

Predictive Study of the Influence of the Position of the Sulfonate Substituent on the Chemical Stability of Some Linear Alkylbenzene Sulfonate Isomers

Jean Missa Ehouman^{*}, Kadjo François Kassi, Georges Stéphane Dembélé,
Lamoussa Ouattara, Yafigui Traoré, Nahossé Ziao

Laboratory of Thermodynamics and Medium Physico-Chemistry, Nangui Abrogoua University, Abidjan, Ivory Coast

^{*}Corresponding author: jeanmissa@gmail.com

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Abstract Molecules from industrial formulations are used as palliative solutions in the treatment and reuse of industrial waste, with very encouraging results in developing countries. However, the lack of knowledge of the physicochemical properties of these molecules constitutes a major obstacle in the search for an effective solution. To contribute to the characterization of their physicochemical properties, twenty molecules of linear alkyl benzenesulphonate isomers of C10 and C13 homologs and their parent structures were the subject of this study. The stability and overall reactivity parameters such as the energy gap (ΔE), the chemical potential (μ), the electrophilic index (ω) as well as the molecular dipole moment (μ_D) are determined by the DFT method with the level B3LYP / 6-311G (d, p) / (water; IEFPCM). The results showed that the meta position of the sulfonate substituent increases overall stability and reactivity and decreases the solubility of the more stable 2C10, 4C10, 2C13 and 3C13 homologues of linear alkylbenzene sulfonates. The parent molecules (2mC10, 4mC10, 2mC13 and 3mC13) obtained more stable and less soluble are in favor of the effects observed in the treatment of industrial waste.

Keywords: linear alkylbenzene sulfonate, metasulfonate position, influence chemical stability, DFT

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1. Introduction

The use and fate of industrial formulation molecules constitute an environmental, health and socio-economic issue in developing countries due to a lack of sanitation facilities [1]. In this context, palliative solutions are possible. To do this, a perfect knowledge of the physicochemical properties of these molecules is essential for their effective and efficient management. Apart from the field of detergents and cosmetics, anionic surfactants are involved in several fields of activity such as petroleum, pharmaceuticals, formulation of phytosanitary products and fertilizers, formulation of paints, synthesis and formulation of materials, plastics, in textile processing etc. [2]. Petrochemical surfactants, including linear alkylbenzenesulphonates, strongly contribute to these industrial and agricultural applications and therefore deserve special attention. [3]. Studies have shown their occurrence in the environment, as a complex mixture of homologues and intermediates in fresh and marine waters, soils and sediments [4,5]. In particular, the homologs C10, C11, C12 and C13, respectively having chains of 10, 11,

12 and 13 carbon atoms [6,7,8]. In-depth analyzes of these homologs, in order to determine their relative proportions in the raw effluents, were the subject of study [6,7,8]. It emerges from these studies that the homologs C10, C11, C12 and C13 are present in the raw effluents in a significant proportion [6,7,8]. Moreover, other studies have revealed the acute and chronic ecotoxicity of these molecules on fish, algae and bacteria [9,10,11]. Fish and algae, the two essential species in the food chain of the aquatic environment, are the most impacted by these micropollutants [9,10,11]. The persistence of linear alkylbenzenesulphonates and their certain environmental impact require perfect knowledge of their chemical stability. These are compounds comprising a linear alkyl chain to which is connected a benzene ring having a sulfonate group (SO_3^-) in the para position. A predictive study of the position of this sulfonate group on the stability and chemical reactivity of these molecules of interest remains essential for an efficient management of these organic micropollutants. The objective of this work is to predict the influence of the sulfonate position on the overall stability and solubility of some homologues of linear alkylbenzene sulfonates (LAS) used in the soap and cosmetic industries.

