

core electrons, e.g., 1s of Na and 2p of K, become more strongly bound by a few electronvolts, ~ 2 eV for Na and K, when the atoms are excited from the ground state to the first excited state, e.g., from 3s to 3p in Na or from 4s to 4p in K. Closely similar energy shifts can be expected with excitation of an outer electron in free ions. These values are of the same order of magnitude as the quantities ΔE_i in Table II and could support our interpretation of ΔE_i around 4 eV in terms of expanded outer electron shells in hydrated ions.

In conclusion, we have calculated hydration energies of core-ionized and Auger-state ions based on an electrostatic model with distance-dependent permittivity. Apart from Mg^{2+} and F^- , agreement between theory and available experimental data is good.

However, a refinement of our approach is desirable for a better treatment of the anions. With the same formalism as used for the hydration energies we have also calculated the extraionic part of the differences between electron promotion work from hydrated and free ions. A comparison of these values with experimental data yields intraionic contributions around 4 eV for several ion families. We interpret this finding by an increase of core electron binding in hydrated ions due to outward extensions of their outer electron shells.

There are still a considerable number of ions without experimental data from core electron and Auger spectroscopy. It would be interesting to compare our predictions for these ions with future experiments.

CHEMICAL KINETICS

Influence of *N*-Cetyl-*N,N,N*-trimethylammonium Bromide Counterions in the Basic Hydrolysis of Negatively Charged Aromatic Esters

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The addition of counterions, Br^- , in the basic hydrolysis of some negatively charged aromatic esters in cationic micelles of *N*-cetyl-*N,N,N*-trimethylammonium bromide displaces the substrates from the micellar phase to the aqueous phase. This effect is related to the different interactions of esters with the micelle.

Introduction

In earlier papers¹⁻³ we have studied the basic hydrolysis of some aromatic esters in cationic micelles of *N*-cetyl-*N,N,N*-trimethylammonium bromide, chloride, and hydroxide (CTABr, CTACl, and CTAOH), and the experimental results were explained by means of the pseudophase ion-exchange model and mass-action model.⁴⁻⁸ Three of the esters, acetylsalicylic acid, 4-acetoxybenzoic acid, and 3-acetoxy-2-naphthoic acid, have a negative charge due to dissociation of the carboxylic acid group present in the molecule. In this case, cationic micelles of CTAX ($\text{X} = \text{Br}^-$, Cl^- , and OH^-) produce a large inhibition effect upon the basic hydrolysis of these esters, while reaction with an uncharged substrate such as 2-naphthyl acetate is less inhibited by these cationic micelles.

Likewise, for charged substrates we find a disparity between the values of the ion binding constant to micelle, K_X' , and ion-exchange equilibrium constants, $K_{\text{Br}}^{\text{OH}}$ and $K_{\text{Cl}}^{\text{OH}}$, with the values reported in the literature. We related this effect to the different interaction and localization of substrates with the micellar surface³ and the values of substrate binding constant to the micelle, K_S .¹⁻³

In this paper we have studied the effect of added counterions, Br^- , upon the basic hydrolysis of acetylsalicylic acid, 4-acetoxybenzoic acid, 3-acetoxy-2-naphthoic acid, and 2-naphthyl acetate in the presence of CTABr micelles. Our aim was to relate the added counterion effect to the different interactions of the four esters with the micellar surface.

Experimental Section

Materials. Acetylsalicylic acid and other reactants such as NaOH and KBr from Merck were used without further purification. Other esters, 4-acetoxybenzoic acid, 3-acetoxy-2-naphthoic acid, and 2-naphthyl acetate, were prepared from 4-hydroxybenzoic acid, 3-hydroxy-2-naphthoic acid, and 2-naphthol, respectively, with acetic anhydride at room temperature, and the products were recrystallized from EtOH according to the general procedure.⁹ The surfactant CTABr (Merck) was recrystallized from MeOH/Et₂O mixtures.¹⁰

Kinetics. All reactions were run at 25 ± 0.1 °C in a thermostated Spectronic 2000 Bausch & Lomb spectrophotometer. The reactions were followed at the wavelengths corresponding to the respective reaction products (surfactant produced only a small shift in λ_{max}): salicylic acid, 296.5 nm; 4-hydroxybenzoic acid, 275.0 nm; 3-hydroxy-2-naphthoic acid, 350.0 nm. For 2-naphthol, for which there is an appreciable shift of its wavelength by cationic micelles, the reaction was followed at 351.0 nm.

