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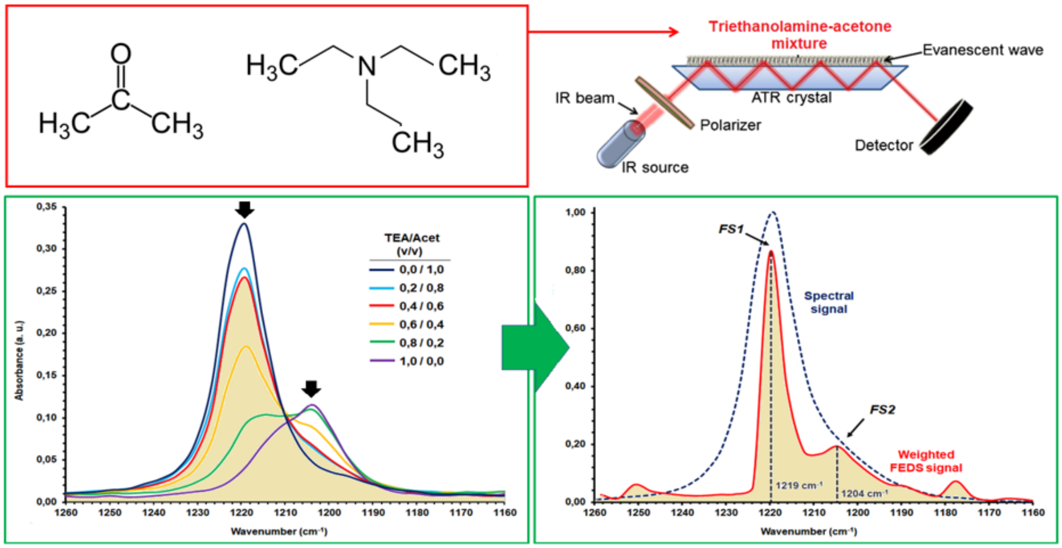
Research Article

Andrés Otálora[1], **Manuel Palencia**[1*]

[1] *Research Group in Science with Technological Applications (GI-CAT), Department of Chemistry, Faculty of Natural and Exact Science, Universidad del Valle, Cali - Colombia*

Corresponding author: manuel.palencia@correounivalle.edu.co

Graphical abstract



Application of functionally-enhanced derivative spectroscopy (FEDS) to the problem of the overlap of spectral signals in binary mixtures: triethylamine-acetone

Abstract

The spectral overlap is a common problem in the study of mixtures by mid-infrared spectroscopy. This creates difficulties for the assignment of spectral signals and, therefore, the correct interpretation of the spectrum. Some common methods for the study of overlap show a high operational complexity, while others have relatively high analytical complexity. Functionally-Enhanced Derivative Spectroscopy (FEDS, for its acronym in English) has been proposed as an easy method of implementation to resolve this problem. FEDS allows the simplification of the spectrum and the identification of signals through the application of different functional transformations. The aim of the present work was to evaluate the applicability of FEDS to the problem of overlap in mid-infrared spectra in binary mixtures using triethylamine/acetone as model system. The results showed that the overlap in the signals of mid-infrared spectra can be resolved by the use of FEDS. It is

Keywords
Spectral overlap
Mid infrared spectroscopy
Functional transformation
Deconvolution
Triethylamine
Acetone

concluded that the methodological strategy based on FEDS allows an accurate study of spectral signals with some grade of overlapping, but also, it is evidenced that the analysis of FTIR spectra of mixture can be improved by smoothing operations and a weighting based on the signal-to-noise ratio.

