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Surface properties of titanate-modified silica gel as measured by inverse gas chromatography

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Silica gel was modified at three temperatures by five titanium coupling agents: tris(isooctadecanoato-*O*)(2-propanolato)titanium, [2-[2-(methoxy-*O*)ethoxy-*O*]ethanolato-*O*]tris(2-methyl-2-propenoato-*O*)titanium, (isooctadecanoato-*O*)bis(2-methyl-2-propenoato-*O*)(2-propanolato)titanium, (4-aminobenzenesulfonato-*O*)bis(dodecylbenzenesulfonato-*O*)(2-propanolato)titanium and tris(dodecylbenzenesulfonato-*O*)(2-propanolato)titanium. Surface properties of these modified materials were measured by inverse gas chromatography and expressed by surface parameters (γ_s^d, K_A, K_D). The influence of the modifier structure and modification temperature on surface parameters is presented and discussed. Relationships between surface parameters and solubility parameters used earlier for the description of the physico-chemical state of the modifier monolayer are also shown.

Introduction

Titanium-containing compounds are known as materials used for surface modification. In contrast to silanes, they are used not only to modify active materials, but also for the modification of inert surfaces. However, in this work the use of titanium coupling agents in a process of bonding of the surface groups of a silica gel is presented. As a result one obtains a monomolecular layer of the titanate on the silica gel surface.[1–3] The physico-chemical properties of solid materials modified in such a way may be characterised by inverse gas chromatography (IGC). The need for the characterisation of silica gel modified with titanium compounds, the usefulness of IGC and the influence of the modifier structure on the properties of the produced monolayer were described earlier.[4] Applications of IGC were also presented in several reviews[5–7] and a number of individual papers.[8–10] Analysis of the parameters calculated from retention data of the test solutes allows the discussion of the influence of the modifier's structure and the modification temperature on the surface properties of the modified material (Fig. 1).

Inverse gas chromatography is useful in the determination of the free surface energy and acid–base properties of the solid materials.[9–11] Intermolecular interactions in an adsorbent–adsorbate system may be generally divided into dispersive and specific. Thus, the free surface energy (γ_s) has two components: specific (γ_s^s) and dispersive (γ_s^d) according to eqn. (1)

$$\gamma_s = \gamma_s^d + \gamma_s^s \tag{1}$$

The standard free energy of transferring a mole of vapour from the gas phase to a standard state on the surface, *i.e.* the adsorption energy, is given by

$$\Delta G^0 = -RT \ln \frac{BV_N}{Sg} \tag{2}$$

where $B = 2.99 \times 10^2$, S is the specific area of the adsorbent, g is the mass of the adsorbent in the column, and V_N is the net retention volume.

For a given system eqn. (2) changes into

$$\Delta G^0 = -RT \ln V_N + \text{const} \tag{3}$$

The adsorption energy has two components: specific (ΔG^s) and dispersive (ΔG^d) according to eqn. (4)

$$\Delta G^0 = \Delta G^d + \Delta G^s \tag{4}$$

For n-alkanes $\Delta G^s = 0$ and $\Delta G^0 = \Delta G^d$. The ΔG^d changes with the number of carbon atoms in their molecules. Its increment corresponding to a methylene group may be calculated from eqn. (5)

$$\Delta G_{CH_2} = -RT \ln \left(\frac{V_{N,n}}{V_{N,n+1}} \right) \tag{5}$$

where $V_{N,n}$ and $V_{N,n+1}$ denote the net retention volumes of n-alkanes having n and $n+1$ atoms respectively.

According to Dorris and Gray[12]

$$\Delta G_{CH_2} = 6.023 \times 10^{23} \times a_{CH_2} \times 2\left(\gamma_s^d \gamma_{CH_2}\right) \tag{6}$$

where a_{CH_2} denotes the surface covered by one methylene group (0.06 nm^2) and γ_{CH_2} is the free surface energy of polyethylene.