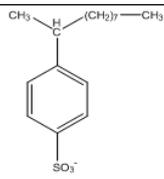
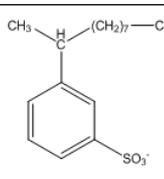
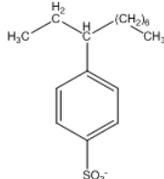
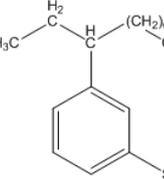
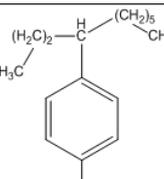
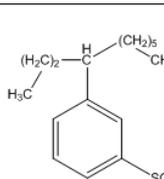
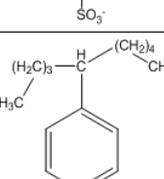
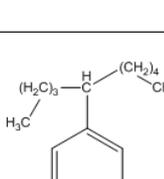
Substitute Sulfonate in para position			Substitute Sulfonate in meta position		
Coded	Structure	name	Coded	Structure	name
2C10		4- (decan-2-yl) benzenesulfonate	m2C10		3- (decan-2-yl) benzenesulfonate
3C10		4- (decan-3-yl) benzenesulfonate	m3C10		3- (decan-3-yl) benzenesulfonate
4C10		4- (decan-4-yl) benzenesulfonate	m4C10		3- (decan-4-yl) benzenesulfonate
5C10		4- (decan-5-yl) benzenesulfonate	m5C10		3- (decan-5-yl) benzenesulfonate

Figure 1. Isomers of the C10 homolog with the sulfonate group in the para and meta position

2. Material and Methods

2.1. Study Material

The linear alkyl benzenesulfonate isomers of C10 and C13 homologs were the subject of this study. For these molecules, the sulfonate substituent was placed in the meta position to generate other molecules in order to gauge the influence of this position on the chemical stability of the isomers of the C10 and C13 homologs. A total of twenty molecules were selected for this work in addition to the previous work carried out for this purpose. [12,13]. These molecules are illustrated by Figure 1 and Figure 2.

The calculation method used within the framework of this study is the DFT method with the level B3LYP / 6-311G (d, p). GAUSSIAN 03 software [14] with its Gauss View 05 graphic interface were used for this purpose. Graphic and statistical processing was carried out using XLSTAT 2016 software.

2.2. Study Methods

Each study molecule is first optimized with a calculation of frequencies in a vacuum. Then a single point calculation taking into account the effects of solvation (solvent: water; IEFPCM method) on each isomer is carried out at the same level of calculation. The overall stability and reactivity parameters (ΔE ; μ ; ω) as

well as the molecular dipole moment (μ_D) are retained for this study. The dipole moment is used to gauge the relative solubility of the isomers studied [15]. This parameter also characterizes the polarity of a molecule. A molecule is said to be more polar when it has a high dipole moment. In addition, a high solubility of a compound in water is reflected in its high dipole moment. [15]. The calculations performed allow us to obtain the energy of the vacant lowest molecular orbital (E_{LUMO}) and that of the highest occupied molecular orbital (E_{HOMO}). These energies provide access to the various stability and chemical reactivity parameters according to Koopmans approximations [16]. Indeed, the energy difference between the energy of the lowest vacant molecular orbital (E_{LUMO}) and that of the highest occupied molecular orbital (E_{HOMO}) is called the energy gap (ΔE). This parameter makes it possible to gauge the overall chemical stability and reactivity of the different study molecules through charge transfer. Thus, the interactions are all the more favored as the value of the gap is small [17]. This energy gap is expressed as:

$$\Delta E = E_{LUMO} - E_{HOMO}. \quad (1)$$

The electronic chemical potential (μ), according to Parr and Pearson (63-65) [18], reflects the capacity of an atom or a molecule to oppose a transfer of its electrons. This descriptor has the following expression:

$$\mu = \frac{1}{2}(E_{LUMO} + E_{HOMO}). \quad (2)$$

Substitute Sulfonate in para position			Substitute Sulfonate in meta position		
Coded	Structure	name	Coded	Structure	name
2C13		4- (tridecan-2-yl) benzenesulfonate	m2C13		3- (tridecan-2-yl) benzenesulfonate
3C13		4- (tridecan-3-yl) benzenesulfonate	m3C13		3- (tridecan-3-yl) benzenesulfonate
4C13		4- (tridecan-4-yl) benzenesulfonate	m4C13		3- (tridecan-4-yl) benzenesulfonate
5C13		4- (tridecan-5-yl) benzenesulfonate	m5C13		3- (tridecan-5-yl) benzenesulfonate
6C13		4- (tridecan-6-yl) benzenesulfonate	m6C13		3- (tridecan-6-yl) benzenesulfonate
7C13		4- (tetradecan-7-yl) benzenesulfonate	m7C13		3- (tetradecan-7-yl) benzenesulfonate

Figure 2. Isomers of the C13 homolog with the sulfonate group in the para and meta position

In the framework of the frontier orbital theory, the global electrophile (ω) is mainly explained by a maximal overlap of vacant lowest molecular orbital of the electrophile and the highest occupied molecular orbital nucleophile [19]. The greater the stabilization energy, the more electrophilic the system. The electrophile of a system can be given by the following relations:

$$\omega = \frac{\mu^2}{2\eta} = \frac{\mu^2}{\Delta E} \quad (3)$$

This parameter therefore defines the energy stabilization of a molecule due to the transfer of electrons. It reflects the capacity of the molecule to bind strongly to a nucleophilic partner by electron transfer.

