TABLE IV: Bond Distances (Å) and Angles (deg) for AlPO₄-54

atoms	distance	atoms	angles
T(1)-O(1)	1.577 (14)	O(1)-T(1)-O(2)	109.3 (10)
T(1) - O(2)	1.655 (10)	O(1)-T(1)-O(3) (2×)	102.7 (6)
T(1)-O(3)(2X)	1.597 (11)	O(2)-T(1)-O(3) (2×)	112.5 (8)
		O(3) - T(1) - O(3)	116.0 (12)
$\langle T(1)-O \rangle$	1.61 (3)		
		O(3) - T(2) - O(4)	119.8 (10)
		O(3) - T(2) - O(5)	91.7 (9)
T(2) - O(3)	1.618 (15)	O(3) - T(2) - O(6)	108.7 (6)
T(2) - O(4)	1.433 (8)	O(4) - T(2) - O(5)	108.8 (7)
T(2) - O(5)	1.703 (12)	O(4) - T(2) - O(6)	116.6 (10)
T(2) - O(6)	1.625 (11)	O(5) - T(2) - O(6)	107.9 (8)
$\langle \hat{T}(2) - \hat{O} \rangle$	1.59 [10]	T(1) - O(1) - T(1)	180.0
		T(1) - O(2) - T(1)	174.4 (21)
		T(1) - O(3) - T(2)	131.0 (7)
		T(2) - O(4) - T(2)	164.5 (15)
		T(2) - O(5) - T(2)	167.6 (16)
		T(2) - O(6) - T(2)	156.4 (10)

T(2), O(2), and O(5) exhibit large displacements normal to the mirror plane joining the 4-rings. This suggests slight deviation from the mirror symmetry, which may be a result of preferential association of water with the T(1)-O(2)-T(1) and T(2)-O(5)-O(5)T(2) linkages. This idea is consistent with the observed contraction of the *a* axis, in that strong association with these linkages might distort the crankshaft chains.

Noncrystalline Component

As mentioned above, an oscillatory component to the total scattering was observed and removed. This scattering function, however, had maxima at d spacings significantly different from those observed in calcined AlPO₄-5 and AlPO₄-11, where short-range order consistent with the framework topologies (possibly from uncrystallized gel) was observed. The first prominent peak in the Fourier transform of the residual scattering from AlPO₄-54 is at $r \sim 2.8$ Å, rather than $\sim 1.5-1.6$ Å. This is consistent with nonperiodic, weak interaction of water with the framework of the second phase. No evidence was found for an Al species, e.g., corundum or boehmite, and it is presumed that the phase seen in electron microscopy is below the detection level.

Conclusions

There are 13 theoretical nets that match the hexagonal geometry of AIPO₄-54 and have geometry constrained by the replacement of edges of the $(4.4.18)_1(4.6.18)_2$ 2D net by crankshaft chains. Rietveld refinement of neutron diffraction data from dehydrated AIPO₄-54 demonstrates that net 520 is the basis of the AlPO₄ framework. This net is the one found in the VPI-5 family of aluminophosphate-based molecular sieves. There are complex structural changes upon heating of the $AlPO_4$ in a Guinier-Lenné camera, and further work is needed to pin down the possible modulation of structural displacements. The structure refinement of dehydrated AlPO₄-54 was complicated by the possible presence of a minor amount of hydrated $AlPO_4$ and by probable presence of displacements of oxygen atoms from the idealized positions for the theoretical net.

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Supplementary Material Available: Table 5, listing anisotropic thermal displacement parameters for AlPO₄-54, and tables of atomic coordinates and equivalent isotropic thermal displacement parameters used to generate the diffraction patterns for Figure 5 (14 pages). Ordering information is given on any current masthead page.

Micellar Effects upon the Reaction of Hydroxide Ion with 2-Phenylethyl Derivatives

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The rate constants for reactions of OH⁻ with para-substituted 2-phenylethyl bromides, i.e., $p-X-C_{6}H_{4}CH_{2}Br$ (X = NO₂, Cl, H), were determined under micellar (k_{ψ}) and nonmicellar $(k_{w'})$ conditions by using hexadecyltrimethylammonium bromide [(CTA)Br] and hydroxide [(CTA)OH)] as the micellar agents. The results can be explained with the pseudophase ion-exchange model. The evaluated second-order rate constants in micelles are greater than the second-order rate constants in water by factors of 3.4, 2.0, and 1.1 for $X = NO_2$, Cl, and H, respectively.

