The influence of the structure of organic compounds on their solubilization by sodium dodecyl sulfate micelles

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Regression analysis of the structural influence of organic compounds on the binding constants in aqueous micellar solutions of sodium dodecyl sulfate (SDS) was performed. Regression equations were obtained using empirical and calculated descriptors that characterize the mechanisms of interaction of substances with micelles and water. For alkanes, compounds with hydroxyl groups (alcohols, phenols, and benzoic acids), and aromatic and aliphatic hydrocarbons without OH groups, the binding constants were described by particular regression equations, which indicate the specificity of solubilization of these types of organic compounds by SDS micelles from aqueous solutions.

Key words: sodium dodecyl sulfate, micelles, solubilization, organic compounds, binding constants, regression analysis.

The capability of increasing solubility of various chemical compounds due to their solubilization in micelles is an important property of aqueous micellar solutions of surfactants. Because of this specific feature, surfactants are widely used in analytical chemistry,[1,2] electrochemistry,[3] biology,[1] oil production,[4] and industrial processes.[1] The solubilizing ability of micellar systems is usually characterized by partition coefficients of substances $K_X = x_m/x_w$ (x_m and x_w are the equilibrium molar fractions of the solubilizate in the micellar pseudophase and water, respectively) and by the binding constants $K_S = C_m/(C_wC_D)$ (C_m and C_w are the equilibrium concentrations (in mol L^{-1}) of the solubilizate bound with micelles and present in the aqueous phase, and C_D is the concentration of the surfactant associated in the micelles[5]).

The K_X and K_S constants have been determined for many compounds in micellar solutions of anionic, cationic, and nonionogenic surfactants.[5–15] During solubilization, different molecules can be localized in either the hydrocarbon core of micelles or the relatively polar region near and on the micellar surface.[1,16] Aqueous micellar solutions of sodium dodecyl sulfate (SDS) are most widely studied, and more than 100 values of K_S and K_X for various organic compounds have been determined.[17] Analysis of the known K_S and K_X values on the basis of the principle of a linear dependence between free solvation energies of substances in different processes has been attempted using empirical parameters (descriptors) that characterize solvation mechanisms.[17–19] Plural regressions describing the $\log K_X$ and $\log K_S$ values of organic compounds have been found for SDS micelles by two research groups.[17,18] The regression coefficients[17,18] are not entirely consistent with each other, which prompted us to refine their values by analysis of newly obtained results[11,15] or those[13,14] not used by the authors of Refs. 17 and 18.

Calculation procedure

The published[11,13–18] K_X and K_S values (25 °C) were averaged, and the K_X values (see Ref. 17) were preliminarily transformed into the K_S values taking into account the difference in standard states ($K_S = K_X/55.5$).[7] Some results[13–15] were presented as free energies ($\Delta G_{tr} = -RT\ln K_X$) of transfer of substances from water into SDS micelles, and the formula $K_S = \exp[-\Delta G_{tr}/(RT)]/55.5$ was used to recalculate them as K_S. After the K_S values were averaged, the $\log K_S$ values were obtained, and their standard deviations were determined, whose average value for 71 compounds was 0.14. The descriptor values for calculations were taken from the literature.[20–22] Some compounds described previously[17] were not analyzed, because some descriptors were absent in several works.[20–22] The regression analysis was performed by the least-squares method using the STATGRAPHICS Plus program. The coefficients at the descriptors, standard errors of calculation of the coefficients, correlation coefficients (r) corrected by the number of degrees of freedom, and selected standard deviations (s) were estimated.

