. Relationship between the Van der Waals volume (VWV) and log k' obtained on a YMC ODS column using 60% tetrahydrofuran–water at 40°C. Symbols and numbers as in Fig. 1.

Fig. 5. Relationship between Van der Waals volume (VWV) and log k' obtained on a YMC phenyl column using 50% tetrahydrofuran–water at 40°C. Symbols and numbers as in Fig. 1.
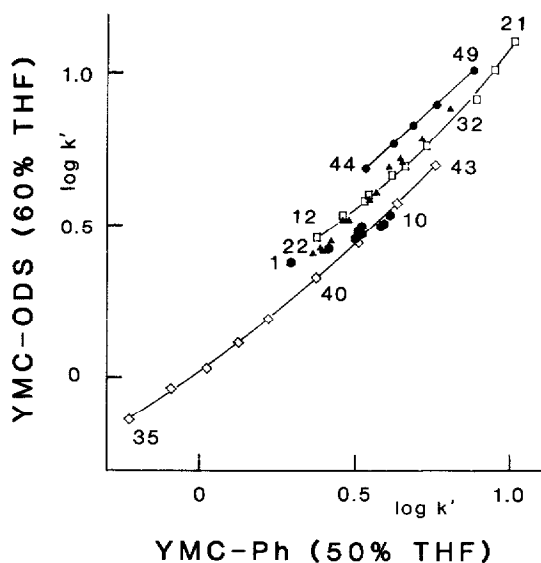
Fig. 6. Selectivity between YMC phenyl and ODS columns in tetrahydrofuran–water mixtures. For details, see Figs. 4 and 5.

10), 0.991 (n = 10), 0.996 (n = 13), 0.999 (n = 9) and 0.9997 (n = 5), respectively, and the capacities of the phenyl-bonded silica gel were 1.1, 0.9, 0.9, 1.0 and 0.7 times, those of the octyl-bonded silica, respectively.

If the retention of alkylbenzenes on both packings was fixed at 1.0, and the selectivity of the packings was re-examined, the polyaromatic hydrocarbons were retained 20% more and the alkanes 20% less on the phenyl-bonded packing using both acetonitrile and tetrahydrofuran–water mixtures. Alcohols were more retained on the phenyl-bonded silica gel in tetrahydrofuran–water mixtures. 1,3,5-Tri-, 1,3,3,5-tetra-, penta- and hexachlorobenzenes were also less retained using tetrahydrofuran–water mixtures. An example of the selectivity using tetrahydrofuran–water on both packings is shown in Fig. 6. The separation of polyaromatic hydrocarbons was very difficult with tetrahydrofuran–water mixtures even with a switch from an aliphatic to an aromatic packing.

A comparison of the retentions of polyaromatic hydrocarbons on phenylbonded silica gel using 60% acetonitrile water and 50% tetrahydrofuran–water mixtures indicated that they were retained up to 20% more than alkylbenzenes using acetonitrile–water mixtures, and the retentions of alcohols and alkanes were similar. However, the retention of halogenated benzenes was 15% less than that of alkylbenzenes. 1,2-Di-, 1,2,4,5-tetra- and hexachlorobenzenes were less retained and 1,4-di- and 1,3,5-trichlorobenzenes were less retained than the average of this group. The selectivity was also examined from the π energy effect, which was derived from the Van der Waals volume and delocalization energy of polyaromatic hydrocarbons[1]. The π energy effect was calculated as follows. The maximum capacity ratio [log k' (Van der Waals) (vwv)] was obtained from the relationship between the logarithm of the capacity ratios and the Van der Waals volumes of the alkanes. The difference (Δlog k') was obtained by subtraction of the value of the observed log k' from the

calculated log k' (vwv). Then the $\Delta\log k'$ values were related to the delocalization energy. The correlation coefficients between $\Delta\log k'$ values obtained from the results on the YMC ODS column and the delocalization energy were 0.921, 0.963 and 0.974 ($n = 11$) in 90, 80 and 70% acetonitrile water mixtures, respectively. The correlation coefficients between the $\Delta\log k'$ values obtained from the results on the YMC phenyl column and the delocalization energy 0.936, 0.975 and 0.984 ($n = 11$) in 70, 60 and 50% acetonitrile–water mixtures, respectively.

