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# GAS CHROMATOGRAPHIC SOLUTE–SORBENT INTERACTIONS ON MACROPOROUS METHACRYLATE ION EXCHANGERS

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## SUMMARY

Solute–sorbent interactions were studied by using the retentions of aliphatic and aromatic hydrocarbons, ethers and alcohols on macroporous methacrylate copolymers ($H^+$, $Li^+$, $Na^+$, $K^+$, $Rb^+$, $Cs^+$ and $Ag^+$) containing sulphopropyl groups. The individual contributions to the overall Kováts index were calculated by multiple linear regression with parameters characterizing the solute (electron polarizability, dipole moment) and sorbent (surface concentration of groups, ionic radius of the cation). In the case of aromatic hydrocarbons and ethers the contribution of the solute is decisive (98%), while for alcohols the contribution of the sorbent increases to as much as 22%. The results confirm classical views according to which low-polarity compounds are separated due to non-specific interactions and polar compounds are separated due to specific solute–sorbent interactions. A similar picture of the interactions was provided by correlations in which the solute was characterized by Hammett and Taft substitution constants.

## INTRODUCTION

According to the theory of sorption[1], the solute–sorbent interactions may be interpreted in terms of specific and non-specific interactions. There are, however, no quantitative relationships regarding the strength of these interactions and the contribution of the solute and sorbent.

In previous papers[2,3] we demonstrated the additivity of such contributions in the case of the Kováts indices, $I$, for a number of solutes. We have now extended those studies by adding further sorbents, which allows the determination of the effect of the effect of the sorbent and some generalizations.

TABLE I

PROPERTIES OF METHACRYLATE ION EXCHANGERS USED

| Ion exchanger | Name | Specific surface area (m²/g) | Pore volume (ml/g) | SO₃H groups | |
|---|---|---|---|---|---|
| | | | | Content (mmol/g) | Surface concentration (μmol/m²) |
| A | G-15-91-SP | 117.2 | 1.246 | 0.468 | 3.99 |
| B | G-40-91-SP | 82.6 | 0.787 | 0.997 | 12.07 |
| C | G-70-85-SP | 30.5 | 1.227 | 0.745 | 24.43 |

## EXPERIMENTAL

### Materials

Methacrylate ion exchangers were prepared from a macroporous copolymer, glycidylmethacrylate–ethylenedimethacrylate[4], by reaction of the hydrolyzed copolymer with propanesulphone in an alkaline medium[5]. Their characteristics are summarized in Table I.

### Chromatographic measurements

Prior to use, the ion exchangers were washed with a 5% HCl solution and distilled water, LiCl, NaCl, KCl, RbCl, CsCl or AgNO₃ solution, again with distilled water and dried. These sorbents, particle size 180–250 μm, were used as the packings in columns 0.5 m long and 0.3 cm in diameter; they were activated at 170°C for 24 h in a stream of helium (50 ml/min). The retention times of a number of solutes (aliphatic, aromatic hydrocarbons, ethers and alcohols) were determined (at 150°C), from which the retention times relative to pentane and Kováts indices were calculated.

The contributions of the interactions between the solute and sorbent to the values of the Kováts indices were separated by multiple linear regression[6] with four parameters using a Wang 2200 computer.

### RESULTS AND DISCUSSION

The retentions of aliphatic and aromatic hydrocarbons, ethers and alcohols were determined on 21 macroporous methacrylate copolymers ($H^+$, $Li^+$, $Na^+$, $K^+$, $Rb^+$, $Cs^+$ or $Ag^+$) with sulphopropyl groups (Table II). The Kováts retention indices calculated from the retention times are given in Table III. The values increase along the homologous series of aromatic hydrocarbons, ethers and alcohols; but the indices of the isomers of alcohols decrease with branching. Increased retentions of methanol and ethanol were observed on sorbent C, especially at temperatures below 100°C. Increased values were also found for unsaturated hydrocarbons on sorbents in the forms $Rb^+$ and $Ag^+$, and for alcohols on sorbents in the hydrogen form. The results may be employed for practical separation of these compounds.