To the mixture of CTABr, NaOH, and KBr at given concentration in the thermostated cuvettes of the spectrophotometer was added 0.1 mL of ester stock solution in acetonitrile (3×10^{-3} M

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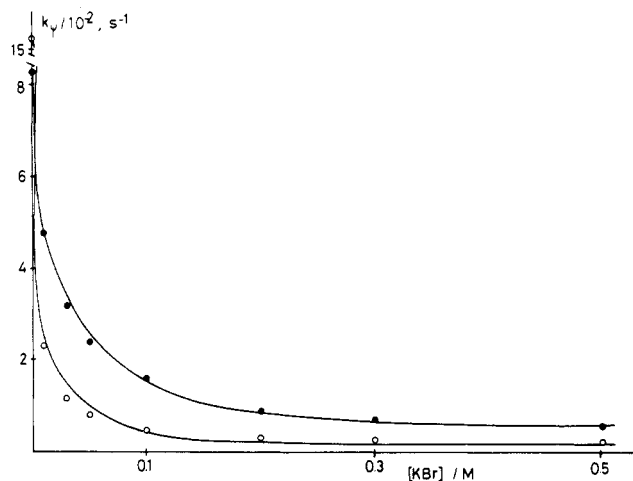


Figure 1. Variation of the pseudo-first-order rate constant k_{ψ} with $[KBr]$ at $[CTABr] = 10^{-2}$ M for the basic hydrolysis of 2-naphthyl acetate: ●, $[NaOH] = 10^{-2}$ M; ○, $[NaOH] = 3 \times 10^{-2}$ M. Lines are the predicted values.

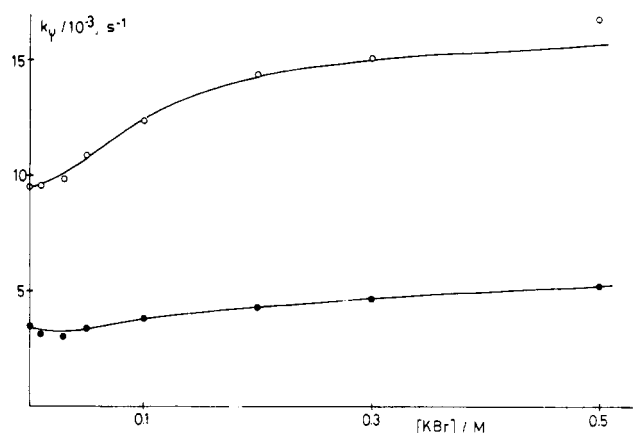


Figure 2. Variation of the pseudo-first-order rate constant k_{ψ} with $[KBr]$ at $[CTABr] = 10^{-2}$ M for the basic hydrolysis of acetylsalicylic acid: ●, $[NaOH] = 3 \times 10^{-2}$ M; ○, $[NaOH] = 8 \times 10^{-2}$ M. Lines are the predicted values.

for acetylsalicylic acid, 3-acetoxy-2-naphthoic acid, and 2-naphthyl acetate and 3×10^{-4} M for 4-acetoxybenzoic acid). The amount of CH_3CN in the total solution volume was 3%. The concentrations of substrates are 10^{-4} M for acetylsalicylic acid, 3-acetoxy-2-naphthoic acid, and 2-naphthylacetate and 10^{-5} M for 4-acetoxybenzoic acid. The hydroxide ion concentration was always in large excess over substrates, and the values of pseudo-first-order rate constants were obtained by a least-squares fit with correlation coefficients greater than 0.999.

Results and Discussion

The second-order rate constants in the aqueous phase, k_w , for the basic hydrolysis of the four esters studied are as follows: acetylsalicylic acid, $0.124 \text{ L mol}^{-1} \text{ s}^{-1}$; 4-acetoxybenzoic acid, $1.48 \text{ L mol}^{-1} \text{ s}^{-1}$; 3-acetoxy-2-naphthoic acid, $0.160 \text{ L mol}^{-1} \text{ s}^{-1}$; 2-naphthyl acetate, $1.61 \text{ L mol}^{-1} \text{ s}^{-1}$.