Introduction

The 2-phenylethyl system seems well suited to the application of kinetic studies in identifying changes in the nature of activated complexes caused by changes in reagent structure or the reaction medium.¹ The phenylethyl derivatives are traditional model compounds in 1,2-elimination-reaction studies on the transitionstate structure and kinetic isotope effects.²⁻⁶ The elimination

reaction under nonmicellar conditions has been studied in detail, and its mechanism is reasonably well understood.⁷⁻⁹ It is known that cationic micelles affect the rates of some E2 processes.^{10,11} A micelle of a choline analogue was reported to favor E2 elimination by inhibiting a competitive S_N^{i} process in reactions of 1-bromo-2-phenylpropane¹²⁻¹⁴ and 3-bromo-3-phenylpropionate

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ion.15 The same micelle was also effective in the Hofmann elimination of (4-nitrophenyl)ethyltrimethylammonium iodide.¹⁶

Most of the kinetic data in micellar systems for many bimolecular reactions and indicator equilibria have been explained in terms of a pseudophase ion-exchange (PIE) model.¹⁷⁻²¹ Not too many reports are available related to application of this theory to the effect of micellar catalysis on the elimination reaction of alkyl halides except for specific examples in the pesticide field.²²⁻²⁵

In the present work, we have studied the elimination reaction of para-substituted 2-phenylethyl bromides p-X-C₆H₄CH₂CH₂Br, where $X = NO_2$, Cl, and H, promoted by hydroxide ion in aqueous solutions of hexadecyltrimethylammonium bromide [(CTA)Br] and hydroxide [(CTA)OH]. The purpose of this work was to describe our experimental kinetic data by means of the PIE model in the best possible way and to compare the obtained results with the available literature data.

Experimental Section

Materials. Reagents and solvents were of commercial grade and were usually purified before use. Commercial 2-phenylethyl bromide (Aldrich Chemical Co.) was purified by distillation (bp = 106 °C at 15 mmHg). 2-(p-Nitrophenyl) ethyl bromide was synthesized by nitration of 2-phenylethyl bromide by the procedure previously described²⁶ (yield, 30%; mp = 70 °C). 2-(p-Chlorophenyl)ethyl bromide was obtained according to the procedure given in²⁷ (yield, 61%; bp = 87 °C at 2 mmHg).

The preparation and purification of hexadecyltrimethylammonium bromide [(CTA)Br] has been described previously.28,29 The surfactant (CTA)OH was prepared by ion exchange from (CTA)Br with anionic resin Wofatyt SBW (GDR). However, the original (CTA)OH solutions did not fulfill the requirements of surface-chemical purity. The stock solutions of (CTA)OH were subjected to a repeated surface purification with a special sucking technique³⁰ until the grade of purity necessary for surface-chemical measurements was achieved. The absence of Br⁻ in (CTA)OH was tested with a silver ion. Solutions of (CTA)OH were stored in a refrigerator and under N_2 and were used within 24 h of preparation.

Measurements. The kinetic measurements were performed in a thermostatically controlled cell compartment of a Specord M 40 spectrophotometer (GDR).

The surface tension measurements were made at 25 ± 0.1 °C by the drop-weight method in a setup constructed for the measurement of equilibrium values. The water used was deionized and thermodistilled twice. The critical micelle concentrations for (CTA)Br and (CTA)OH were 9×10^{-4} and 9.6×10^{-4} M, respectively. These were in good agreement with literature values.³¹

The concentrations of NaOH and (CTA)OH were determined by titration with standard HCl solutions, with conductometric use of a OK-102 conductivity meter (Radelkis, Hungary).

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Figure 1. Reaction of 2-(p-nitrophenyl)ethyl bromide with OH⁻: in (CTA)Br, (O) [NaOH] = 0.025, (\diamond) [NaOH] = 0.05, (∇) [NaOH] =0.075, (\Box) [NaOH] = 0.1, (\bullet) [NaOH] = 0.2 M; in (CTA)OH, (∇) [NaOH] = 0.00, (*) [NaOH] = 0.02 M. Lines are predicted values.



Figure 2. Reaction of 2-(p-chlorophenyl)ethyl bromide with OH⁻: in (CTA)Br, (O) [NaOH] = 0.025, (\diamond) [NaOH] = 0.05, (∇) [NaOH] =0.075, (\Box) [NaOH] = 0.1, (\bullet) [NaOH] = 0.2 M; in (CTA)OH, (∇) [NaOH] = 0.00, (*) [NaOH] = 0.02 M. Lines are predicted values.