Usually γ_{CH_2} is taken as 35.6 mJ m^{-2} or is calculated according to eqn. (7)

$$\gamma_{CH_2} = 35.6 + 0.058(293 - T) \tag{7}$$

The dispersive component of surface free energy can be calculated from eqn. (8) with the use of experimentally determined ΔG_{CH_2} values:

$$\gamma_s^d = \frac{\Delta G_{CH_2}}{4 \times (6.023 \times 10^{23})^2 \times a_{CH_2}^2 \times \gamma_{CH_2}} \tag{8}$$

The acid–base properties of the examined surface can be determined after calculating the specific component of the adsorption energy, ΔG^s. From its temperature dependence one may calculate the enthalpy of specific interactions ΔH^s which is used to calculate the acid–base properties of the examined surface.

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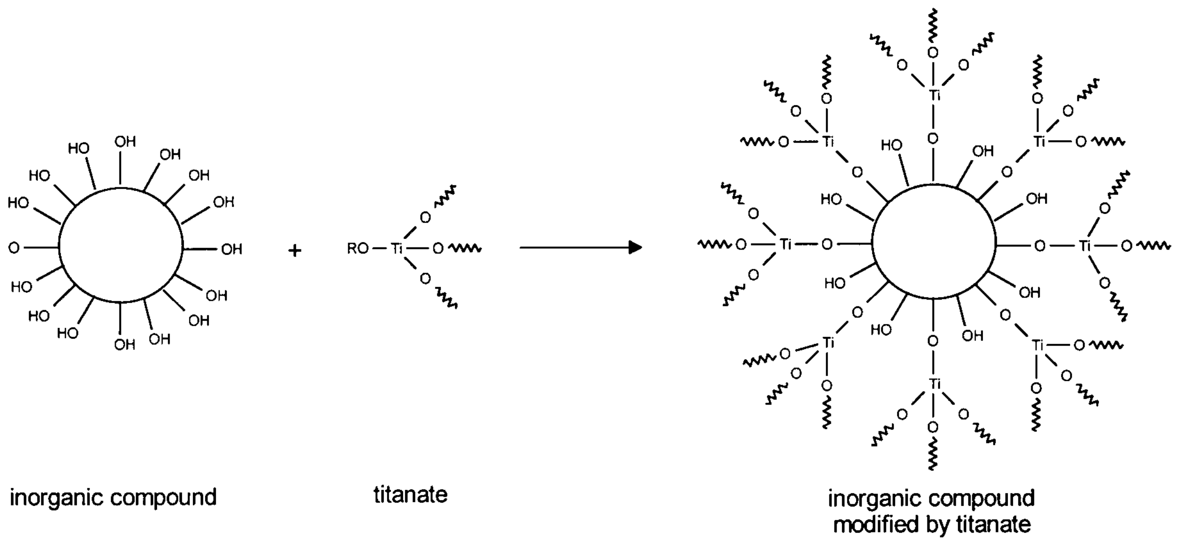


Fig. 1 The reaction of the monoalkoxy titanium modifier with the surface proton of the inorganic compound.

The specific component of the adsorption energy, ΔG^s, can be determined according to several procedures. Generally, it is calculated as the difference between the adsorption energies of polar test compounds and a hypothetical n-alkane having the same dispersive or other properties. As a measure of these properties a few parameters were proposed. Saint Flour and Papirer[13] proposed the use of the logarithm of the saturated vapour pressure (log p^o). Thus the specific component of the adsorption energy, ΔG^s, according to Papirer can be calculated by subtracting from the adsorption energy ΔG of a polar probe the adsorption energy of a hypothetical n-alkane having the same value of the logarithm of the saturated vapour pressure (log p^o).

Another approach was proposed by Dong, Brendle and Donnet.[14] According to them

$$RT\ln V_N + C = C'P_{DS}P_{DP} - \Delta G^s \tag{9}$$

where C and C' are constants, P_{DS} and P_{DP} are the molar deformation polarisation of the solid and probe, respectively.

For n-alkanes (where $\Delta G^s = 0$)

$$RT\ln V_N + C = C'P_{DS}P_{DP} \tag{10}$$

Dong *et al.* proved that $RT\ln V_N$ is proportional to P_{DP}. This dependence is linear and the slope of the line is equal to $C'P_{DS}$. Here the parameter $C'P_{DS}$ is a measure of the ability of a surface being characterised to undergo dispersive interactions. The specific component of the adsorption energy, ΔG^s, may be also calculated with the use of eqn. (9). Similarly to the procedure proposed by Saint Flour and Papirer, ΔG^s is calculated by subtracting from the adsorption energy ΔG of a polar test solute the adsorption energy of a hypothetical n-alkane having the same value of $C'P_{DS}$ as the polar probe.