The experimental pseudo-first-order rate constants, k_{ψ} , for reactions at fixed CTABr and NaOH concentrations and added KBr amounts are represented by dots in Figures 1–4 for the esters studied. For the reaction of the uncharged substrate, 2-naphthyl acetate, an increase of Br^- concentration produces a decrease in the pseudo-first-order rate constant (Figure 1), which is the normal behavior found in the literature^{11–13} for noncharged substrates. However, the values of the pseudo-first-order rate constants in-

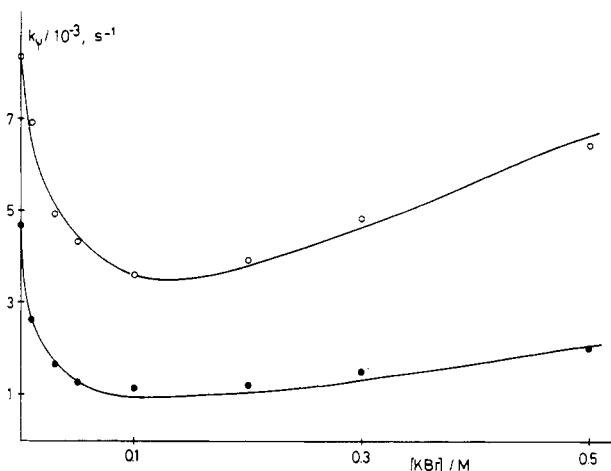


Figure 3. Variation of the pseudo-first-order rate constant k_{ψ} with $[KBr]$ at $[CTABr] = 10^{-2}$ M for the basic hydrolysis of 3-acetoxy-2-naphthoic acid: ●, $[NaOH] = 3 \times 10^{-2}$ M; ○, $[NaOH] = 8 \times 10^{-2}$ M. Lines are the predicted values.

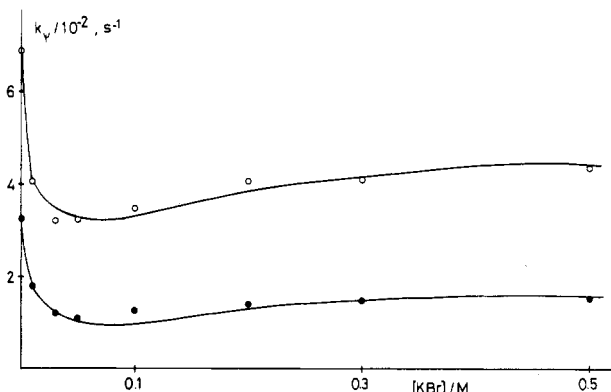
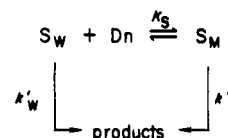


Figure 4. Variation of the pseudo-first-order rate constant k_{ψ} with $[KBr]$ at $[CTABr] = 10^{-2}$ M for the basic hydrolysis of 4-acetoxybenzoic acid: ●, $[NaOH] = 10^{-2}$ M; ○, $[NaOH] = 3 \times 10^{-2}$ M. Lines are the predicted values.

SCHEME I



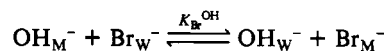
crease with the unreactive counterion concentration for the charged substrates (Figures 2–4).

It is possible to explain the experimental results for 2-naphthyl acetate by means of the pseudophase ion-exchange model developed by Bunton⁶ and Romsted,^{5,7} which considers the total volume of micelles as a separate phase uniformly distributed in the aqueous phase and the reaction occurring in both phases according to Scheme I, where the subscripts W and M denote the aqueous and micellar phases, K_S is the binding constant of substrate, and k'_W and k'_M are the pseudo-first-order rate constants in the aqueous and micellar phases, given by

$$k'_W = k_w[OH_W^-] \quad (1)$$

$$k'_M = k_m[OH_M^-]/[Dn] \quad (2)$$

When two ions compete for the micellar surface, Romsted^{5,7} supposes that this interaction is governed by an ion-exchange equilibrium such as



considering the fraction of micellar surface neutralized, β , as a constant with values between 0.7 and 0.8 when the micellar counterions are halide ions.^{5,7,14} With this pseudophase ion-ex-