For the calculation of the π energy effect for the other compounds, benzene, naphthalene, phenanthrene, chrysene and tetrasene were selected for octadecyl-bonded silica gels and benzene, naphthalene, fluorene, phenanthrene and chrysene for the phenyl-bonded silica gel. The π energy effect is given in Table I.

The calculated π energy effects obtained on the different packings were similar, and the correlation coefficient for polyaromatic hydrocarbons observed on Develosil and Hypersil ODS columns was 0.982 ($n = 10$)[1], When the value of anthracene was rejected, the correlation coefficient was 0.997 ($n = 9$). The correlation coefficient between the YMC and Hypersil ODS columns was 0.999 ($n = 10$) and the difference of the π energy effect was within 2%. The selectivity for the retention of polyaromatic hydrocarbons has been reported[10], but the π energy effect observed was very constant.

The correlation of the π energy effect for alkylbenzenes was also very good. The correlation coefficient between Develosil and Hypersil ODS columns was 0.999 ($n = 8$) and that between YMC and Hypersil ODS columns was 0.996 ($n = 10$). The π energy effect of polyaromatic hydrocarbons and alkylbenzenes was reasonably constant using different acetonitrile water mixtures, and the mean values for halogenated benzenes were also similar. The correlation coefficient between Develosil and Hypersil ODS columns for alkylbenzenes was 0.992 ($n = 13$) and that between YMC and Hypersil ODS columns was 0.980 ($n = 13$). However, the solvent effect cannot be neglected for the halogenated benzenes, as a decrease in the concentration of acetonitrile increased the π values.

These values of the π energy effect using octadecyl-bonded packings were constant, and can be used for the optimization of liquid chromatography. The inductive effect of substitutes may be additive, but the resonance effect at present is not predictable. Further investigations are required to improve the precision.

The order of elution of polyaromatic hydrocarbons from both phenyl and ODS columns was same, but the selectivity within the polyaromatic hydrocarbons was slightly different. The correlation coefficient for the π energy effect between YMC phenyl and ODS columns was 0.981 ($n = 10$). In acetonitrile–water mixtures, naphthalene, anthracene and tetrasene were more retained and benzene, phenanthrene, chrysene and benzopyrene were less retained on the phenyl-bonded silica gel than was expected from their Van der Waals volumes and delocalization energies. The correlation coefficient for alkylbenzenes was 0.834 ($n = 10$), which indicates nonlinearity of the π energy effects between the two columns.

Several values for chlorobenzenes could not be calculated in highly concentrated acetonitrile eluents, and their values are not given in Table I.

The above approach could not be used with tetrahydrofuran–water mixtures owing to the very weak selectivity within the polyaromatic hydrocarbons.

CONCLUSION

Selectivity of the packings and the solvents was observed for the chromato-graphic behavior of chlorobenzenes. The order elution of the dichlorobenzenes from the ODS column was 1,2- < 1,4- < 1,3-dichlorobenzenes, and that from the phenyl column was 1,2- < 1,3- ≤ 1,4-dichlorobenzenes using acetonitrile–water mixtures, and this tendency was also observed with multi-substituted chlorobenzenes.

In tetrahydrofuran–water mixtures, the elution order was mono- < 1,2- di- < 1,3-di- < 1,4-di- < 1,2,4-tri- < 1,2,3,4-tetra- < 1,3,5-tri- < 1,2,3,5-tetra- < 1,2,4,5-tetra- < penta- < hexa-substituted chlorobenzenes for the phenyl-bonded column, and mono- < 1,2-di < 1,3-di- ≤ 1,4-di- < 1,2,4,-tri- < 1,2,3,4-tetra- < 1,3,5-tri- < 1,2,4,5-tetra. < 1,2,3,5-tetra- < penta- < hexa-substituted chloroben-zenes for the ODS column. The selectivity for the separation of isomers observed on the phenyl-bonded packing using acetonitrile–water mixtures and on the ODS pack-ing using tetrahydrofuran–water mixtures was enhanced on the phenyl-bonded pack-ing using tetrahydrofuran–water mixtures.

The compounds with a strong dipole moment were well solvated by the organic modifier and eluted faster. It seems that the direct dipole–dipole interaction between the solutes and the organic phase of the packings was not a predominant force for their retention.

The π energy effect on a phenyl-bonded silica gel derived from the Van der Waals volume and the delocalization energy was not the same as that obtained on octadecyl-bonded silica gels, and further experiments are required.

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