Aplicación de la Espectroscopía Derivativa Mejorada Funcionalmente (FEDS) al problema del solapamiento de señales espectrales en mezclas binarias: trietilamina-acetona

Resumen

El solapamiento espectral es un problema habitual en el estudio de mezclas por espectroscopía de infrarrojo medio (EIRm), éste dificulta o imposibilita la identificación de señales espectrales y, por ende, la correcta interpretación del espectro. Algunos métodos comunes para el estudio del solapamiento presentan complejidad operativa, mientras que otros poseen cierta complejidad analítica. Recientemente, se ha propuesto la Espectroscopía Derivativa Mejorada Funcionalmente (FEDS, por sus siglas en inglés) como un método de fácil implementación que permite la simplificación del espectro y la identificación de las señales de mayor contribución mediante la aplicación de diferentes transformaciones funcionales. El objetivo del presente trabajo fue evaluar la aplicabilidad de FEDS al problema del solapamiento de señales obtenidas mediante FEDS, usando el sistema trietilamina/acetona como modelo de estudio. Para esto, se seleccionó una región espectral en la que existía un posible fenómeno de solapamiento en este tipo de mezclas, se analizó la respuesta de la metodología FEDS sobre ésta y, en adición, se estudió la conexión del ruido de espectro final, la relación señal/ruido y el proceso de suavizado espectral con la respuesta de FEDS. Los resultados mostraron que el solapamiento de las bandas en los espectros obtenidos por EIRm puede ser abordado por la metodología FEDS, permitiendo una adecuada asignación de señales y siendo posible la mejora de su respuesta por medio de una ponderación basada en la relación señal-ruido y por el proceso de suavizado espectral.

Palabras clave
Solapamiento espectral
Espectroscopía infrarroja media
Transformación funcional
Desconvolución
Trietiamina
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Corresponding author:
manuel.palencia@correounivalle.edu.co

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Application of functionally-enhanced derivative spectroscopy (FEDS) to the problem of the overlap of spectral signals in binary mixtures: triethylamine-acetone

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Abstract

The spectral overlap is a common problem in the study of mixtures by mid-infrared spectroscopy. This creates difficulties for the assignment of spectral signals and, therefore, the correct interpretation of the spectrum. Some common methods for the study of overlap show a high operational complexity, while others have relatively high analytical complexity. Functionally-Enhanced Derivative Spectroscopy (FEDS, for its acronym in English) has been proposed as an easy method of implementation to resolve this problem. FEDS allows the simplification of the spectrum and the identification of signals through the application of different functional transformations. The aim of the present work was to evaluate the applicability of FEDS to the problem of overlap in mid-infrared spectra in binary mixtures using triethylamine/acetone as model system. The results showed that the overlap in the signals of mid-infrared spectra can be resolved by the use of FEDS. It is concluded that the methodological strategy based on FEDS allows an accurate study of spectral signals with some grade of overlapping, but also, it is evidenced that the analysis of FTIR spectra of mixture can be improved by smoothing operations and a weighting based on the signal-to-noise ratio.

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1. Introduction

Infrared spectroscopy is one of the most used spectroscopic techniques in the structural analysis of organic compounds, mixtures and materials. Mid-infrared spectroscopy (MIR spectroscopy) provides qualitative and quantitative information of the different vibrational modes of the molecules into a system, which are associated with functional groups, bonds and structural arrangements of them [1-3]. However, the amount of information obtained from this type of spectra is limited when complex systems are studied, such as mixtures or biological systems. Part of this information remains hidden due to instrumental limitations such as the resolution, the signal-to-noise ratio or physical phenomena in which a measurement can be distorted by unwanted contributions from neighboring measurements, giving rise to a phenomenon of spectral band overlap (SBO) [4-5]. One of the first solutions for the SBO is the improvement of the resolution and the signal-to-noise ratio, however, these characteristics are often limited to specific cases. For example, in an infrared spectrophotometer the opening of the slits improves the signal-noise ratio which in turn decreases its resolution [6]. On the other hand, in most cases, SBO is due to intrinsic physical phenomena of the system and the problem is addressed by the modification of sample by different strategies, e.g., the change of solvent or change in the relative composition of analyte and the interferent. But also, by mathematical methodologies, like spectral derivatization and deconvolution by Fourier transform this problem can be studied and resolved in some cases [7].