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TABLE I: Pseudo-First-Order Rate Constants for the Basic Hydrolysis of Acetylsalicylic Acid at $[\text{NaOH}] = 3 \times 10^{-2} \text{ M}$ in the Absence and Presence of CTABr

[KBr]/M	$k_{\psi}/10^{-3} \text{ s}^{-1}$	
	[CTABr] = 0 M	[CTABr] = 10^{-2} M
0.01		3.15
0.03		3.13
0.05		3.38
0.10	4.23	3.85
0.20	4.66	4.33
0.30	4.78	4.71
0.50	5.10	5.26

change model the pseudo-first-order rate constant, k_{ψ} , is given by⁵⁻⁷

$$k_{\psi} = \frac{k_w[\text{OH}_T^-] + (k_M K_S - k_w)m_{\text{OH}}[\text{Dn}]}{1 + K_S[\text{Dn}]} \quad (3)$$

where m_{OH} can be obtained by

$$m_{\text{OH}}^2 + m_{\text{OH}} \left[\frac{[\text{OH}_T^-] + K_{\text{Br}}^{\text{OH}}[\text{Br}_T^-]}{(K_{\text{Br}}^{\text{OH}} - 1)[\text{Dn}]} - \beta \right] - \frac{\beta[\text{OH}_T^-]}{(K_{\text{Br}}^{\text{OH}} - 1)[\text{Dn}]} = 0 \quad (4)$$

The observed variation of pseudo-first-order rate constant with Br^- concentration for the reaction with 2-naphthyl acetate can be explained with this model because when the total unreactive counterion concentration is increased, the micelle-bound hydroxide ion concentration decreases due to the ion-exchange equilibrium.

The values of the parameters k_M , K_S , $K_{\text{Br}}^{\text{OH}}$, and β are determined by simulation,¹⁴ and the best fit values are $k_M = 0.36 \text{ s}^{-1}$, $K_S = 680 \text{ M}^{-1}$,³ $K_{\text{Br}}^{\text{OH}} = 8$,³ and $\beta = 0.8$, and solid lines in Figure 1 represent the values of k_{ψ} calculated with these parameters by eq 3 and 4. Comparison of these parameter values with the ones obtained for the basic hydrolysis of 2-naphthyl acetate in CTABr in the absence of added counterions³ shows a disparity in the value of k_M ($k_M = 0.53 \text{ s}^{-1}$), which can be rationalized by assuming that k_M is affected by changes of the structure of CTABr micelles at high ion concentration,¹⁵⁻²⁰ because it is not possible to fit the experimental results by assuming a variation in K_S and β according to other approaches in the literature.^{21,22}

For reactions with the charged substrates, the k_{ψ} -[CTABr] profiles are very different; the values of the pseudo-first-order rate constant increase as Br^- concentration increases. Like other results with charged substrates in the literature,²³⁻²⁷ the solubilization sites of these negatively charged esters will also be near to or at the positively charged micellar surface. For this reason, added Br^- will displace the substrates from micellar surface to aqueous phase, increasing the k_{ψ} values. To test this assumption, we also studied the effect of added bromide ions upon the basic hydrolysis

TABLE II: Pseudo-First-Order Rate Constants for the Basic Hydrolysis of 4-Acetoxybenzoic Acid at $[\text{NaOH}] = 1 \times 10^{-2} \text{ M}$ in the Absence and Presence of CTABr

[KBr]/M	$k_{\psi}/10^{-2} \text{ s}^{-1}$	
	[CTABr] = 0 M	[CTABr] = 10^{-2} M
0.01		1.78
0.03		1.19
0.05		1.09
0.10	1.25	1.27
0.20	1.39	1.38
0.30	1.44	1.42
0.50	1.52	1.54

TABLE III: Pseudo-First-Order Rate Constants for the Basic Hydrolysis of 3-Acetoxy-2-naphthoic Acid at $[\text{NaOH}] = 3 \times 10^{-2} \text{ M}$ in the Absence and Presence of CTABr

[KBr]/M	$k_{\psi}/10^{-3} \text{ s}^{-1}$	
	[CTABr] = 0 M	[CTABr] = 10^{-2} M
0.01		2.61
0.03		1.65
0.05		1.26
0.10	5.05	1.15
0.20	5.51	1.20
0.30	5.68	1.48
0.50	5.93	2.01

rate constants of acetylsalicylic acid, 4-acetoxybenzoic acid, and 3-acetoxy-2-naphthoic acid in water. Tables I-III show the values of the pseudo-first-order rate constants at different KBr concentrations in the presence and absence of CTABr micelles for the three charged esters.