The binding constants of para-substituted phenylethyl bromides to (CTA)Br in the absence of hydroxide ion were corrected by (¹H, FT) NMR measurements³² with the Tesla Model BS 567A 100-MHz instrument (Czechoslovakia).

Chromatographic analyses were carried out with a gas-liquid chromatograph Giede Model 18.3.6 equipped with a flame-ionization detector. Metallic columns (3-mm diameter and 1.5-m length) were filled with 10% carbowax 20 M on Chrom G/AW-DVCS, 60-80 mesh.

Kinetic Procedure. A 15- μ L stock solution of each substrate $(1 \times 10^{-2} \text{ M in acetonitrile})$ was added by microsyringe to 3 mL of sodium hydroxide and a given surfactant. The rate constants were determined by following the para-substituted styrenes' ap-

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Figure 3. Reaction of 2-phenylethyl bromide with OH^- : in (CTA)Br, (\bigtriangledown) [NaOH] = 0.075, (\square) [NaOH] = 0.1, (\textcircledo) [NaOH] = 0.2 M; in (CTA)OH, (\bigtriangledown) [NaOH] = 0.00, (*) [NaOH] = 0.02 M. Lines are predicted values.



Figure 4. Reaction of 2-(p-nitrophenyl)ethyl bromide with OH⁻ at a fixed (CTA)Br concentration: (\diamond) 0.01; (O) 0.02 M. Lines are predicted values.

pearance $(p\text{-NO}_2, 318; p\text{-C}l, 253; H, 248 \text{ nm})$. The temperature for the kinetic runs was maintained at 25 °C within ±0.1 °C. Individual pseudo-first-order rate constants were obtained from linear plots of ln $(A_{\infty} - A_i)$ vs time. All of these plots showed good linearity up to >80% of the reaction (60% for the slower reactions), and the correlation coefficients were greater than 0.99. The second-order rate constants, k_w , for dehydrobromination reactions of $p\text{-X}-C_6H_4CH_2CH_2Br$ are 261.0, 5.24, and $3.1 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ for X = NO₂, Cl, and H, respectively. The obtained values are in accordance with the cited literature.⁷⁻¹¹ Additionally, the quantitative chromatographic product analysis has been performed in all cases, and it indicated that the unsaturated compound is exclusively the reaction product.

Results and Discussion

The experimental pseudo-first-order rate constants, k_{ψ} , for the investigated reactions in micellar solutions of (CTA)Br and (CTA)OH are shown in Figures 1-3 at different hydroxide ion and surfactant concentrations. The variations of pseudo-first-order rate constants with hydroxide ion concentration at fixed concentration of (CTA)Br are shown in Figures 4-6.

The effect of unreactive counterion surfactant such as (CTA)Br upon the reaction of hydroxide ion with many organic reagents can be explained by means of the pseudophase ion-exchange model.¹⁷⁻²¹ This model considers that ions bind to micelles according to the exchange model developed for resins and that the



Figure 5. Reaction of 2-(p-chlorophenyl) ethyl bromide with OH⁻ at a fixed (CTA)Br concentration: (\diamond) 0.01; (O) 0.02 M. Lines are predicted values.



Figure 6. Reaction of 2-phenylethyl bromide with OH^- at a fixed (CTA)Br concentration: (\diamond) 0.01; (O) 0.02 M. Lines are predicted values.

mole ratio of reactive ion to micellar head group (β) can be taken as a constant when one of the ions in solution binds very strongly to micelles. A high charge density ion such as hydroxide is readily displaced from a cationic micelle by a low charge density ion such as bromide. The ion-exchange constant for this system can be expressed by

$$K_{Br}^{OH} = [OH_{M}^{-}][Br_{W}^{-}]/[OH_{W}^{-}][Br_{M}^{-}]$$
(1)

where M and W denote the micellar and aqueous pseudophases, respectively. Then, we can describe the concentration of reactive ion in the micelle in terms of an assumed constancy of β and K_{Br}^{OH19} and analyze the reaction rates in terms of these parameters, i.e., the substrate binding constant, K_{s} ,³³ and the second-order rate constants, k_{W} and k_{M} .³⁴ Thus, the first-order rate constants, k_{W} and k_{M} are written below as second-order rate constants, k_{W} and k_{M}

$$k_{\rm W}' = k_{\rm W}[\rm OH^-_{\rm T}] \tag{2}$$

$$k_{\rm M}' = k_{\rm M} [\rm OH^{-}_{\rm M}] / ([\rm D] - cmc)$$
 (3)

where cmc is the critical micelle concentration; [D] is the total surfactant concentration; $\beta = m_{OH} + m_{Br}$, while the mole ratios