Results and Discussion

A regression equation describing the partition of many organic compounds between water and SDS micelles (Eq. (1)) has previously[17] been obtained

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$$\log K_X = 1.280 + 0.484R_2 - 0.431\pi_2{}^H - 0.183\Sigma\alpha_2{}^H - \\ - 1.721\Sigma\beta_2{}^\circ + 2.878V_X, \quad (1)$$

$$n = 138,\ r = 0.9808,\ s = 0.192,$$

where R_2, $\pi_2{}^H$, $\Sigma\alpha_2{}^H$, and $\Sigma\beta_2{}^\circ$ are descriptors that reflect the dispersion (expressed as an excess molar refraction), dipole-dipole, proton-donor, and proton-acceptor (by the formation of a H bond) interaction of the solubilizates with the medium, respectively,[20—22] and V_X is the characteristic volume of the substance (10^{-2} cm^3 mol^{-1}), which is calculated by the McHowen method.[20] Equation (1) is also appropriate for the description of solubilization of some alkanes (CH_4—C_6H_{14}). When six alkanes were eliminated from the selection, the statistical indicators of the regression were improved, and Eq. (1) gained the form[17]

$$\log K_X = 1.201 + 0.542R_2 - 0.400\pi_2{}^H - 0.133\Sigma\alpha_2{}^H - \\ - 1.580\Sigma\beta_2{}^\circ + 2.793V_X, \quad (2)$$

$$n = 132,\ r = 0.9849,\ s = 0.171,$$

which better describes the $\log K_X$ values for SDS micelles in water.

The following equation was obtained[18] for the binding constants of various organic compounds, including lower alkanes, in aqueous micellar solutions of SDS:

$$\log K_S = -0.62 + 0.32R_2 - 0.57\pi_2{}^H - 0.08\Sigma\alpha_2 - \\ - 1.84\Sigma\beta_2 + 3.25V_X, \quad (3)$$

$$n = 66,\ r = 0.9895,\ s = 0.13,$$

where $\Sigma\alpha_2$ and $\Sigma\beta_2$ are descriptors corresponding to $\Sigma\alpha_2{}^H$ and $\Sigma\beta_2{}^\circ$ in Eqs. (1) and (2).[17]

Due to the difference in standard states, Eqs. (1)—(3) can statistically significantly differ by their free terms only, but as the authors[17,18] used selections differing in composition, the coefficients of the descriptors in Eqs. (1)—(3) differ substantially from one another.

The combined regression analysis of the $\log K_S$ values performed in this work for 122 compounds, including alkanes, by the model equation in the form

$$\log K_S = a_0 + a_1R_2 + a_2\pi_2{}^H + a_3\Sigma\alpha_2{}^H + a_4\Sigma\beta_2 + a_5V_X, \quad (4)$$

shows (Tables 1—5) that the total regression is characterized by high standard deviations (s = 0.33) and low correlation coefficients (r = 0.966) and, hence, it is unreasonable to use it. Systematic deviations from Eq. (4) are observed for higher alkanes, alcohols, and ketones with alkyl groups from C_7H_{15} and with a great number of carbon atoms, as well as for some other compounds. Estimation of the $\log K_S$ values of alkanes by Eqs. (1) and (3) indicates that these equations are inappropriate for higher alkanes (see Table 1).

Table 1. Calculated and observed $\log K_S$ values of alkanes and some nonpolar gases in aqueous micellar solutions of SDS

Compound	$\log K_S$				Reference
	Calculation by regression equations			Experiment	
	(1)[a]	(3)	(4.1)[b]		
Ar (**1**)	0.08	0	−0.19	−0.115±0.015	17, 18
O_2 (**2**)	0.06	−0.03	−0.22	−0.133±0.027	17, 18
Methane (**3**)	0.25	0.19	0.09	0.0740±0.003	17, 18
Ethane (**4**)	0.66	0.65	0.73	0.787±0.008	15, 17, 18
Propane (**5**)	1.06	1.11	1.37	1.355±0.010	15, 17, 18
Butane (**6**)	1.47	1.56	2.01	2.035±0.012	15, 17
Pentane (**7**)	1.88	2.02	2.65	2.555±0.145	15, 17
Hexane (**8**)	2.28	2.48	3.29	2.802±0.306	15, 17
Heptane (**9**)	2.69	2.94	3.93	3.984	15
Octane (**10**)	3.09	3.40	4.57	4.667	15
Nonane (**11**)	3.50	3.85	5.21	5.263	15
Decane (**12**)	3.90	4.31	5.86	5.823	15
Undecane (**13**)	4.31	4.77	6.50	6.910	15
Dodecane (**14**)	4.71	5.23	7.14	6.927	15

[a] The calculation took into account that $\log K_S = \log K_X - \log 55.5$.