For acetylsalicylic acid and 4-acetoxybenzoic acid, values of pseudo-first-order rate constants in the presence and absence of CTABr micelles are similar at $[\text{KBr}] \geq 0.1 \text{ M}$ (Tables I and II). It can be concluded that added Br^- displaces these substrates from the micellar surface to the aqueous phase, and the observed increase in k_{ψ} values can be related to an ionic strength effect. For acetylsalicylic acid and 4-acetoxybenzoic acid, the rate constant values in aqueous solution in the presence of KBr effectively agree with the extended Debye-Hückel law²⁸

$$\log k = \log k_0 + 1.018z_+z_- \frac{I^{1/2}}{1 + BI^{1/2}}$$

where I is the ionic strength and B has the values 2.6 and 2.5 for acetylsalicylic acid and 4-acetoxybenzoic acid respectively.

However, for 3-acetoxy-2-naphthoic acid measured values of the pseudo-first-order rate constants at different KBr concentrations in the absence of CTABr are higher than the ones in the presence of surfactant (see Table III). That means that this substrate is not fully displaced from the micellar to aqueous phase. For this substrate, the experimental results can be adapted to the pseudophase ion-exchange model by assuming that K_S decreases linearly with added [KBr], according to an empirical equation given by

$$K_S = K_S^0 - L[\text{KBr}] \quad (5)$$

where K_S^0 is the binding constant for the substrate in CTABr without added KBr and L is an adjustable parameter. The values of parameters that fit the experimental results with eq 3-5 are $K_{\text{Br}}^{\text{OH}} = 5$,² $K_S^0 = 500 \text{ M}^{-1}$,² $\beta = 0.8$, $k_M = 1.3 \times 10^{-2} \text{ s}^{-1}$, $L \approx 670 \text{ M}^{-2}$, and the k_w value was corrected according to the extended Debye-Hückel considering the parameter $B = 2.4$. The solid lines in Figure 3 represent the values of k_{ψ} with these parameters.

Equations 3-5 can also be used to simulate the reaction of acetylsalicylic acid and 4-acetoxybenzoic acid, and the values of parameters that best fit the results are $K_{\text{Br}}^{\text{OH}} = 2$,^{1,2} $K_S^0 = 120 \text{ M}^{-1}$, $s^{1,2}$ $\beta = 0.8$ $k_M = 9.2 \times 10^{-3} \text{ s}^{-1}$, and $L \approx 4000 \text{ M}^{-2}$ for acetylsalicylic acid and $K_{\text{Br}}^{\text{OH}} = 16$,³ $K_S^0 = 320 \text{ M}^{-1}$,³ $\beta = 0.8$, $k_M = 0.55 \text{ s}^{-1}$, and $L \approx 3000 \text{ M}^{-2}$ for 4-acetoxybenzoic acid; the ex-

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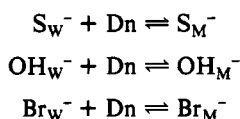
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tended Debye-Hückel law was used to correct the k_w values for these esters. The solid lines in Figures 2 and 4 represent the values of k_ψ (calculated with these parameters).

According to the high value of parameter L , we estimated that $K_S = 0$ at low KBr concentration ($[KBr] \geq 0.1$ M for 4-acetoxybenzoic acid and $[KBr] \geq 0.01$ M for acetylsalicylic acid). Above these $[KBr]$ all the observed rate constants are for reaction in water and not in micelles, in agreement with the values of the rate constants in Tables I and II. It can be deduced that these less hydrophobic substrates are displaced to the aqueous phase more efficiently than 3-acetoxy-2-naphthoic acid, according to the different values of binding constant K_S° for these esters.