The graphic treatments will be carried out using the

XLSTAT 2016 software. These histograms will make it possible for each parameter and for each isomer and its parent structure of given homolog, to make relative comparisons.

Also, the specific case of the most stable molecules will hold our attention. For these specific molecules, the effect of the influence of the meta position of the sulfonate substituent will be quantity per the variation of a global stability parameter (ΔP) according to the relation.

$$\Delta P = P_{meta} - P_{para} \quad (4)$$

In this relation, is the Parameter (P); the Parameter calculated when the substituent is in the para position (P_{para}); the Parameter calculated when the substituent is in the meta position (P_{meta}).

3. Results and Discussion

All the investigations concern isomers with the sulfonate substituent (SO_3^-) in the para position and the parent structures of the isomers of the C10 and C13 homologs, when the sulfonate substituent is in the meta position, which homologs are called respectively mC10 and mC13. In order to analyze the influence of the position of the substituent on the chemical stability of linear alkylbenzene sulfonate isomers, the same overall stability and reactivity parameters are calculated under the same conditions and with the same level of calculation. The results obtained for these two series of calculations are given in the tables below.

Table 1. Energy parameters (eV) and the dipole moment (D) of the C10 and mC10 isomers calculated at the B3LYP / 6-311G (d, p) level taking into account solvation (Solvent: water; IEFPCM).

Parameters	E_{LUMO}	E_{HOMO}	ΔE	μ	ω	μ_D
m2C10	-0.539	-6.706	6.167	-3.623	2.128	25.263
2C10	-0.460	-6.612	6.153	-3.536	2.032	27.533
m3C10	-0.514	-6.674	6.161	-3.594	2.097	25.862
3C10	-0.454	-6.598	6.144	-3.526	2.023	26.676
m4C10	-0.487	-6.670	6.183	-3.578	2.071	24.970
4C10	-0.454	-6.579	6.125	-3.517	2.019	25.163
m5c10	24.970	-6.680	6.147	-3.606	2,116	23.828
5C10	-0.442	-6.574	6.132	-3.508	2.007	24.802

Table 2. Energy parameters (eV) and dipole moment (D) of the C13 and mC13 isomers calculated at the B3LYP / 6-311G (d, p) level taking into account solvation (Solvent: water; IEFPCM).

Parameters	E_{LUMO}	E_{HOMO}	ΔE	μ	ω	μ_D
m2C13	-0.540	-6.694	6.154	-3.617	2.126	30.351
2C13	-0.543	-6.631	6.088	-3.587	2.113	32.291
m3C13	-0.529	-6.680	6.151	-3.605	2,113	27.990
3C13	-0.453	-6.587	6.134	-3.520	2.020	30.115
m4C13	-0.464	-6.645	6.181	-3.554	2.044	23.456
4C13	-0.456	-6.581	6.125	-3.519	2.022	28.328
m5C13	-0.530	-6.634	6.104	-3.582	2.102	24.066
5C13	-0.441	-6.573	6.132	-3.507	2.006	27.623
m6c13	-0.459	-6.617	6.157	-3.538	2.033	23.854
6C13	-0.441	-6.572	6.131	-3.507	2.006	26.867
m7C13	-0.530	-6.661	6.131	-3.596	2.109	23.547
7C13	-0.441	-6.571	6.130	-3.506	2.005	26.662

3.1. Influence of the Meta Position of the Sulfonate Substituent on the Chemical Stability and Solubility of Isomers of C10 and C13 Homologs

The variations in the overall chemical stability and solubility parameters of the study molecules due to the change in the position of the sulfonate group in meta are illustrated in Figure 3 and Figure 4.

