Data Article

Mass spectrometric data on the cluster ions formed in mixtures of sodium dodecyl sulfate with divalent metal salts

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A B S T R A C T

This paper reports the data obtained from electrospray mass spectra of sodium dodecyl sulfate (SDS) recorded at different concentrations of electrolytes in the positive and negative ion mode, for five different times of acquisition. Using the Excel program, we show the changes in intensities of the peak assigned to a given cluster ion with increasing acquisition time and increasing salt concentration. Moreover, for DS monomers and dimers the correlations were found between the relative peak intensities, \( P_{\text{Me}/\text{Na}} \), and concentration ratios, \([\text{Me}] / [\text{DS}]\) ([Me] and [DS] are concentrations of metal and dodecyl sulfate ions, respectively). The \( P_{\text{Me}/\text{Na}} \) values are numerical measures of the competition between metal, Me, and sodium, Na, cations in their binding with DS monomers and dimers. Generally, the data presented herein may be used to predict the type of cluster ions formed in a given mixture of an anionic surfactant with a divalent metal salt and a possible correlation between the peak height of a given cluster ion and the electrolyte concentration and acquisition time. For a broad discussion of the dataset obtained for \([\text{Me}] / [\text{DS}] = 1\), please refer to the research article "Interactions of divalent metal cations with headgroups of monomers, dimers, and trimers of anionic surfactant" (Jakubowska, 2021).

Abbreviations: \( P_{\text{Me}/\text{Na}} \), the relative peak intensities.
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Specifications Table

| Subject | Chemistry |
|---------|-----------|
| Specific subject area | Mass spectrometry of anionic surfactants in the presence of metal salts |
| Type of data | Table |
| How the data were acquired | Mass spectrometry with electrospray ionization (ESI-MS): electrospray mass spectra were recorded on a ZQ single-quadrupole mass spectrometer (Waters & Micromass, Manchester, UK) equipped with an electrospray interface and a probe. Data were collected and analyzed using Excel. The Excel file with data analyzed has been uploaded as a supplementary file. |
| Description of data collection | The flow rate of the solution studied was 80 μL min⁻¹. Nitrogen was used as the nebulizing (80 L min⁻¹), cone (100 L h⁻¹), and desolvation gas (300 L h⁻¹). The temperatures of the ion source and the desolvation gas were 120 °C and 200 °C, respectively. The electrospray capillary voltage was set to 3000 V. The cone voltage was 30 V, the times of acquisition, t, were 0.1, 0.2, 0.3, 0.4, and 0.5 min. Ten scans were summed to obtain the representative spectrum. |
| Data source location | • Adam Mickiewicz University |
| Data accessibility | With the article |
| Related research article | A. Jakubowska, Interactions of divalent metal cations with headgroups of monomers, dimers, and trimers of anionic surfactant, J. Mol. Liquids 336 (2021) 116,331. https://doi.org/10.1016/j.molliq.2021.116331 [1]. |

Value of the Data

- The data presented provide an insight into: (1) the types of the cluster ions formed in a given mixture of an anionic surfactant with a divalent metal salt, (2) the effect of the electrolyte concentration and acquisition time on the peak height of a given cluster ion.
- The data presented should be of particular use to researchers dealing with spectrometric studies of surfactant compounds in the presence of electrolytes.
- The data can be used in the study of the binding of the divalent cations with the headgroups of monomers, dimers, and trimers of an anionic surfactant.
- They can be reused for further insights on interactions of the cations with the micelle surface of anionic surfactants.

1. Data Description

 Fifteen .zip files are hosted on the data repository [2]. One .zip file is for one given electrolyte studied and names of the files are: SDS_with_BeCl2.zip, SDS_with_MgCl2.zip, SDS_with_CaCl2.zip, SDS_with_SrCl2.zip, SDS_with_BaNO3.zip, SDS_with_MnCl2.zip, SDS_with_FeCl2.zip, SDS_with_CoCl2.zip, SDS_with_NiCl2.zip, SDS_with_CuCl2.zip, SDS_with_ZnCl2.zip, SDS_with_CdCl2.zip, SDS_with_HgNO3.zip, SDS_with_SnCl2.zip, and
SDS_with_PbCl2.zip. Each .zip file contains 50 .raw files with raw data linked to electro-spray mass spectra of SDS recorded in the presence of a given electrolyte studied. More specifically, for five different concentrations of a given salt, the ESI mass spectra of SDS were collected for five different acquisition times, both in the positive and negative ion mode. It means that ten spectra were recorded (and 10 .raw files were generated) for each concentration ratio of the metal to DS.