Essentially, the spectral derivatization is based on the analysis of its first orders of derivation, with the second order being the most used [8]. This process allows to observe changes in the slope and in the rate of change to the experimental spectrum, leading to the presence of overlapping peaks which can be clearly seen. However, this method decreases the signal-to-noise ratio and generates a more complex spectra than the original spectrum [4, 7, 8].

On the other hand, deconvolution by Fourier transform is based on the idea that the original spectrum is a convolution of a "line function" or base function of the real spectrum. The objective is to obtain the real spectrum by a deconvolution operation with inverse Fourier transform from different base functions, such as Gaussian, Lorentzian, and Voight functions [9]. This procedure is generally used in conjunction with different curve fitting methods, which helps to identify the overlapping of bands and their contribution to the real spectrum [10]. However, it presents high operational complexity and the basic functions may vary depending on the system to be studied.

By the above, it is clear that for some complex samples these procedures allow a better analysis because it provides more information than those contained in the original spectra. However, with this improvement in the analysis and the amount of information obtained, the complexity in the application and inherent limitations of the method appear like critical aspects to be considered. For this reason, easy-to-use mathematical algorithms have been proposed. In this context, FEDS has emerged as a simple and easy-to-implement method that allows the simplification of spectrum and identification of greater signals by a set of functional transformations.

The central idea of this methodology is that by FEDS is possible to construct a function, called Function P, from a series of simple functions, equation (1), allowing the modification of spectrum by a narrowing of the spectral bands. But also, the above is directly associated with a function of the critical points (maximum and minimum points) without a change of its relative position.

$$P_i = (1 + A_i)\left(\left|\frac{1}{A_i}\right| - \left|\frac{1}{A_{i-1}}\right|\right)^{-1/2} \qquad (1)$$

where P_i es the value of function P for i-absorbance A_i.

Recently, the application of FEDS to the qualitative analysis of several systems has been studied, such as water, aqueous solutions of acetic acid and some organic compounds (ethanol, butanol, hexanol, formic acid, among others). Additionally, it was successfully used in the quantitative analysis of the dimerization of acetic acid [5]. In order to advance with the study FEDS transform, the applicability of FEDS in the study of the overlap of spectral bands in the medium infrared using the triethylamine/acetone system (TEA/Acet) as research model was studied.

2. Experimental section

For this study, 99.8 % acetone (Merck, Darmstadt, Germany) and 99 % triethylamine (J.T. Baker, New Jersey, United States) were used. Fourier transform infrared (FTIR) spectra were recorded in the range of 4000-600 cm^{-1} using attenuated total reflectance (ATR) technique in an IRAffinity-1S spectrophotometer (Shidmazu Co, Kyoto, Japan) using a resolution of 2 cm^{-1} and 16 scans. The data processing was carried out in Excel spreadsheets (Microsoft Co).

2.1 Choice of study system and analysis window

From the ATR-FTIR spectra of the TEA/Acet mixtures at different volume ratios (1.0/0.0, 0.8/0.2, 0.6/0.4, 0.4/0.6, 0.2/0.8, 0.0/1.0), the system that presented greater visual overlap in the range of 1260 to 1160 cm^{-1} was chosen due to a possible SBO phenomenon in this analysis window.

2.2 Application of FEDS methodology

Using Excel spreadsheets, a pre-treatment of the data was performed using a moving-average smoothing technique with a 3-data window, equation 2, and a subsequent normalization process based on the maximum and the minimum [11] of the absorbance values, calling the new variable b, equation 3.

$$A_i = \frac{1}{3}\sum_i^{i+2} A_i \qquad (2)$$

$$b_i = \frac{A_i - A_{min}}{A_{max} - A_{min}} \qquad (3)$$

Next, the process of functional transformation of the normalized signal was carried out by the Function P, equation 4. In addition, it was normalized with respect to its maximum value [5].

$$P_i = (1 + b_i)\left(\left|\frac{1}{b_i}\right| - \left|\frac{1}{b_{i-1}}\right|\right)^{-1/2} \qquad (1)$$

Here, b denotes the normalized absorbance.