In our previous work[2], very good correlations were obtained between the Kováts retention indices and the number of methylene groups and the steric require-

TABLE II

RELATIVE RETENTION TIMES (PENTANE REFERENCE) OF SOLUTES ON METHACRYLATE ION EXCHANGERS AT 150°C

Sorbents A–C as in Table I.

| Solute | Form $H^+$ | | | Form $Li^+$ | | | Form $Na^+$ | | | Form $K^+$ | | | Form $Rb^+$ | | | Form $Cs^+$ | | | Form $Ag^+$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | A | B | C | A | B | C | A | B | C | A | B | C | A | B | C | A | B | C | A | B | C |
| Pentane | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| Hexane | 2.3 | 2.0 | 2.0 | 2.7 | 1.5 | 2.0 | 2.3 | 1.7 | 1.0 | 2.7 | 1.5 | 2.5 | 2.3 | 1.5 | 2.0 | 2.6 | 1.3 | 2.0 | 2.4 | 1.5 | 2.0 |
| Heptane | 5.7 | 3.0 | 2.0 | 5.7 | 3.0 | 3.5 | 4.5 | 2.5 | 1.5 | 6.0 | 2.0 | 3.0 | 4.0 | 2.5 | 3.8 | 5.2 | 3.7 | 5.3 | 6.2 | 3.0 | 3.5 |
| Octane | 9.7 | 4.5 | 5.0 | 14.3 | 4.0 | 5.5 | 11.3 | 5.0 | 2.0 | 14.0 | 3.0 | 6.5 | 12.3 | 4.0 | 6.5 | 6.4 | 3.3 | 10.0 | 16.6 | 3.0 | 6.0 |
| Nonane | 32.0 | 10.0 | 7.5 | 26.0 | 7.0 | 7.5 | 28.0 | 7.0 | 3.0 | 46.3 | 6.0 | 13.5 | 16.0 | 6.0 | 12.5 | 23.2 | 5.3 | 20.0 | 35.6 | 5.5 | 12.0 |
| Decane | 65.3 | 12.0 | 14.0 | 41.0 | 12.0 | 11.0 | 75.5 | 22.0 | 7.0 | 66.3 | 11.0 | 27.0 | 45.0 | 10.0 | 24.0 | 56.0 | 10.0 | 40.0 | 68.0 | 10.0 | 23.0 |
| Benzene | 4.3 | 5.5 | 4.0 | 4.3 | 2.5 | 4.0 | 4.0 | 6.0 | 1.0 | 4.0 | 4.0 | 2.5 | 5.3 | 4.0 | 4.0 | 4.4 | 5.3 | 2.7 | 6.8 | 5.0 | 3.0 |
| Toluene | 9.0 | 9.0 | 5.0 | 7.7 | 3.5 | 7.0 | 9.2 | 6.0 | 1.0 | 9.3 | 5.0 | 4.5 | 10.0 | 6.0 | 7.0 | 9.6 | 7.3 | 5.3 | 18.4 | 8.0 | 5.0 |
| p-Xylene | 20.0 | – | 7.0 | 18.8 | 6.0 | 12.5 | 24.8 | 6.0 | 2.0 | 23.1 | 5.0 | 10.0 | 20.0 | 6.5 | 11.5 | 22.4 | 8.7 | 10.7 | 23.4 | 8.0 | 10.0 |
| Ethylbenzene | 23.0 | – | 7.0 | 19.0 | 5.5 | 13.0 | 26.4 | 8.0 | 3.0 | 21.3 | 6.0 | 9.5 | 20.0 | 6.0 | 11.5 | 25.0 | 7.3 | 8.7 | 21.0 | 10.0 | 8.0 |