The specific component of the adsorption energy, ΔG^s, is calculated for all polar probes at three temperatures. The specific component of the enthalpy of adsorption, ΔH^s, required can be obtained from eqn. (11):

$$\frac{\Delta G^s}{T} = \frac{\Delta H^s}{T} - \Delta S^s \tag{11}$$

i.e., as the slope of the plot $\Delta G^s/T$ versus $1/T$.[9]

The specific component of the enthalpy of adsorption, ΔH^s, is further correlated to parameters characterising the examined surface[15]

$$-\Delta H^s = K_D AN^* + K_A DN \tag{12}$$

where ΔH^s is the specific component of the enthalpy of adsorption, AN^* and DN are the acceptor and donor numbers of the test solute, and K_A and K_D reflect the ability of the examined surface to act as an electron acceptor and electron donor, respectively.

Eqn. (12) is an extended version of the Gutman relationship.[16] The parameters K_A and K_D are calculated with the use of the transformed eqn. (12). For example, when calculating K_A, eqn. (12) changes into

$$\frac{(-\Delta H^s)_i}{AN_i^*} = K_A \frac{DN_i}{AN_i^*} + K_D \tag{13}$$

where index 'i' means the parameters of different test compounds.

The surface character may also be determined as the ratio of the K_D and K_A parameters

$$S_C = K_D/K_A \tag{14}$$

If $S_C < 1$ the examined surface exhibits acidic (electron acceptor) properties while for basic (electron donor) surfaces this parameter is $S_C > 1$.

Experimental

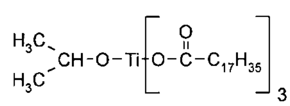
Materials

Five titanium coupling agents were used to modify the silica gel. They have the formulae given in Fig. 2. All titanium coupling agents were supplied by Kenrich Petrochemicals, Inc. (USA).

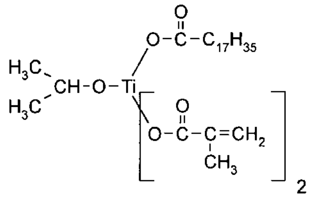
Silica gel (Fluka, Silica gel 60, 0.2–0.5 mm (35–70 mesh)) was modified in CCl_4 solution at three temperatures: room temperature (~20 °C), 50 °C and 70 °C. This process was carried out for 2 h. All the titanates (as delivered by the manufacturer) were used in 20 : 100 proportion to silica gel. After modification the adsorbed excess of titanate was extracted with CCl_4 in a Soxhlet apparatus.

IGC experiments

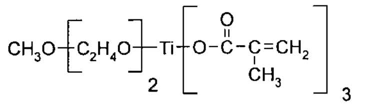
The inverse gas chromatography experiments were carried out under the following conditions: column stainless steel, 1 m × 3 mm I.D., measurement temperatures 120, 130 and 140 °C, temperature of the FID detector and injector 160 °C; carrier gas helium, at a flow rate of 40 ml min^{-1}, Chrom 5 gas chromatograph (Kovo, Czech Republic). The choice of the volatile test compounds used in the experiments was limited because of the highly acidic properties of the silica gel. Thus the



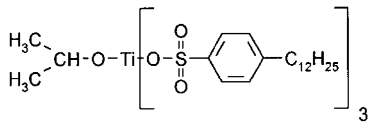
KR TTS - tris(isooctadecanoato-*O*)(2-propanolato)titanium



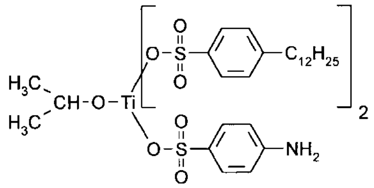
KR 7 - (isooctadecanoato-*O*)bis(2-methyl-2-propenoato-*O*)(2-propanolato)titanium



KR 33DS - [2-[2-(methoxy-*O*)ethoxy-*O*]ethanolato-*O*]
tris(2-methyl-2-propenoato-*O*)titanium



KR 9S - tris(dodecylbenzenesulfonato-*O*)(2-propanolato)titanium



KR 26S - (4-aminobenzenesulfonato-*O*)bis(dodecylbenzenesulfonato-*O*)
(2-propanolato)titanium

Fig. 2 Chemical formulae of the modifiers.

test probes showing basic properties could not be used and only n-alkanes from n-pentane to n-nonane, as well as benzene, carbon tetrachloride, chloroform and methylene chloride, were chosen as the test compounds. The amount of column filling varied from 4.198 to 7.515 g. The amount of injected compounds was from 0.1 to 1.0 μl of vapour to achieve a region of infinite dilution.