In the Excel file uploaded as a supplementary file, at first, the main cluster ions whose mass peaks were recorded at a given m/z (m and z are, respectively, the mass and the charge of the ion), are given for all salts studied. In the positive-ion mass spectrum of SDS in the presence of MeX$_2$, the signals assigned to the [Me(DS)]$^+$, [Na(DS)MeX]$^+$, [MeX]$^+$, and [Na$_2$(DS)]$^+$ ions were found. On the other hand, in the negative-ion mass spectrum of SDS in the presence of MeX$_2$, the peaks assigned to the [(DS)]$^-$, [X]$^-$, [Me(X)$_3$]$^-$, [MeX(DS)$_2$]$^-$, [Me(X)$_2$(DS)]$^-$, [Me(DS)$_3$]$^-$, and [Na(DS)$_2$]$^-$ ions were found. For all salts studied, the intensities, I, of the mass peaks at specific m/z assigned to the above-mentioned ions are collected for the five times, t, of acquisition at a given [Me]/[DS] ratio. The correlations between the peak intensities, I, times, t, and concentration ratios, [Me]/[DS], are shown. The slopes, dI/dt, and the square of the correlation coefficients, $r^2$, are also given for the each relation $I = f(t)$. As can be seen, the values of I generally increase linearly with increasing acquisition time, t. For the [Me(DS)]$^+$, [Na(DS)MeX]$^+$, and [Me(DS)$_3$]$^-$ ions, due to too low peak intensities, the linear courses of the plots $I = f(t)$ are disturbed. On the other hand, the changes in I with the concentration ratio, [Me]/[DS], at a given time of acquisition, are more complex. For the [Me(DS)]$^+$ (except for Me = Hg, Sn, and Pb), [MeX]$^+$, [X]$^-$, [Me(X)$_3$]$^-$, and [Me(X)$_2$(DS)]$^-$ ions, the peak intensities increase with increasing salt concentration. For the [Na$_2$(DS)]$^+$, [(DS)]$^-$, and [Na(DS)$_2$]$^-$ ions, the values of I decrease with increasing [Me]/[DS] ratio. For the [Me(DS)$_3$]$^-$ ions (except for Me = Hg, Sn, and Zn) the peak intensities increase initially and then decrease with increasing metal concentration, while for the [Na(DS)MeX]$^+$ and [MeX(DS)$_2$]$^-$ ions, the change in the peak intensities with increasing [Me]/[DS] ratio depends on the electrolyte metal, Me.

Moreover, in the Excel program, the relative peak intensities, $P_{\text{Me/Na}}$, were calculated on the basis of the intensities of the mass peaks assigned to the [Me(DS)]$^+$, [Na(DS)MeX]$^+$, and [Na$_2$(DS)]$^+$ ions for DS monomers, and the [MeX(DS)$_2$]$^-$ and [Na(DS)$_2$]$^-$ ions for DS dimers. The $P_{\text{Me/Na}}$ values for DS monomers and dimers were determined for all electrolytes studied for each acquisition time and concentration ratio, [Me]/[DS]. For each metal concentration in a given salt studied, the averaged values of the relative peak intensities were calculated from five $P_{\text{Me/Na}}$ values obtained for five different acquisition times. The obtained plots of the $P_{\text{Me/Na}}$ averaged values as a function of increasing concentration ratio, [Me]/[DS], are presented for DS monomers and dimers in Figs. 1 and 2, respectively.

Fig. 1. shows that in the presence of most electrolytes studied, the relative peak intensities for DS monomers increase to the maximum values starting from the [Me]/[DS] = 1. While, as follows from Fig. 2, in the presence of most salts studied, the changes in the $P_{\text{Me/Na}}$ values for DS dimers with increasing metal to DS concentration ratio, i.e. values of $d(P_{\text{Me/Na}})/d([\text{Me}]/[\text{DS}])$, are the greatest up to [Me]/[DS] = 1. At higher metal concentrations the changes in relative peak intensities with [Me]/[DS] become smaller.