| Isopropylbenzene | 40.5 | 7.5 | 8.0 | 39.0 | 7.0 | 19.0 | 55.2 | 10.0 | 4.0 | 32.5 | 7.0 | 14.0 | 29.3 | 7.0 | 14.0 | 33.6 | 6.7 | 14.0 | 37.2 | 8.0 | 15.0 |
| 1,2,4-Trimethyl-benzene | 68.7 | 11.5 | 14.0 | 41.0 | 7.3 | 23.0 | 85.0 | 14.0 | 6.0 | 53.0 | 8.0 | 19.0 | 37.7 | 9.0 | 27.0 | 56.0 | 10.0 | 21.3 | 82.8 | 14.0 | 22.5 |
| Methanol | 1.0 | 6.5 | 22.0 | 1.3 | 10.8 | 23.3 | 1.4 | 8.5 | 8.0 | 1.0 | 5.0 | 29.0 | 1.0 | 7.0 | 34.3 | 1.2 | 6.0 | 20.0 | 1.0 | 4.0 | 17.0 |
| Ethanol | 1.8 | 10.0 | 48.0 | 3.0 | 12.0 | 15.0 | 2.2 | 10.5 | 11.0 | 2.5 | 6.0 | 35.0 | 2.2 | 9.0 | 50.0 | 2.0 | 6.7 | 28.0 | 2.2 | 7.0 | 22.5 |
| Propanol | 5.0 | 16.5 | 80.0 | 5.3 | 19.0 | 7.0 | 6.2 | 19.0 | 3.0 | 4.8 | 9.5 | 16.0 | 5.0 | 13.0 | 38.5 | 4.6 | 10.7 | 23.3 | 5.2 | 10.0 | 9.0 |
| n-Butanol | 9.0 | 30.0 | – | 18.0 | 31.0 | 11.0 | 13.4 | 35.0 | 5.0 | 13.0 | 19.0 | 16.0 | 11.3 | 24.0 | 27.0 | 10.6 | 24.7 | 20.0 | 10.0 | 21.0 | 12.5 |
| Isobutanol | 8.0 | 15.0 | – | 13.0 | 10.0 | 8.0 | 11.0 | 18.5 | 3.2 | 8.5 | 11.0 | 13.5 | 87.0 | 16.0 | 16.5 | 8.2 | 18.7 | 11.3 | 9.4 | 11.0 | 7.0 |
| tert.-Butanol | 1.0 | 5.0 | – | 6.0 | 5.0 | 5.0 | 6.0 | 5.5 | 2.0 | 5.5 | 4.0 | 6.5 | 5.3 | 5.5 | 11.0 | 4.8 | 4.7 | 6.0 | 1.0 | 4.0 | 5.0 |
| Diethyl ether | 2.3 | 2.5 | 4.7 | 1.5 | 3.0 | 1.5 | 1.4 | 4.5 | 1.0 | 1.5 | 1.3 | 1.5 | 1.7 | 2.5 | 2.0 | 1.6 | 3.0 | 2.0 | 1.8 | 2.5 | 1.5 |
| Di(isopropyl) ether | 5.0 | 1.5 | 2.0 | 3.5 | 2.0 | 3.5 | 7.2 | 1.8 | 1.5 | 4.5 | 2.0 | 4.0 | 3.7 | 2.0 | 4.0 | 4.4 | 2.0 | 3.3 | 4.4 | 2.5 | 3.0 |
| Di-(n-butyl) ether | 30.0 | 7.5 | 12.0 | 29.8 | 11.0 | 13.0 | 38.4 | 8.0 | 4.5 | 34.3 | 6.0 | 16.0 | 28.3 | 8.0 | 15.5 | 25.6 | 7.5 | 14.7 | 36.2 | 8.0 | 14.5 |

TABLE III

KOVÁTS RETENTION INDICES OF SOLUTES ON METHACRYLATE ION EXCHANGERS AT 150°C

Sorbents A–C as in Table I.