Results and discussion

The most important characteristics discussed here are the parameters describing the surface properties of the modified materials. There are two groups of surface parameters: (i) dispersive parameters—dispersive increment of the surface energy γ_s^d and the Donnet parameter $C'P_{DS}$; (ii) specific interaction parameters. Values of the dispersive parameters are presented in Table 1 while the specific surface parameters (K_D, K_A, S_C) are given in Table 2. The accuracy of calculating the dispersive parameters is satisfying while in the case of the specific interaction parameters the relative errors are somewhat higher. This problem is connected to the method of calculation of the specific component of the enthalpy of adsorption, ΔH^s, from the temperature dependence of the specific component of the adsorption energy ΔG^s. Here the Donnet approach gives more accurate results than the Papirer method of calculation. Moreover, there are no negative values of the surface parameters determined with the use of the Donnet procedure.

Table 1 Values of the increment of the adsorption energy for a methylene group, the dispersive component of the surface free energy γ_s^d and the Donnet parameter $C'P_{DS}$ (calculated for measurements carried out at 130 °C; confidence level calculated at $\alpha = 0.05$)

Modifier	Modification temperature/°C	ΔG_{CH_2}/J mol^{-1}	γ_s^d/mJ m^{-2}	$C'P_{DS}$/J cm^{-3}
—	—	2064±13	28±1	425±3
KR TTS	20	2015±8	27±1	416±1
	50	2041±6	27±1	419±1
	70	2039±2	27±1	420±1
KR 7	20	1930±2	24±1	402±2
	50	1926±25	24±1	398±5
	70	1934±43	25±1	401±7
KR 33DS	20	1970±15	25±1	401±2
	50	1964±38	25±1	401±7
	70	1999±19	26±1	411±2
KR 9S	20	2042±16	27±1	424±2
	50	2008±49	26±1	416±7
	70	2100±31	29±1	432±6
KR 26S	20	1982±7	26±1	411±1
	50	2010±25	26±1	415±7
	70	1983±33	26±1	408±4

Dispersive parameters

Surface modification should decrease the number of active sites. It should be accompanied by a decrease of the dispersive increment of the surface free energy.[17,18] Although the changes of γ_s^d are relatively small one may find an influence of the modifier structure. All γ_s^d values vary from 21 to 31 mJ m^{-2}. These values are lower than those reported earlier for, *e.g.*, A130 or XOB75.[19] The highest values of γ_s^d were found for non-modified silica gel and decrease in the order: silica gel ⩾ silica gel modified with KR 9S > silica gel modified with KR TTS > silica gel modified with KR 26S > silica gel modified with KR 33DS > silica gel modified with KR 7. Values of the Donnet parameter $C'P_{DS}$ change in the same order. The temperature of modification is important for the final properties of the modified materials but its influence is different for different modifiers. Lowest values of γ_s^d for silica gel modified with KR 7 were found after processing at 50 °C while for KR TTS derivatives the lowest values were found after modification at 70 °C. For silica gel probes modified with KR 7 and KR 33DS the increase of the modification temperature from 50 to 70 °C caused an increase of the γ_s^d value while for KR 9S and KR 26S the values of γ_s^d were similar and did not change considerably with the modification temperature.