[b] For parameters of regression equation (4.1), see Table 5.

The $\log K_S$ values for alkanes are described by an equation of a simple linear regression (4.1) (see Table 5) with the V_X descriptor. It should be expected that the behavior of alkanes solubilized, unlike other compounds, in the hydrophobic core of micelles[16] is unusual. Regression (4.1) also describes molecules of nonpolar gases (Ar and O_2).

Elimination of alkanes from the selection analyzed by Eq. (4) allowed us to obtain regressions (4.2) and (4.3) (see Table 5), whose statistical indicators (s, r) are very close. Regression (4.3), containing only four descriptors (without $\Sigma\alpha_2{}^H$), is preferable. The two-parametric (with the V_X and $\Sigma\beta_2{}^H$ descriptors) regression (4.4) is presented in Table 5, and its value of standard deviation (s) is insignificantly higher than those for Eqs. (4.2) and (4.3).

Regression equations (4.2)—(4.4) were found for a selection including compounds (n = 108) with various structures. Solubilization of some types of compounds is specific in the mechanism of their interaction with micelles or by the region of their localization in micelles, whereas statistical indicators of regressions can be improved for selections consisting of single-type compounds. Therefore, the data presented in Tables 2—4, taking into account the specific features of the compounds, were grouped into three selections: I, compounds with the hydroxyl group (see Table 2) that are capable of forming hydrogen bonds with anionic head groups; II, aromatic compounds without OH groups and solubilized near the micellar surface[16] (see Table 3); and III, aliphatic compounds containing no OH groups but bearing polar bonds that favor their localization in the relatively polar region of micelles (see Table 4).

The results of analysis (see Table 5) indicate a certain specificity of solubilization of these types of organic compounds by SDS micelles from the aqueous phase. For selections I—III, the main regression equations

Table 2. Calculated and observed $\log K_S$ values of compounds bearing hydroxyl groups in aqueous micellar solutions of SDS