From these results and according to other approaches in the literature,^{29,30} it appears that it is possible to consider these charged substrates as ions. We considered for these substrates an ionic distribution equilibrium between micellar and aqueous phase similar as for ions in solution, so that, for OH^- as reactive ion and Br^- as counterion, the following equilibria can be written



with equilibrium constants, K_S' , K_{OH}' , and K_{Br}' given by

$$\begin{aligned} K_S' &= \frac{[S_M^-]}{[S_w^-]([Dn] - [OH_M^-] - [Br_M^-] - [S_M^-])} \\ K_{OH}' &= \frac{[OH_M^-]}{[OH_w^-]([Dn] - [OH_M^-] - [Br_M^-] - [S_M^-])} \\ K_{Br}' &= \frac{[Br_M^-]}{[Br_w^-]([Dn] - [OH_M^-] - [Br_M^-] - [S_M^-])} \end{aligned}$$

which reduce to

$$K_S'[S_M^-]^2 - (K_S'[Dn] + K_S'[S_T^-] - K_S'[OH_M^-] - K_S'[Br_M^-] + 1) [S_M^-] + K_S'[S_T^-]([Dn] - [OH_M^-] - [Br_M^-]) = 0 \quad (6)$$

$$K_{OH}'[OH_M^-]^2 - (K_{OH}'[Dn] - K_{OH}'[OH_T^-] - K_{OH}'[S_M^-] - K_{OH}'[Br_M^-] + 1) \times [OH_M^-] + K_{OH}'[OH_T^-]([Dn] - [S_M^-] - [Br_M^-]) = 0 \quad (7)$$

$$K_{Br}'[Br_M^-]^2 - (K_{Br}'[Dn] - K_{Br}'[Br_T^-] - K_{Br}'[S_M^-] - K_{Br}'[OH_M^-] + 1)[Br_M^-] + K_{Br}'[Br_T^-]([Dn] - [S_M^-] - [OH_M^-]) = 0 \quad (8)$$

Equations 6–8 can be solved simultaneously with an iterative calculation method to give the values of $[S_M^-]$, $[OH_M^-]$, and $[Br_M^-]$ as a function of K_S' , K_{OH}' , and K_{Br}' for each surfactant and ion concentration. This ionic model, which predicts a variation of the fraction of micellar head groups neutralized, β , explains the observed variation of k_ψ with $[KBr]$ for acetylsalicylic acid and 4-acetoxybenzoic acid. However, it is not possible to fit the experimental results for 3-acetoxy-2-naphthoic acid, and this behavior is in agreement with the high hydrophobicity of this substrate, for which it is deduced that the electrostatic forces are less important than the hydrophobic ones.

The values of parameters that best fit the experimental results, with eq 6–8, for acetylsalicylic acid are $k_M = 9.2 \times 10^{-3} \text{ s}^{-1}$, $K_S' = 1000 \text{ M}^{-1}$, $K_{OH}' = 380 \text{ M}^{-1}$, and $K_{Br}' = 760 \text{ M}^{-1}$ and for 4-acetoxybenzoic acid $k_M = 0.55 \text{ s}^{-1}$, $K_S' = 1200 \text{ M}^{-1}$, $K_{OH}' = 230 \text{ M}^{-1}$, and $K_{Br}' = 3680 \text{ M}^{-1}$. The values of k_ψ so calculated are represented in Figures 2 and 4 by the same solid lines because the fit is similar. In these cases, it is not necessary to suppose an empirical variation in the K_S' value to explain the experimental results.

From all these results, we can conclude that for charged substrates in the binding to ionic micelles both electrostatic and hydrophobic forces are important. The extent of displacement of charged esters from the micellar phase to the aqueous phase, when the unreactive counterion concentration increases, depends on the values of substrate binding constant to micelle. This effect should be directly related to the different interaction and localization of substrates to an ionic micelle, according to the electrostatic and hydrophobic forces balance.

Registry No. Br^- , 24959-67-9; CTABr, 57-09-0; acetylsalicylic acid, 50-78-2; 4-acetoxybenzoic acid, 2345-34-8; 3-acetoxy-2-naphthoic acid, 5464-07-3; 2-naphthyl acetate, 1523-11-1; 4-hydroxybenzoic acid, 99-96-7; 2-naphthoic acid, 93-09-4; 2-naphthol, 135-19-3.

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