Specific interaction parameters

It is well known that the silica gel surface exhibits highly acidic properties. Here, K_A is the parameter expressing the ability of the surface to interact as an electron acceptor, *i.e.* Lewis acid, in intermolecular interactions. Very high K_A values were found for silica gel: 38.45 (Papirer procedure) and 54.07 (Donnet procedure). These values significantly decrease after modification with the use of any titanate modifier in the following order: silica gel > silica gel modified with KR 26S ≈ silica gel modified with KR9S > silica gel modified with KR7 > silica gel modified with KR TTS > silica gel modified with KR 33DS. One should also expect that the values of the K_D parameter, expressing the surface's ability to act as an electron donor (Lewis base), would be very low for the silica gel. These values should become higher for the modified silica gels, because of the presence of the modifier chains having "electron rich" functional groups. Indeed, this is true! The values of the K_D parameter decrease in the order: silica gel modified with KR 26S ≈ silica gel modified with KR 33DS ≈ silica gel modified with KR 7 > silica gel modified with KR TTS ≈ silica gel modified with KR 9S > silica gel. The low value of the K_D parameter [equal to 0.163 for silica

Table 2 Surface parameters calculated according to the Papirer and Donnet procedures (confidence level calculated at $\alpha = 0.05$)

		Papirer			Donnet		
Modifier	Modification temperature/°C	K_D	K_A	S_C	K_D	K_A	S_C
—	—	0.163 ± 0.141	38.45 ± 10.89	0.004 ± 0.005	0.639 ± 0.191	54.07 ± 9.59	0.012 ± 0.004
KR TTS	20	0.156 ± 0.141	34.61 ± 5.31	0.004 ± 0.004	0.601 ± 0.108	49.15 ± 6.82	0.012 ± 0.004
	50	0.240 ± 0.071	17.20 ± 2.02	0.014 ± 0.004	0.615 ± 0.070	29.02 ± 1.90	0.021 ± 0.001
	70	0.247 ± 0.108	16.62 ± 11.18	0.015 ± 0.015	0.673 ± 0.142	30.39 ± 10.46	0.022 ± 0.011
KR 7	20	0.494 ± 0.083	27.22 ± 2.06	0.018 ± 0.004	0.906 ± 0.245	40.46 ± 3.15	0.022 ± 0.005
	50	0.231 ± 0.070	20.75 ± 2.45	0.011 ± 0.002	0.640 ± 0.050	33.99 ± 3.24	0.019 ± 0.001
	70	—	2.88 ± 6.46	—	0.265 ± 0.148	13.54 ± 6.40	0.020 ± 0.017
KR 33DS	20	0.280 ± 0.207	4.91 ± 9.77	0.057 ± 0.321	0.745 ± 0.309	20.14 ± 13.66	0.037 ± 0.011
	50	0.292 ± 0.045	3.78 ± 6.51	0.077 ± 0.197	0.764 ± 0.063	19.26 ± 6.49	0.040 ± 0.013
	70	0.569 ± 0.103	14.16 ± 4.44	0.041 ± 0.008	0.424 ± 0.132	35.69 ± 5.06	0.012 ± 0.008
KR 9S	20	—	12.00 ± 2.71	—	0.176 ± 0.056	23.29 ± 2.57	0.008 ± 0.003
	50	0.243 ± 0.053	29.87 ± 4.14	0.008 ± 0.002	0.682 ± 0.166	44.03 ± 2.12	0.015 ± 0.004
	70	0.029 ± 0.074	22.87 ± 5.46	0.001 ± 0.003	0.437 ± 0.081	35.86 ± 5.10	0.012 ± 0.004
KR 26S	20	0.255 ± 0.073	30.98 ± 1.99	0.008 ± 0.003	0.766 ± 0.122	47.89 ± 4.50	0.016 ± 0.001
	50	0.318 ± 0.027	31.07 ± 1.11	0.010 ± 0.001	0.779 ± 0.032	46.14 ± 1.27	0.017 ± 0.001
	70	0.176 ± 0.032	24.78 ± 5.23	0.007 ± 0.001	0.654 ± 0.067	40.42 ± 5.84	0.016 ± 0.002

gel (Papirer)] increases after the modification at 50 °C to the values given in Table 3.

The increase of the value of the K_D parameter is relatively low. Much higher changes are observed for the K_A parameter. While the values of the K_D parameter seem to be properly determined the values of the K_A parameters are probably somewhat overestimated due to the electron acceptor properties of the test compounds. However, the change of the character of the examined surfaces appears to be due to blocking of the silanol groups ($K_A\downarrow$) and introduction of groups with electron donor properties ($K_D\uparrow$). Here, the use of the Donnet procedure led to the unexpected statement that modification with KR TTS caused a decrease of the surface basic character (?).