Compound	$\log K_S$				Reference
	Calculation by regression equations*			Experiment	
	(4.5)	(4.6)	(4.7)		
Methanol (**15**)	−0.44	−0.45	−0.47	−0.534±0.196	11, 17, 18
Ethanol (**16**)	−0.08	−0.06	−0.08	−0.116±0.158	11, 17, 18
Propanol (**17**)	0.32	0.34	0.32	0.309±0.139	11, 17, 18
Propan-2-ol (**18**)	0.23	0.23	0.20	0.296±0.253	17, 18
Butanol (**19**)	0.72	0.74	0.72	0.717±0.100	11, 17, 18
2-Methylpropanol (**20**)	0.74	0.75	0.72	0.806±0.159	17
Butan-2-ol (**21**)	0.63	0.64	0.60	0.691±0.204	17
tert-Butyl alcohol (**22**)	0.60	0.59	0.55	0.544±0.232	17
Pentanol (**23**)	1.12	1.14	1.12	1.205±0.107	11, 17, 18
Pentan-2-ol (**24**)	1.03	1.03	1.01	0.951±0.276	17
Pentan-3-ol (**25**)	1.04	1.04	1.01	0.686	17
3-Methylbutanol (**26**)	1.13	1.14	1.12	1.149±0.018	17, 18
2-Methylbutan-2-ol (**27**)	1.01	1.00	0.95	0.846	17
Hexanol (**28**)	1.52	1.54	1.52	1.644±0.098	11, 17, 18
Hexan-2-ol (**29**)	1.44	1.44	1.41	1.586	17
Heptanol (**30**)	1.93	1.94	1.92	2.036±0.091	17, 18
Heptan-2-ol (**31**)	1.85	1.84	1.81	1.956	17, 18
Octanol (**32**)	2.33	2.34	2.32	2.457±0.027	17, 18
Decanol (**33**)	3.14	3.14	3.12	2.666	17
2-Butoxyethanol (**34**)	1.17	1.10	1.19	1.296	17
Benzyl alcohol (**35**)	1.05	1.11	1.13	1.086±0.172	17
2-Phenylethanol (**36**)	1.30	1.36	1.40	1.398±0.191	17
3-Phenylpropanol (**37**)	1.69	1.74	1.77	1.678±0.081	17
4-Phenylbutanol (**38**)	2.10	2.14	2.17	2.048±0.191	17
5-Phenylpentanol (**39**)	2.51	2.55	2.57	2.485±0.235	17
6-Phenylhexanol (**40**)	2.89	2.93	2.95	2.883±0.259	17
Phenol (**41**)	1.11	1.11	1.09	1.129±0.374	17, 18
2-Methylphenol (**42**)	1.49	1.53	1.49	1.329±0.010	17, 18
3-Methylphenol (**43**)	1.47	1.47	1.45	1.370±0.038	17, 18
4-Methylphenol (**44**)	1.50	1.51	1.47	1.526±0.319	17, 18
2,3-Dimethylphenol (**45**)	1.88	1.89	1.82	1.776	17
2,4-Dimethylphenol (**46**)	1.85	1.84	1.77	1.816	17
2,5-Dimethylphenol (**47**)	1.89	1.88	1.80	1.816	17
2,6-Dimethylphenol (**48**)	1.77	1.85	1.77	1.776	17
3,5-Dimethylphenol (**49**)	1.88	1.86	1.82	1.816	17
4-Ethylphenol (**50**)	1.82	1.82	1.82	1.859±0.310	17
4-Propylphenol (**51**)	2.22	2.22	2.20	2.436	17
4-*tert*-Butylphenol (**52**)	2.61	2.59	2.57	2.576	17
4-Fluorophenol (**53**)	1.17	1.20	1.25	1.225±0.011	17, 18
4-Chlorophenol (**54**)	1.54	1.56	1.58	1.554±0.049	17, 18
4-Bromophenol (**55**)	1.71	1.74	1.74	1.811±0.021	17, 18
4-Iodophenol (**56**)	2.03	2.06	1.98	2.130±0.054	17, 18
3,5-Dichlorophenol (**57**)	2.14	2.12	2.11	1.976	17
4-Formylphenol (**58**)	1.25	1.16	1.35	1.106	17
4-Methoxyphenol (**59**)	1.30	1.30	1.41	1.186	17
4-Cyanophenol (**60**)	1.24	1.25	1.54	1.186	17
4-Nitrophenol (**61**)	1.36	1.37	1.65	1.263±0.042	17, 18
1-Naphthol (**62**)	2.27	2.23	2.05	2.159±0.171	17, 18
2-Naphthol (**63**)	2.21	2.17	2.01	2.233±0.248	17, 18
Benzoic acid (**64**)	1.41	1.38	1.40	1.542±0.088	17, 18
3-Methylbenzoic acid (**65**)	1.82	1.78	1.80	1.918±0.002	17, 18
4-Methylbenzoic acid (**66**)	1.84	1.81	1.83	2.048±0.299	17, 18
4-Ethylbenzoic acid (**67**)	2.24	2.22	2.23	2.656	17

* For parameters of Eqs. (4.5)—(4.7), see Table 5.