| Solute | Form H+ | | | Form Na+ | | | Form K+ | | | Form Rb+ | | | Form Cs+ | | | Form Ag+ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | A | B | C | A | B | C | A | B | C | A | B | C | A | B | C | A | B | C |
| Benzene | 668 | 826 | 776 | 683 | 853 | 500 | 649 | 804 | 600 | 724 | 800 | 714 | 674 | 900 | 631 | 709 | 846 | 672 |
| Toluene | 783 | 886 | 800 | 778 | 853 | 500 | 751 | 873 | 752 | 782 | 900 | 811 | 830 | 950 | 700 | 806 | 962 | 766 |
| p-Xylene | 860 | – | 883 | 900 | 853 | 800 | 840 | 873 | 859 | 922 | 914 | 887 | 889 | 979 | 810 | 845 | 1000 | 874 |
| Ethylbenzene | 871 | – | 883 | 899 | 910 | 900 | 835 | 900 | 852 | 922 | 900 | 887 | 908 | 950 | 778 | 830 | 962 | 841 |
| Isopropylbenzene | 930 | 866 | 910 | 967 | 931 | 934 | 869 | 927 | 905 | 960 | 932 | 964 | 942 | 939 | 849 | 907 | 962 | 939 |
| 1,2,4-Trimethylbenzene | – | 1000 | 1000 | – | 961 | 982 | 933 | 946 | 949 | 984 | 977 | 1017 | 1000 | 1000 | 910 | – | 1056 | 997 |
| Methanol | 500 | 846 | 1086 | 542 | 916 | 1015 | 500 | 873 | 1011 | 500 | 932 | 1045 | 520 | 921 | 900 | 500 | 846 | 954 |
| Ethanol | 572 | 900 | 1183 | 594 | 941 | 1051 | 593 | 900 | 1041 | 600 | 977 | 1090 | 573 | 939 | 949 | 589 | 942 | 997 |
| Propanol | 685 | 1050 | 1255 | 735 | 988 | 800 | 671 | 977 | 925 | 720 | 1048 | 1058 | 681 | 1015 | 922 | 683 | 1000 | 858 |
| n-Butanol | 783 | 1078 | – | 820 | 1188 | 960 | 789 | 1155 | 924 | 792 | 1154 | 1015 | 839 | 1176 | 900 | 749 | 1112 | 906 |
| Isobutanol | 761 | 1055 | – | 798 | 986 | 908 | 741 | 1000 | 900 | 769 | 1098 | 943 | 818 | 1128 | 818 | 742 | 1015 | 822 |
| tert.-Butanol | 500 | 814 | – | 733 | 827 | 900 | 689 | 840 | 800 | 724 | 878 | 880 | 687 | 875 | 720 | 500 | 846 | 784 |
| Diethyl ether | 600 | 650 | 883 | 542 | 783 | 500 | 542 | 556 | 544 | 564 | 700 | 600 | 549 | 756 | 600 | 568 | 756 | 550 |
| Di(isopropyl) ether | 685 | 560 | 600 | 753 | 618 | 700 | 663 | 700 | 737 | 688 | 643 | 710 | 674 | 659 | 651 | 663 | 756 | 672 |
| Di(n-butyl) ether | 894 | 866 | 975 | 930 | 910 | 948 | 875 | 900 | 924 | 956 | 955 | 933 | 911 | 957 | 856 | 904 | 962 | 929 |

ments of the solute. The fact that the retention indices are correlated with the electron polarizability, $\alpha$, of the solute molecules[7,8] indicates the role played by non-specific interactions. Specific interactions will be proportional, among other things, to the dipole moment, $\mu$, of the molecules[1].

The objective of this study was to determine the strength of these interactions and the individual contributions of the solute and sorbent. For this purpose we used multiple linear regression[5] of the Kováts indices with parameters characterizing the solute (electron polarizability and dipole moment)[9] and sorbent (content of groups, $c_p$, and type of cation, $R$) (Table IV) by means of the relationship:

$$I = I_\alpha \alpha + I_\mu \mu + I_{c_p} c_p + I_R R \tag{1}$$

The Kováts retention indices are related to thermodynamic quantities, $\Delta\Delta G^E(CH_2)$; consequently, this relationship is analogous to the linear free energy relationships used in organic chemistry in the correlation of kinetic data[5].