S_C changes in the order: silica gel < silica gel modified with KR 7 ≈ silica gel modified with KR 9S ≈ silica gel modified with KR 26S < silica gel modified with KR TTS < silica gel modified with KR 33DS. This is a result of changes in the values of both earlier discussed surface parameters. Despite the influence of the used modifier the surface of the modified silica gel remains highly acidic: the S_C values are always lower than 0.1. Only for KR 33DS (at all modification temperatures) were the S_C values from the Papirer procedure found to be higher than those from the Donnet approach.

As previously discussed[10,11] the use of two different reference states led to two different numerical values of the specific surface parameters. However, the direction of changes shown by the two sets of surface parameters is the same. The values of the surface parameters found according to the Donnet procedure are almost always higher than those calculated from the Papirer procedure.

Influence of the modifier structure

The ability of the examined surfaces to undergo specific interactions depends on the structure of the modifier. Silica gel modified with all the modifiers having long alkyl chains (KR TTS, KR 9S and KR 26S) exhibits a high ability to undergo specific interactions while for other modifiers (KR 7 and KR 33DS) this ability is less in comparison to the parent silica gel.

Table 3 K_D Parameter values after modification at 50 °C

Modifier	Value of K_D after modification
KR TTS	0.240
KR 7	0.231
KR 33DS	0.292
KR 9S	0.243
KR 26S	0.318

For the specific interaction parameters it is possible to distinguish a few effects influencing the character of the modified silica gel. The value of the K_A parameter depends mainly on the quantity of the blocked surface silanol groups. The influence of the modifier structure is therefore hidden and impossible to determine for this parameter.

For the K_D parameter the influence of the modifier structure is clear. All the modifiers have basic carbonyl or sulfonyl groups. However, for most of the modifiers the basic character of these groups is reduced due to the inductive influence of the titanium atom. In the KR TTS molecule there are also acidic hydrogen atoms (in the α position to the carbonyl group) which lower the basic properties of the silica gel modified with this modifier. Neither of these effects influence the properties of the KR 33DS modifier. The inductive effect is reduced by the presence of a double bond and there is no acidic hydrogen atom. Thus silica gel modified with KR 33DS exhibits, in comparison to the parent silica, a much greater ability to undergo basic interactions. Similarly, high values of the K_D parameter characterise the silica gel modified with KR 26S. However, this is caused by the presence of the highly basic amino group in one of the modifier's chains.

Influence of the modification temperature

The influence of the modification temperature is different for each modifier and parameter (Fig. 3 and 4). Values of the K_D parameter decreased with the increase of the modification temperature when KR 7 was used as the modifier. This decrease is almost linear. For the silica gels modified with KR TTS, KR 9S, KR 26S and KR 33DS the increase of modification temperature from 20 to 50 °C caused a small increase of the discussed parameter. Further increase of the modification temperature to 70 °C led to a sharp decrease of the K_D value for the silica gels modified with KR 33DS, KR 9S and KR 26S, respectively but a slight increase for the silica gels modified with KR TTS (Fig. 3B). The K_A values decrease with an increase of the modification temperature from 20 to 50 °C for the silica gels modified with KR TTS, KR 7, KR 33DS and KR 26S, respectively and increase for the silica gel modified with KR 9S (Fig. 3D). Further increase of the reaction temperature caused a decrease of the K_A value for the silica gels modified with KR 7, KR 9S and KR 26S, a small increase for the silica gel modified with KR TTS and a sharp increase for the silica gel modified with KR 33DS. The final result, *i.e.*, the changes of the S_C parameter, are presented in Fig. 4B. The increase of the