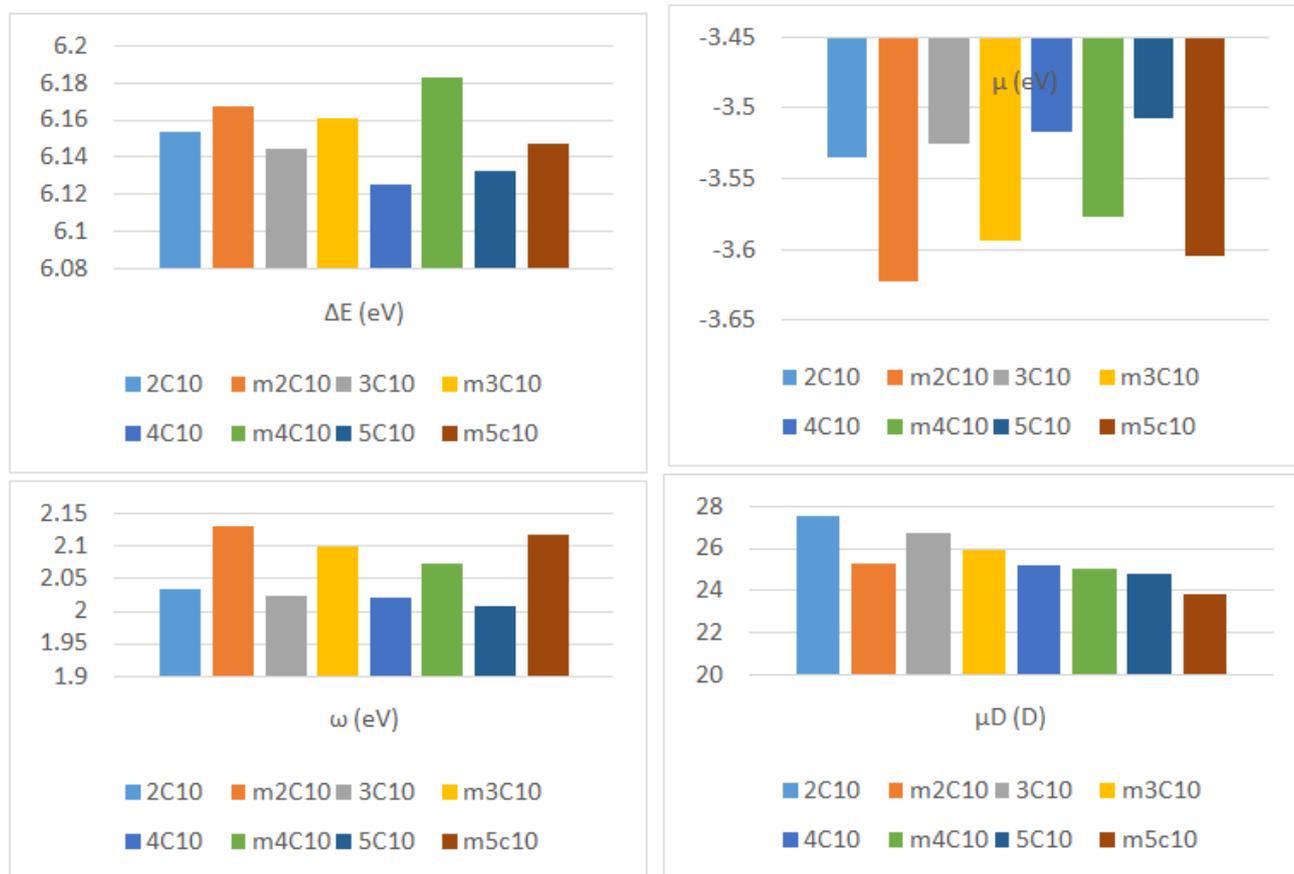


Figure 3. Influence of meta position of the meta group on the overall stability and reactivity parameters and the molecular dipole moment of C10 isomers