The relative peak intensities, $P_{\text{Me/Na}}$, are a measure of the competition between a metal cation (derived from the electrolyte added) and the sodium cation (derived from SDS) in their interactions and binding with DS monomers and dimers. So, intensity quotients indicate the exchange of the ions derived from the surfactant for the ions derived from the salt added, and the peak intensity quotients can be called relative selectivity constants or exchange constants. A broader discussion of the $P_{\text{Me/Na}}$ values obtained for DS monomers and dimers in the presence of fifteen electrolytes at [Me]/[DS] = 1 is available in Ref. [1].
Fig. 1. The dependence of the relative peak intensities, \( P_{\text{Me/Na}} \), on the concentration ratio \([\text{Me}]/[\text{DS}]\) obtained for DS monomers in the presence of a given electrolyte studied.

Fig. 2. The dependences of the relative peak intensities, \( P_{\text{Me/Na}} \), on the concentration ratio \([\text{Me}]/[\text{DS}]\) obtained for DS dimers in the presence of the salts studied.
2. Experimental Design, Materials and Methods

The salts of MeX_2 (where Me is a divalent metal cation and X is chloride or nitrate anion), i.e. BeCl_2, MgCl_2, CaCl_2, SrCl_2, Ba(NO_3)_2, MnCl_2, FeCl_2, CoCl_2, NiCl_2, CuCl_2, ZnCl_2, CdCl_2, Hg(NO_3)_2, SnCl_2, PbCl_2 (P.P.H. Polish Chemical Reagents “POCH” Gliwice, all compounds p.a.), and sodium dodecyl sulfate, SDS (Merck, purity > 99%) were used without further purification. All solutions were prepared with deionized water, whose conductivity was less than 0.05 μS cm\(^{-1}\).

For each salt the five solutions were prepared in the electrolyte concentrations: 2\( \times 10^{-5}\), 4.47\( \times 10^{-5}\), 1\( \times 10^{-4}\), 2.24\( \times 10^{-4}\), and 5\( \times 10^{-4}\) M, respectively. Each solution studied contained 1\( \times 10^{-4}\) M SDS. Therefore, in the five solutions of a given electrolyte, the metal to DS concentration ratio, [Me]/[DS], was equal to: 0.2, 0.447, 1, 2.24, and 5, respectively.

The mass spectra were recorded using a mass spectrometer with electrospray ionization (ESI-MS method). The ESI mass spectra of SDS in the presence of a salt at a given concentration were collected for five acquisition times, \(t = 0.1, 0.2, 0.3, 0.4, \text{ and } 0.5 \text{ min}\), both in the positive and negative ion mode. Each spectrum was the sum of ten scans.

Excel was used to (1) collect the intensities of the mass peaks assigned to the given cluster ions, (2) show the relations between the peak intensities, the concentration ratios, [Me]/[DS], and the acquisition times, and (3) determine the dependences between the relative peak intensities, \(P_{\text{Me/Na}}\), and the concentration ratios, [Me]/[DS]. The \(P_{\text{Me/Na}}\) values for DS monomers and dimers were calculated according to equations given in supplementary file.

Data Availability

The mass spectra of sodium dodecyl sulfate in the presence of divalent metal cations (Original data) (Mendeley Data).

Ethics Statements

The study complied with all applicable codes of ethics.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT Author Statement

Anna Jakubowska: Conceptualization, Formal analysis, Data curation, Writing – original draft, Visualization.

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Supplementary Materials

Supplementary material associated with this article can be found in the online version at doi:10.1016/j.dib.2022.107943.
References

[1] A. Jakubowska, Interactions of divalent metal cations with headgroups of monomers, dimers, and trimers of anionic surfactant, J. Mol. Liq. 336 (2021) 116331, doi:10.1016/j.molliq.2021.116331.

[2] [dataset] A. Jakubowska, The mass spectra of sodium dodecyl sulfate in the presence of divalent metal cations, Mendeley Data, v1, 2021. doi:10.17632/vzbvbsswnx.1.