Table 3. Calculated and observed $\log K_S$ values of aromatic compounds containing no hydroxyl groups in aqueous micellar solutions of SDS

Compound	$\log K_S$				Reference
	Calculation by regression equations*			Experiment	
	(4.8)	(4.9)	(4.10)		
Benzene (**68**)	1.42	1.45	1.39	1.386±0.180	11, 13, 17, 18
Toluene (**69**)	1.85	1.86	1.88	1.755±0.113	11, 17, 18
Ethylbenzene (**70**)	2.25	2.25	2.34	2.344±0.148	11, 17, 18
Propylbenzene (**71**)	2.67	2.67	2.83	2.655	11
Butylbenzene (**72**)	3.10	3.08	3.32	3.074	11
Pentylbenzene (**73**)	3.52	3.50	3.81	3.406	11
p-Xylene (**74**)	2.21	2.22	2.31	2.321±0.112	17, 18
Anisole (**75**)	1.56	1.63	1.65	1.462	18
Nitrobenzene (**76**)	1.57	1.64	1.59	1.239±0.234	14, 18
Fluorobenzene (**77**)	1.57	1.58	1.56	1.900	13, 18
Chlorobenzene (**78**)	2.06	2.05	2.02	1.904±0.071	13, 18
Bromobenzene (**79**)	2.21	2.21	2.14	2.302	13, 18
Iodobenzene (**80**)	2.46	2.46	2.34	2.531	13, 18
Benzonitrile (**81**)	1.30	1.39	1.37	1.282±0.444	14, 18
1,2-Dichlorobenzene (**82**)	2.59	2.56	2.53	2.483±0.331	14, 17
1,3-Dichlorobenzene (**83**)	2.65	2.61	2.59	2.723	14
1,4-Dichlorobenzene (**84**)	2.64	2.60	2.59	2.856	14
Naphthalene (**85**)	2.58	2.60	2.50	2.454±0.184	13, 17, 18
1-Methylnaphthalene (**86**)	3.01	3.02	2.99	3.068±0.008	17, 18
Biphenyl (**87**)	3.25	3.26	3.27	3.093±0.019	17, 18
Anthracene (**88**)	3.81	3.83	3.61	3.701±0.206	13, 17, 18
Phenanthrene (**89**)	3.74	3.75	3.61	3.856	17
Pyrene (**90**)	4.28	4.30	3.97	4.456	17
Aniline (**91**)	0.83	0.80	0.69	0.714±0.232	14, 17, 18
4-Methylaniline (**92**)	1.16	1.14	1.12	1.287±0.013	17, 18
Acetanilide (**93**)	1.31	1.15	1.23	1.364	17, 18
Benzamide (**94**)	0.91	0.77	0.74	0.881	18
Benzaldehyde (**95**)	1.13	1.25	1.21	0.901	14
Acetophenone (**96**)	1.23	1.37	1.41	1.542±0.163	17, 18
Propiophenone (**97**)	1.58	1.72	1.84	1.820±0.225	17, 18
Benzophenone (**98**)	2.81	2.92	3.00	2.686±0.044	17, 18

* For parameters of Eqs. (4.8)—(4.10), see Table 5.

Table 4. Calculated and observed $\log K_S$ values of aliphatic compounds containing no hydroxyl groups in aqueous micellar solutions of SDS