⁽³³⁾ K_s is the binding constant of the substrate to the micelle written in terms of micellized surfactant: $K_s = [S_M]/([S_w][D_s])$ where D_s is the micellized surfactant whose concentration is given by $[D_s] = [D_T] - cmc$; cmc is the critical micelle concentration. (34) Bunton, C. A.; Carrasco, N.; Huang, S. K.; Paik, C. H.; Romsted,

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TABLE I: Parameters That Best Fit the Kinetic Results for p-X-C₆H₄CH₂CH₂Br in (CTA)Br at 25 °C

X	[NaOH], M	$k_{\rm M} \times 10^4$, s ⁻¹	β	K _s , ^a M ⁻¹	K ^{OH} Br
NO ₂	0.025	640	0.77	290	32
*	0.050	640	0.77	348	32
	0.075	640	0.77	382	32
	0.1	640	0.77	404	32
Cl	0.025	7.5	0.76	255	27
	0.050	7.5	0.76	303	27
	0.075	7.5	0.76	345	27
	0.1	7.5	0.76	367	27
	0.2	7.4	0.76	415	27
н	0.075	2.5	0.77	295	32
	0.1	2.5	0.77	325	32
	0.2	2.4	0.77	375	32

"The NMR values of K_s in the absence of OH⁻ were 230, 200, and 150 M⁻¹, respectively, for $X = NO_2$, Cl, and H.

 $m_{\rm OH} = [OH_{\rm M}^{-}]/([D] - cmc)$ and $m_{\rm Br} = [Br_{\rm M}^{-}]/([D] - cmc)$; and $k_{\rm M}$ is written in terms of the mole ratio of micellar-bound OH⁻ to micellar head groups.

The pseudo-first-order rate constant^{17,35-37} is easily derived as

$$k_{\psi} = \frac{k_{\rm W}[{\rm OH}^-_{\rm T}] + (k_{\rm M}K_{\rm s} - k_{\rm W})m_{\rm OH}([{\rm D}] - {\rm cmc})}{1 + K_{\rm s}([{\rm D}] - {\rm cmc})}$$
(4)

where m_{OH} is expressed by

$$m_{\rm OH}^{2} + m_{\rm OH} \left[\frac{[\rm OH^{-}_{T}] + K_{\rm Br}^{\rm OH}[\rm Br^{-}_{T}]}{(K_{\rm Br}^{\rm OH} - 1)([\rm D] - \rm cmc)} - \beta \right] - \frac{\beta[\rm OH^{-}_{T}]}{(K_{\rm Br}^{\rm OH} - 1)([\rm D] - \rm cmc)} = 0 (5)$$

where subscript T denotes total concentration. Equation 5 has the same general form as that used previously.³⁸⁻⁴⁰

The experimental rate constants were adapted to eq 4 and 5 by simulating on a computer the variation of k_{ψ} with surfactant and reactive ion concentrations while parameters such as cmc, $k_{\rm W}$, and β were fixed and $k_{\rm M}$, $K_{\rm s}$, $K_{\rm Br}^{\rm OH}$ adjustable.

This approach is oversimplified because the reported light scattering measurements suggest that β increases with addition of counterions in the solution,⁴¹ and even for ions that bind very strongly to the micelle, it is only an approximation to consider β as a constant.

The cmc value of (CTA)Br decreases with NaOH addition. The surface tension isotherms of the (CTA)Br aqueous solutions do not show minima at the cmc environment until $[OH^-] = 0.5$ M of NaOH. The deep minimum in the surface tension isotherm is invoked by occurence of the Hofmann elimination of (CTA)Br, i.e., the presence of unsaturated compounds.⁴² The cmc affected by the hydroxide ion addition were taken into account with the same empirical expression as reported in ref 43.