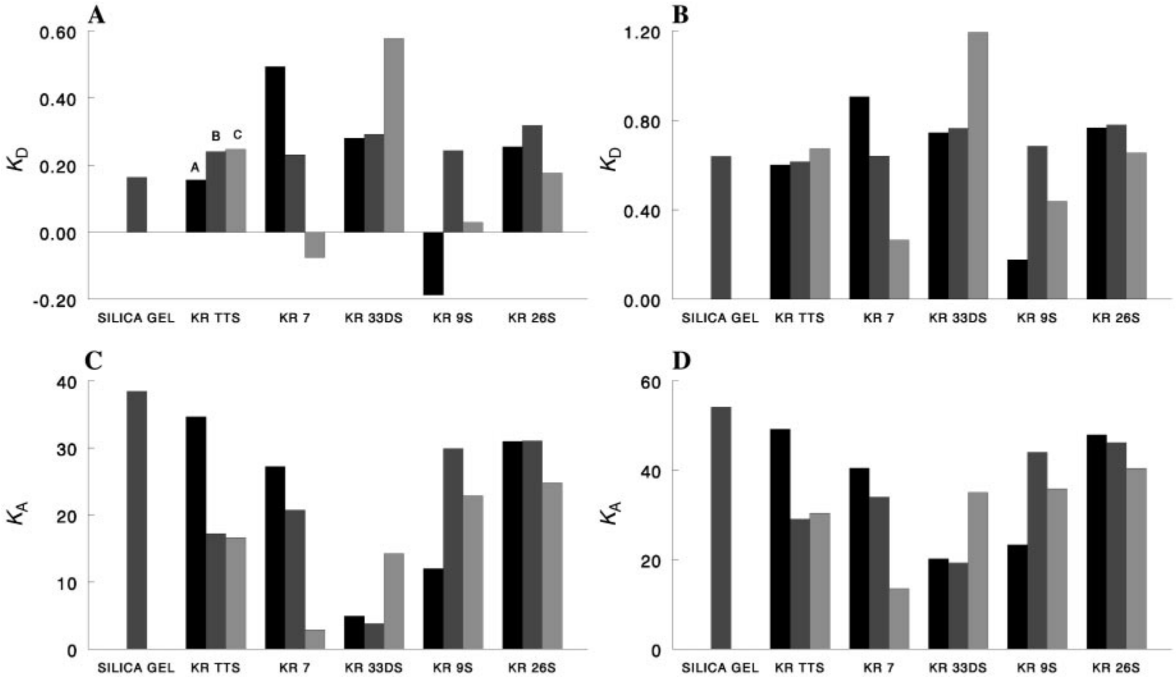


Fig. 3 Values of: A, K_D (Papirer); B, K_D (Donnet); C, K_A (Papirer); D, K_A (Donnet). Columns A, B and C refer to modification temperatures of 20, 50 and 70 °C, respectively.

modification temperature seems to be profitable: it leads to the maximum changes in the surface properties after modification. The nucleophilic character of the modified surface generally increases with increasing the temperature of the modification process. The highest increase of the S_C values was found after the modification of the silica gel with KR 33DS at 50 °C. In this case, further increase of reaction temperature seems to cause some degradation processes. These processes probably lead to the decrease of the surface ability to undergo nucleophilic interactions and a sharp increase of the electron acceptor properties. The surface character of the silica gel surface modified with KR 33DS at 70 °C is very similar to that found for raw silica gel.

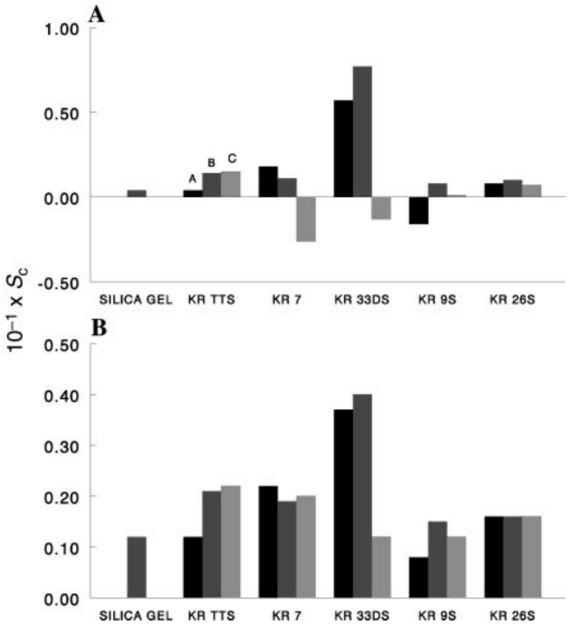


Fig. 4 Values of: A, S_C (Papirer); B, S_C (Donnet). Columns A, B and C refer to modification temperatures of 20, 50 and 70 °C, respectively.