Compound	$\log K_S$				Reference
	Calculation by regression equations[a]			Experiment	
	(4.11)	(4.12)	(4.13)		
Propionamide (**99**)	0.21	0.19	0.06	0.496	17
Butyramide (**100**)	0.70	0.69	0.520.542±0.241		17
Acetone (**101**)	−0.13	−0.14	−0.07−0.122±0.117		11, 15, 17, 18
Butanone (**102**)	0.33	0.33	0.390.367±0.193		17, 18
Pentan-2-one (**103**)	0.83	0.83	0.860.850±0.166		17, 18
Pentan-3-one (**104**)	0.84	0.83	0.86	0.686	17
4-Methylpentan-2-one (**105**)	1.28	1.30	1.31	1.110	17
Hexan-2-one (**106**)	1.29	1.30	1.311.317±0.105		11, 15, 18
Heptan-2-one (**107**)	1.79	1.79	1.781.770±0.114		11, 17, 18
Octan-2-one (**108**)	2.27	2.28	2.24	2.214	15
Nonan-2-one (**109**)	2.76	2.77	2.70	2.780	11
Decan-2-one (**110**)	3.25	3.26	3.17	3.371	15
Dichloromethane (**111**)	0.54	0.52	0.570.549±0.012		17, 18
Trichloromethane (**112**)	1.12	1.08	1.031.041±0.059		17, 18
Iodoethane (**113**)	1.11	0.90	0.90	1.342	18
Iodobutane (**114**)	2.09	1.88	1.83	2.057	18
Halotane[b] (**115**)	1.45	1.55	1.42	1.041	18
Tetrafluoromethane (**116**)	0.10	0.29	0.09	0.376	17, 18
Tetrachloromethane (**117**)	1.52	1.43	1.431.421±0.328		17, 18
Dioxane (**118**)	0.17	0.06	0.140.059±0.083		17, 18
Butyronitrile (**119**)	-0.40	0.45	0.650.0634±0.002		17, 18
Nitrobutane (**120**)	1.04	1.09	1.30	1.256	15
Nitropentane (**121**)	1.52	1.58	1.77	1.674	15
Nitrohexane (**122**)	2.01	2.07	2.23	2.142	15

[a] For parameters of Eqs. (4.11)—(4.13), see Table 5.

[b] 2-Bromo-2-chloro-1,1,1-trifluoroethane.

Table 5. Parameters in regression equations (4.1)—(4.13)

Compound	Equation	a_0	a_1	a_2	a_3	a_4	a_5	s	r	n
1—14[a]	(4.1)	−1.05±0.11	—	—	—	—	4.55±0.10	0.20	0.997	14
15—122[b]	(4.2)	−0.55±0.09	0.40±0.07	−0.44±0.09	−0.18±0.08	−1.75±0.12	3.05±0.09	0.20	0.974	108
	(4.3)	−0.57±0.09	0.39±0.07	−0.49±0.09	—	−1.81±0.12	3.09±0.09	0.21	0.973	108
	(4.4)	−0.72±0.09	—	—	—	−2.13±0.12	3.22±0.09	0.24	0.965	108
15—67[c]	(4.5)	−0.85±0.29	0.38±0.12	−0.67±0.17	0.65±0.44	−1.21±0.33	2.88±0.09	0.14	0.980	53
	(4.6)	−0.45±0.12	0.34±0.12	−0.49±0.12	—	−1.61±0.18	2.86±0.09	0.15	0.979	53
	(4.7)	−0.67±0.11	—	—	—	−1.43±0.16	2.84±0.09	0.16	0.973	53
68—98[d]	(4.8)	−0.48±0.16	0.33±0.08	—	0.73±0.34	−3.34±0.25	3.03±0.19	0.17	0.984	31
	(4.9)	−0.45±0.17	0.33±0.09	—	—	−2.95±0.18	2.95±0.20	0.18	0.981	31
	(4.10)	−0.70±0.19	—	—	—	−2.90±0.22	3.48±0.17	0.22	0.972	31
99—122[e]	(4.11)	−1.01±0.15	0.51±0.24	−0.66±0.23	0.76±0.35	−1.36±0.28	3.49±0.18	0.19	0.975	24
	(4.12)	−0.92±0.16	—	−0.48±0.24	0.86±0.38	−1.58±0.28	3.47±0.19	0.21	0.970	24
	(4.13)	−0.96±0.16	—		—	−1.77±0.23	3.28±0.19	0.23	0.964	24

[a] See Table 1. [b] See Tables 2—4. [c] See Table 2. [d] See Table 3. [e] See Table 4.