Table I gives the values of parameters that best fit the experimental results in (CTA)Br solutions at a given β , but to fit them, K, must be allowed to vary. As reported for other micelle-catalyzed reactions,38 small variations in the parameters' values also give acceptable fits of the experimental results. We calculated the parameter K_s for a given $[OH_T]$ from eq 4 and 5 that in-

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Figure 7. Variation of K_s with hydroxide ion concentration in (CTA)Br for $p-X-C_6H_5CH_2CH_2Br$: (0) $X = NO_2$; (*) X = Cl; (Δ) $X = H_2$.

TABLE II:	Parameters	for the	Relationship	between K,	and
Hydroxide l	on Concentr	ation		-	

Х	-A	В	С	D	
NO ₂	108	105	1110	21	
CI -	208	107	1570	44	
Н	340	122	1584	62	

TABLE III: Parameters That Best Fit the Kinetic Results for p-X-C₆H₄CH₂CH₂Br in (CTA)OH at 25 °C

 X	[NaOH], M	$k \times 10^4$, s ⁻¹	K _s , M ⁻¹	K _{OH} '	
NO ₂	0.00	640	250	30	
2	0.02	640	250	30	
Cl	0.00	7.5	230	30	
	0.02	7.4	230	30	
н	0.00	2.5	200	30	
	0.02	2.5	210	30	

creased as shown in Figure 7 with the hydroxide ion concentration. It seems to be in accord with a salting-out effect previously observed in ref 39 and 44. We found that the following relationship in the best way describes this empirical increase of K_s :

$$K_{\rm s} = A + B[\ln (C[\rm OH^-_{\rm T}] + D)]$$
(6)

The A-D values are given in Table II. Thus, the variation of the pseudo-first-order rate constants at fixed (CTA)Br with hydroxide ion concentrations can be fitted with the PIE model through the evaluated increase of K_s . However, we should not regard the above work as support for the PIE model unless the empirical expression for K_s could be replaced by a theoretically meaningful salting-out model. The applied approach can only be regarded as anything more than an useful tool for predicting and comparing the experimental kinetic data of the reactions under study.

It should be stated here that the parameters A-D have no physical meaning, and they only lead to the best possible fit of kinetic experiments to the theory. In the elimination of pesticides,²⁵ a linear relationship of K_s vs $[OH_T]$ was used to adapt the pseudo-first-order rate constant, k_{ψ} , with the hydroxide ion concentration. However, it did not work out in the case of our computation procedure.

The kinetic data for reactive counterion micelles as (CTA)OH can be treated on the assumption that the distribution between water and micelles of hydroxide ion follows a mass-action equation44,45

$$K_{\rm OH}' = [\rm OH^-_{\rm M}] / \{[\rm OH^-_{\rm w}]([\rm D_n] - [\rm OH^-_{\rm M}])\}$$
(7)

which reduces to

 $K_{\rm OH'}[\rm OH^-_{M}]^2 - \{K_{\rm OH'}([\rm D] - cmc) + K_{\rm OH'}[\rm OH^-] + 1\} \times$ $[OH_{M}] + K_{OH'}([D] - cmc)[OH_{T}] = 0$ (8)

This approach predicts that β given by $[OH_M^-]/([D] - cmc)$ will

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TABLE IV: Second-Order Rate Constants for Reactions of p-X-C₆H₄CH₂CH₂Br with OH⁻ in Water and Micelles

 <u> </u>	$k_{2}^{m} \times 10^{5}$, M ⁻¹ s ⁻¹	k., ^m /k	
 NO	8896	3.4	
Cl	10.5	2.0	
н	3.4	1.1	

increase with the surfactant concentration. The application of this mass-law treatment to the reaction of hydroxide ion with para-substituted phenylethyl derivatives in (CTA)OH is illustrated in Figures 1-3. The lines are calculated taking parameters that are shown in Table III, cmc = 9.6×10^{-3} M with no NaOH added, and cmc = 6×10^{-4} M in 0.02 M NaOH.