Relationship between solubility and surface parameters

We have been looking for relationships between solubility parameters describing the properties of the modifier monolayer[4] and surface parameters exhibiting its ability to undergo different interactions with, *e.g.*, an adsorbate when a modified material is used as the adsorbent in the sample preparation procedure, or a polymer when the modified material acts as the filler. Such relationships were really found (Fig. 5). The K_D values slightly increase with the increase of the corrected solubility parameter δ_T and its specific increment δ_s. Similar relationships were found for the K_D values determined

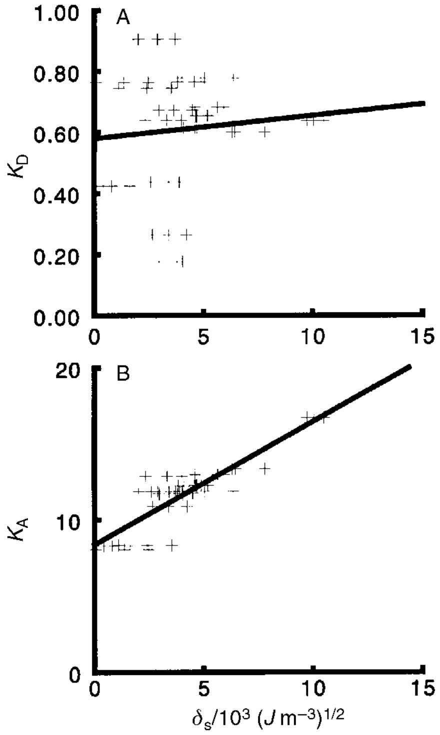


Fig. 5 Relationship between A, K_D (Donnet); B, K_A (Donnet) and the specific increment of the solubility parameter (δ_s).

Table 4 Correlation coefficients for the relationship between the parameters characterising the surface properties of the adsorbent and the modifier monolayer

Temperature of IGC measurement/°C	Correlation coefficient for K_D *vs.* δ_s plot	Correlation coefficient for K_A *vs.* δ_s plot
120	0.647	0.872
130	0.417	0.928
140	0.821	0.855

according to both discussed (Papirer and Donnet) procedures. The increase of the K_A values is accompanied by an increase of the corrected solubility parameter δ_T and its specific increment δ_s. The slope of the linear relationship K_D *vs.* δ_s is lower than that for the relationship K_A *vs.* δ_s. Therefore, the increase of the specific increment of the solubility parameter causes a decrease of the surface character parameter S_C. This means that the increase of the specific activity of the modifier monolayer leads to the decrease of the nucleophilic character of the modified surface (K_D and S_C) while the basic (electron acceptor) properties increase (K_A). The specific increment of the solubility parameter is defined in such a way that it is difficult to discriminate between the influences of electron acceptor and electron donor abilities on the value of this parameter (δ_s). However, as we mentioned above, the increase of the S_C parameter for the modified silica gel was a result of the increase of the values of the K_D parameter accompanied by the decrease of the electron acceptor properties of the adsorbent surface (K_D). The relationship between K_D and δ_s is not a statistically valid linear relationship while the relationship between K_A and δ_s is almost linear. Taking these facts into account, we may conclude that the specific increment of the solubility parameter δ_s characterises mainly the electrophilic properties of the monolayer.

We may also notice that the values of the correlation coefficient of the linear relationship between K_D and δ_s are higher when the values of this coefficient decrease for the respective relationships between K_A and δ_s (Table 4). This can be caused by the fact that δ_s reflects both acidic and basic properties of the monolayer. The decrease of the correlation coefficient for the relationship K_A *vs.* δ_s is accompanied by the increase of the correlation coefficient of the K_D *vs.* δ_s relationship.

A statistically valid relationship was not found between the dispersive increment of the solubility parameter δ_d and the dispersive increment of the surface free energy γ_s^d. The experimental points are randomly distributed around a hypothetical straight line.

Conclusions

It has been shown that surface parameters (both dispersive and specific ones) may be successfully used for the "screening" of the properties of silica gels modified with titanium coupling agents. The choice of the method of calculation (Papirer and Donnet) of the specific surface parameters (K_A, K_D, S_C) leads to different numerical values but the direction of changes (caused by the modification of examined materials) remains the same. The analysis of the surface parameter values permits one to discuss the influence of the modifier structure on the final product properties. It was also found that the temperature of the modification process significantly affects these properties. Linear relationships were found between the solubility parameters describing the properties of the monolayer and the surface parameter K_A.

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