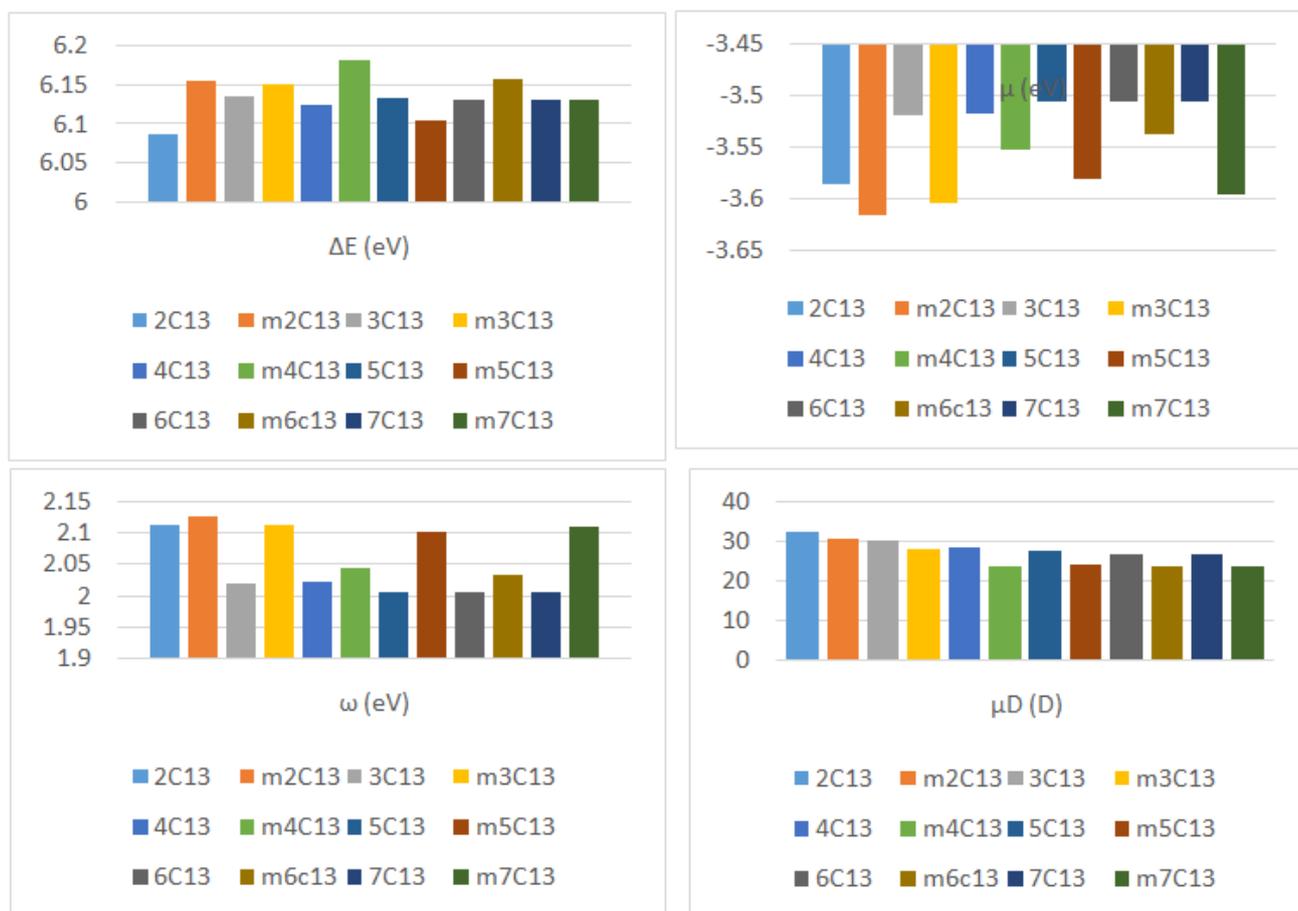


Figure 4. Influence of meta position of the meta group on the overall stability and reactivity parameters and the molecular dipole moment of C13 isomers

Analysis of the results reveals that all the calculated physicochemical parameters vary when the substituent is in the meta position. These variations in values are observed at the level of all of all the homologous C10 and C13 isomers studied. It can therefore be said that the position of the sulfonate substituent in the meta position has an influence on the chemical stability and the solubility of the linear C10 and C13 alkylbenzene sulfonate isomers. In general, the meta position of the substituent influences the order of stability of the isomers. Indeed, Figure 3 illustrates this influence on the stability and the overall reactivity of the isomers of the C10 homolog and of its parent structures obtained from the meta position of the sulfonate substituent. Analysis of the histograms in Figure 3 reveals that the 2C10 isomer exhibits the energy gap (ΔE) and electrophilia (ω) the highest. Also, this isomer registers the chemical potential (μ) the lowest. Therefore the charge transfers within the 2C10 isomer are the most difficult. It is therefore the most stable. In addition, this same isomer presents the highest dipole moment. The 2C10 isomer is therefore the most soluble. It emerges from this first analysis that the 2C10 molecule has the advantage of being the most stable, the least reactive and the most soluble among all the isomers. of the C10 homolog when the sulfonate group is in the para position. Moreover, the meta position of the sulfonate group increases the energy gap and the electrophile of all the isomers of the C10 homolog, in particular the 2C10 isomer (Figure 3). On the other hand, this position decreases the chemical potential and the dipole moment of these isomers. The