The multiple linear regression enabled the separation of the individual correlations. The best fit was found for a dependence between the measured properties and the surface concentration of functional groups $-SO_3^- M^+$, $c_p$ ($\mu$mol/m$^2$), calculated as the ratio of the group content to the specific surface area of the sorbent. The type of cation $M^+$ bound was characterized by its ionic radius, $R$ (nm). The multiple linear regression simplifies the problem, as it does not include higher-order interactions between the variables. The calculated values of the coefficients $I_\alpha$, $I_\mu$, $I_{c_p}$ and $I_R$ and the contributions $I_\alpha \bar{\alpha}$, $I_\mu \bar{\mu}$, $I_{c_p} \bar{c}_p$ and $I_R \bar{R}$ for homologous series of aromatic hydrocarbons, alcohols and ethers are summarized in Table V.

The values of the coefficients vary with the solute and sorbent used, the effect of the solute being the most important . In the series of aromatic hydrocarbons, ethers and alcohols, the coefficient $I_\alpha$ corresponding to non-specific interactions decreases while the coefficient $I_\mu$ related to specific interactions of the solute, e.g., formation of hydrogen bonds in the case of alcohols, increases.

TABLE IV

ELECTRON POLARIZABILITY, $\alpha$, AND DIPOLE MOMENT, $\mu$, OF SOLUTES USED IN EQN. 1

| Solute | $\alpha \cdot 10^{23}$ | $\mu$ | Solute | $\alpha \cdot 10^{23}$ | $\mu$ |
|---|---|---|---|---|---|
| Pentane | 1.0013 | 0.0 | Benzene | 1.0370 | 0.0 |
| Hexane | 1.1835 | 0.0 | Toluene | 1.2320 | 0.36 |
| Heptane | 1.3689 | 0.0 | p-Xylene | 1.4269 | 0.0 |
| Octane | 1.5520 | 0.0 | 1,2,4-Trimethyl- | 1.6128 | 0.59 |
| Nonane | 1.7782 | 0.0 | benzene | | |
| Decane | 1.9208 | 0.0 | Isopropylbenzene | 1.6021 | 0.79 |
| Average of interval | 1.46 | 0.0 | | 1.30 | 0.4 |
| Methanol | 0.3278 | 1.70 | Diethyl ether | 0.8851 | 1.15 |
| Ethanol | 0.5132 | 1.69 | Diisopropyl ether | 1.2612 | 1.21 |
| Propanol | 0.6944 | 1.68 | Dibutyl ether | 1.6231 | 1.17 |
| Butanol | 0.88779 | 1.66 | | | |
| Amyl alcohol | 1.0626 | | | | |
| Average of interval | 0.6 | 1.62 | | 1.26 | 1.18 |

TABLE V

COEFFICIENTS CALCULATED USING EQN. 1 AND AVERAGE CONTRIBUTIONS TO THE KOVÁTS INDICES

| | Solute interaction | | Sorbent interaction | | Average contribution (%) | | | |
|---|---|---|---|---|---|---|---|---|
| | $I_\alpha$ | $I_\mu$ | $I_{c_p}$ | $I_R$ | $I_\alpha\bar{\alpha}$ | $I_\mu\bar{\mu}$ | $I_{c_p}\bar{c}_p$ | $I_R R$ |
| Aromatic hydrocarbons* | 633 | − 90 | − 0.23 | 17 | 93.9 | 4.1 | 0.3 | 1.6 |
| Ethers** | 427 | 161 | 1.16 | 2.5 | 72.3 | 25.5 | 1.9 | 0.3 |
| Alcohols*** | 171 | 356 | 13.8 | −29 | 12.3 | 65.9 | 19.0 | 2.8 |

Mean square deviations: * 76.5; ** 86.1;*** 140.0.