Different values of the ion-exchange parameter, K_{Br}^{OH} , have been used in the literature, and there are significant differences between the values adopted by different groups.²¹ However, for the most widely studied systems, values of K_{Br}^{OH} are between 10 and 20. From our results, it can be deduced that organic reagents may affect the binding of hydroxide ion to (CTA)Br micelles very affect the binding of hydroxide ion to (CTA) of micenes very strongly and the value of K_{Br}^{OH} is higher. We obtained the value of K_{Br}^{OH} that is in the range calculated for pesticides: DDT, DDD,³⁹ and p,p'-methoxychlor,²⁵ i.e., 32, 30, and 24, respectively. The value of K_{OH}^{OH} = 30 M⁻¹ is similar to the reported values for DDT and DDD of 30 and 35, respectively.³⁹ It differs,

however, from other values reported in the literature for reagents such as benzoic anhydride,⁴⁵ 5-nitroindole,⁴⁶ N-methyl-4-cyanopyridinium tetrafluoroborate⁴⁷ for which the value of 55 M⁻¹ has been found.

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The second-order rate constants, $k_{\rm M}$, are given with the concentrations written as a mole ratio. The constants can be converted into k_2^m [M⁻¹ s⁻¹] by taking into account the volume element of the reaction in the micelles, which is assumed to be that of a Stern layer, with a molar volume of ca. 0.14 L.³⁴

The second-order rate constants for all the investigated reagents with hydroxide ion in (CTA)Br and (CTA)OH, k_2^m , given in Table IV, are about the same order of magnitude as the second-order rate constants for reaction in the aqueous phase, k_w . Thus, the effect of cationic micelles on the reaction of hydroxide ion with para-substituted phenylethyl bromides is mainly due to the concentration of both reactants in the small volume of the Stern layer of the micelle.

Para substituents in the benzene ring of the investigated organic reagents do not introduce any significant influence on the PIE parameters' values.

Recently, D. G. Hall⁴⁸ proposed a new theory based on the equilibrium formulation of transition-state theory where all attention is focused on the partition coefficients of reactants and activated complexes between micellar and aqueous environments. The present authors will consider this alternative theory to explain micellar catalysis of the elimination reaction in terms of transition-state theory in a further publication.

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Registry No. p-X-C₆H₄CH₂CH₂Br (X = NO₂), 5339-26-4; p-X- $C_6H_4CH_2CH_2Br$ (X = Cl), 6529-53-9; p-X- $C_6H_4CH_2CH_2Br$ (X = H), 103-63-9.

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Chemical Structure and Thermodynamics of Amphiphile Solutions. 1. Solubility of Alkylthiooligooxyethylene Glycols in Water

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Solubilities of individual alkylthiooligooxyethylene glycols $C_nH_{2n+1}SCH_2CH_2(OCH_2CH_2)_2OH$ (alkyl: $n-C_4H_9$, ..., $n-C_9H_{19}$; and z = 0, ..., 3) in water at 298.15 K have been determined. A quantitative correlation has been found between the standard free energy for transfer from aqueous solution to pure liquid phase, ΔG° , and the structure of the studied sulfides and of oligooxyethylenated alcohols as well by using the appropriate multiple regression equation. It has been found that the thioethylene group, $-SCH_2CH_2-$, is hydrophobic. The standard free energy contribution, $\Delta G^{\circ}_{1}[-SCH_2CH_2-]$, is -3.4 kJ mol⁻¹. The interaction between methylene groups, $-CH_2-$, of the hydrocarbon chain and the $-OCH_2CH_2^{-}$ groups of the oligooxyethylene chain is statistically significant and has an influence on the total value of ΔG°_{t} . Furthermore, the ΔG°_{t} [-OCH₂CH₂-] and ΔG°_{t} [-CH₂-] are not constant. For the sulfides studied, ΔG°_{t} [-OCH₂CH₂-] increases linearly with hydrocarbon chain length. For example, $\Delta G^{\circ}_{,}$ [-OCH₂CH₂-] for the series of butyl and nonyl derivatives is +0.24 and +0.81 kJ mol⁻¹, respectively. The ΔG°_{t} [-CH₂-] for the series of alkyl-2-hydroxyethyl sulfides (z = 0) and alkylthiotetraoxyethylene glycol (z = 3) is -3.43 and -3.10 kJ mol⁻¹, and the ΔG°_{t} [-OCH₂CH₂-] and ΔG°_{t} [-CH₂-] for the group of oxyethylenated alcohols are +0.53 and -3.13 kJ mol⁻¹, respectively.

Introduction

The number of scientific reports and publications on solubility, micellization, and surface activity of oligooxyethylene nonionics has rapidly increased in recent several years, mainly due to the expansion of their application field and the increased availability of well-characterized compounds for the research.¹⁻¹⁰

In our previous works, we have investigated the surface activity of individual ω -alkylthiooligooxyethylene glycols at the aqueous

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