(4.5), (4.8), and (4.11) corresponding to the model equation (4) are characterized by lower s values and increased correlation coefficients r (see Table 5), as compared to the general equation (4.2), whose parameters are presented in Table 5. The $\log K_S$ values calculated from the regression equations of different forms are compared with those observed experimentally (see Tables 2—4).

The coefficients of descriptors reflect the degree of influence of the corresponding interactions on the $\log K_S$ value. For all groups of compounds, the a_5 at the V_X descriptor is the most significant (see Table 5). Its influence on the K_S value is related to a change in the energy necessary for the formation of a cavity during localization of the molecule in the aqueous phase and in micelles. The positive sign at the a_5 coefficient indicates that the cavity is more easily formed in micelles than in water, and this favors solubilization of substances by micelles. The higher (as compared to other groups of compounds) a_5 value for alkanes agrees with their solubilization in the hydrophobic core of micelles, whereas the a_5 values are the lowest for compounds with hydroxyl groups. Decreased a_5 coefficients are also characteristic of aromatic compounds solubilized near the micellar surface.[16] The a_4 coefficient, second in absolute value, is negative for all groups of compounds, which is due to the suppression of the proton-acceptor interaction of organic bases with water in micelles. The dipole-dipole interaction of substances with the medium resulting in a negative value of the a_2 coefficient is similarly suppressed in micelles. In the case of aromatic compounds solubilized near the micellar surface,[16] this interaction is not suppressed, which leads to the absence of its contribution to the ΔG_{tr} value and insignificance (absence) of a_2. The positive a_1 coefficient for all selections reflects an increase in the dispersion interaction of substances with the medium in the micellar pseudophase.

The a_3 coefficient at the $\Sigma\alpha_2^H$ descriptor in regression equations (4.5), (4.8), (4.11), and (4.12) is positive (see Table 5), but it is negative in general equations (1)—(3) and (4.2). The $\Sigma\alpha_2^H$ descriptor describes the proton-donor mechanism of interaction of substances with the medium, and the a_3 value is determined by the contribution of this mechanism to the ΔG_{tr} value during transfer of substances from water into micelles. The positive a_3 values indicate the formation of stronger H bonds in micelles by proton donors, which is defined by the participation of bicharged SDS anions in the formation of H bonds. Evidently, general equations (1)—(3) and (4.2) reflect incorrectly the proton-donor interaction of substances with SDS micelles.

In addition to the main regressions (4.5), (4.8), and (4.11), regression equations with a lower number of descriptors were obtained for all selections. When some descriptors (R_2, π_2^H, $\Sigma\alpha_2^H$) are eliminated from the analysis, the statistical indicators (s, r) of regressions (see Table 5) change sufficiently weakly. Even for the two-parametric regressions with the $\Sigma\beta_2^H$ and V_X descriptors, the r values remain higher than 0.96, and the s value is lower than the double average error (see Calculation procedure) of the experimental data (0.14). This is due to substantially higher values of the a_4 and a_5 coefficients as compared to a_1, a_2, and a_3. The r^2 values show the fraction of variation of the $\log K_S$ variable described by the descriptors used in the equation. In particular, for regressions (4.7) and (4.10), two descriptors explain about 95%, and for regressions (4.4) and (4.13), they explain 93% of the $\log K_S$ variations. The total fraction of the influence of the three remaining descriptors is not higher than 2% and, hence, the role of the latter is comparatively small.

The regression equations obtained make it possible to estimate unknown K_S and K_X values of organic compounds for aqueous micellar solutions of SDS. Two-parametric equations (4.1), (4.4), (4.7), (4.10), and (4.13) provide wide possibilities for prognostication of the K_S and K_X values (see Table 5), and their use is facilitated by the fact that the $\Sigma\beta_2{}^H$ descriptor is known[20–23] for several hundred organic compounds, and the V_X descriptor can easily be calculated.[20]

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