meta position of the sulfonate substituent thus enhances the chemical stability of the C10 isomers while reducing their solubility in water. The m2C10 isomer is therefore more stable and less soluble than the 2C10 isomer because of the meta position of the sulfonate group. It should be noted the very significant influence of the meta position on the energy gap of the 4C10 isomer (Figure 3). This position further enhances its stability by making it the most stable among the C10 isomers and its parent structures in terms of internal electron transfer. It should be noted the very significant influence of the meta position on the energy gap of the 4C10 isomer (Figure 3). This position further enhances its stability by making it the most stable among the C10 isomers and its parent structures in terms of internal electron transfer. It should be noted the very significant influence of the meta position on the energy gap of the 4C10 isomer (Figure 3). This position further enhances its stability by making it the most stable among the C10 isomers and its parent structures in terms of internal electron transfer.

3.2. Specific Cases of Stable Isomers 2C10, 4C10, 2C13 and 3C13

This study concerns the specific case of the 2C10, 4C10, 2C13 and 3C13 isomers and their parent structures m2C10, m4C10, m2C13 and m3C13 when the sulfonate substituent is in the meta position. The variations of the parameters due to the change in the meta position of the sulfonate substituent are shown in Table 3 below.

Table 3. Variation of the overall stability and reactivity parameters of the 2C10, 4C10, 2C13 and 3C13 isomers when the sulfonate substituent is in the meta position

Parameters	ΔE (eV)	μ (eV)	ω (eV)	μD (D)
m2C10	6.167	-3.623	2.128	25.263
2C10	6.153	-3.536	2.032	27.533
$\Delta P2C10$(eV)	+0.014	-0.087	+0.096	-2.270
m4C10	6.183	-3.578	2.071	24.970
4C10	6.125	-3.517	2.019	25.163
$\Delta P4C10$(eV)	+0.058	-0.421	+0.052	-0.193
m2C13	6.154	-3.617	2.126	30.350
2C13	6.088	-3.587	2.113	32.291
$\Delta P2C13$ (eV)	+0.066	-0.030	+0.013	-2.000
m3C13	6.151	-3.605	2.113	27.990
3C13	6.134	-3.520	2.020	30.115
$\Delta P3C13$ (eV)	+0.017	-0.085	+0.093	-2.125

For the 2C10 isomer, the meta position of the substituent slightly increases the energy gap by (+0.014 eV). However, this increase is more significant for the electrophilic index of (+0.096 eV). On the other hand, this position of the substituent decreases the chemical potential of (-0.087 eV) and the dipole moment (-2.270 D). These different variations of the stability and overall reactivity parameters show that the meta position of the sulfonate group enhances the stability of the 2C10 isomer by reducing its solubility. However, the effect of this position is much stronger for the 4C10 isomer in terms of energy gap (+0.058 eV) and chemical potential (-0.421 eV). The meta position further decreases the transfer of electrons within the 4C10 isomer by enhancing its chemical stability. However, this position has less influence on its solubility (-0.193 D). In addition, the analysis Table 3 for the 2C13 and 3C13 isomers shows similar observations as the 2C10 isomer. The meta position of the sulfonate substituent enhances the stability of the 2C13 and C13 isomer by reducing their solubilities. These results are in agreement with those of our previous studies relating to isomers 2C11, 3C11 and 2C12 [12]. Overall, the sulfonate substituent in the meta position enhances the stability of the 2C10, 4C10, 2C13 and 3C13 isomers by making them less soluble. The most stable and least soluble isomers m2C10, m4C10, m2C13 and m3C13.

4. Conclusion

This study reveals that the meta position of the sulfonate substituent increases overall stability and reactivity and decreases the solubility of linear alkylbenzene sulfonate homologues, specifically the more stable 2C10, 4C10, 2C13 and 3C13. These results are consistent with those obtained on the more stable homologs 2C12, 2C11 and 3C11. The meta position of the substituent therefore modifies the chemical stability and the solubility of the homologues of linear alkylbenzene sulfonates. These studies provide essential information on the behavior of these micropollutants, opening up research fields for the management of their use and occurrence. Also, the parent molecules (2mC10, 4mC10, 2mC13 and 3mC13) obtained, more stable and less soluble, will they be studied in order to predict their physicochemical surfactant properties? The identification of the meta

position of linear alkylbenzene sulfonate molecules constitutes real progress in understanding the mode of action of micropollutants involved in the treatment and reuse of industrial liquid wastes within the framework of the circular economy.

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