Using the averages of the individual contributions to the Kováts indices, it is possible to obtain an idea of the extent of interaction between the solute and sorbent. While with aromatic hydrocarbons and ethers the interactions are almost exclusively those of the solute (about 98%), in the case of alcohols an increasingly important role is played by the sorbent (up to 22%). In this case the type of active group on the sorbent, as characterized by the ionic radius, is more important than its surface concentration.

TABLE VI

EXPERIMENTAL AND CALCULATED VALUES OF KOVÁTS INDICES ON COPOLYMERS A–C IN THE LITHIUM FORM

| Aromatic hydrocarbons | | | Ethers | | | Alcohols | | |
|---|---|---|---|---|---|---|---|---|
| Exptl. | Calc.* | Calc.** | Exptl. | Calc.* | Calc.** | Exptl. | Calc.* | Calc.** |
| 661 | 665 | 198 | 542 | 566 | 522 | 526 | 702 | 262 |
| 733 | 756 | 652 | 633 | 737 | 791 | 615 | 732 | 555 |
| 840 | 912 | 633 | 935 | 885 | 628 | 688 | 761 | 503 |
| 848 | 857 | 588 | 700 | 576 | 561 | 840 | 787 | 523 |
| 990 | 952 | 633 | 660 | 746 | 829 | 705 | 748 | 677 |
| 1000 | 1003 | 588 | 983 | 895 | 666 | 965 | 815 | 359 |
| 653 | 663 | 302 | 550 | 590 | 619 | 1000 | 844 | 651 |
| 750 | 755 | 733 | 700 | 761 | 888 | 1100 | 873 | 598 |
| 872 | 910 | 741 | 1021 | 909 | 725 | 1181 | 899 | 619 |
| 856 | 855 | 692 | | | | 840 | 860 | 774 |
| 900 | 950 | 733 | | | | 1094 | 986 | 507 |
| 904 | 1001 | 692 | | | | 1039 | 1016 | 800 |
| 600 | 661 | 461 | | | | 878 | 1045 | 746 |
| 776 | 752 | 893 | | | | 1000 | 1071 | 767 |
| 1016 | 908 | 900 | | | | 779 | 1031 | 922 |
| 1021 | 852 | 852 | | | | | | |
| 1068 | 947 | 897 | | | | | | |
| 1092 | 998 | 852 | | | | | | |
| − | 76.5*** | 250.1*** | − | 86.1*** | 191.6*** | − | 140.0*** | 328.0*** |

\* Calculated by means of eqn. 1.
\*\* Calculated by means of eqn. 2.
\*\*\* Mean square deviation.

The separation of the contribution from sorption effects helps us to understand the mechanism of sorption. The results show that interactions occur mainly between molecules of the solute on the polymer surface; in the case of polar molecules, the interaction between the solute and sorbent must also be taken into account.

A similar, though less accurate (as evidenced by the mean square deviations in Table VI) picture of the interactions was provided by a correlation of the Kováts indices with Hammett ($\sigma$) and Taft substitution constants ($E$) characterizing the solute

$$I = I_\sigma \sigma + I_E E + I_{c_p} c_p + I_R R \tag{2}$$

and also by correlation of $\ln t_R$ and $\Delta\Delta G^E(CH_2)$.

The results confirm quantitatively the classical views of sorption processes in which low-polarity compounds are separated due to non-specific interactions comprising solute–solute dispersion forces on the surface of the sorbent. In the case of polar compounds, specific interactions take place, e.g., hydrogen bonding in alcohols, giving rise to space where solute–sorbent interactions may occur.

The values of the coefficients of eqn. 1 can be used not only for the evaluation of solute–sorbent interactions, but also for the calculation of unknown Kováts indices by using only a few constants characterizing the solute and sorbent. This may help in the prediction of separation conditions. The contribution of the sorbent, represented by constants $I_{c_p}$ and $I_R$, in this case is a measure of the sorbent polarity. Such a classification of the polarity of polymeric sorbents is being evaluated.

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