2.3. Effect of final spectrum noise and signal-to-noise ratio

The study of the effect of the final spectrum noise and the signal/noise ratio in the FEDS response for two different spectral signals was carried out. From a geometric definition of noise (r), the distribution of this was calculated through the analysis window, equation 5; in the same way for the signal-to-noise ratio (R) was done, equation 6.

$$r_{i+1} = \frac{|b_{i+1} - b_i|}{2} \qquad (5)$$

$$R_{i+1} = \frac{b_{i+1}}{r_{i+1}} \qquad (6)$$

From the previous analysis, a FEDS signal weighting criterion was established based on R, equation 7, calling the new function with weighted function P (P_w).

$$P_w = \frac{(1+b)}{P_{max}\sqrt{|p|}} \times R = \frac{(1+b)}{P_{max}\sqrt{|p|}} \times \left(\frac{b}{r}\right) \qquad (7)$$

2.4. Effect of the data number in both the analysis window and smoothing

In addition, the effect of the number of data within the analysis window was studied by performing a data simulation process, in which intermediate data (b_{int}) was included into the original data since these were an average of the adjacent data, equation 8. This process was performed for every 1 and 3 intermediate data points for every two consecutive original data. In addition, the effect of moving-average smoothing with a 3-data window, equation 2, was considered for 5, 10 and 20 loops.

$$b_{int} = \frac{b_j + b_i}{2} \qquad (8)$$

2.5 Quantitative approximation

To evaluate the accuracy of the assignment of the FEDS signals, the TEA/Acet molar fraction was calculated from the maximum absorbance values of bands involved in the overlap. For this, by means of the law of Beer-Lambert, equation 9, the system of equations for the maximum absorbances in terms of the amount of acetone and triethylamine present in the system was proposed, equations 10 and 11.

$$A_v = \varepsilon_{v,x} b C_x = k_{v,x} C_x \qquad (9)$$

where A_v is absorbance value at wavenumber v, $\varepsilon_{v,x}$ is the molar absorptivity coefficient of substance x in $M^{-1}cm^{-1}$ at wavenumber v, b in this case is the optic path length in cm^{-1}, C_x is the concentration of substance x expressed in M and $k_{v,x}$ is a constant obtained from $\varepsilon_{v,x} - b$ product in M^{-1}, which was determined from ATR-FTIR spectra of each reactive.

$$A_1 = k_{1,TEA} C_{TEA} + k_{1,Acet} C_{Acet} \qquad (10)$$

$$A_2 = k_{2,TEA} C_{TEA} + k_{2,Acet} C_{Acet} \qquad (11)$$

Finally, the system of equations was solved for TEA/Acet molar fraction, equation 12, considering that C_{TEA} and C_{Acet} can be expressed as n_{TEA}/V_T and n_{Acet}/V_T, respectively. Here, A_1 and A_2 are the maximum absorbance values identified by FEDS, n is moles number and V_T total volume of the mixture.

$$n_{TEA}/n_{Acet} = \frac{k_{1,Acet} - (A_1/A_2)k_{2,Acet}}{(A_1/A_2)k_{2,TEA} - k_{1,TEA}} \qquad (12)$$

To compare the result obtained by equation 12, the TEA/Acet molar fraction was calculated considering the mixed volumes of reactants and their concentrations, according to equation 13; where ρ represent density at room temperature

(0.726 and 0.7845 g/cm^3 at 25 °C for TEA and acetone [12, 13], respectively) and M is the molecular weight in g/mol.

$$\frac{n_{TEA}}{n_{Acet}} = \frac{\rho_{TEA} V_{Acet} M_{Acet}}{\rho_{Acet} V_{TEA} M_{TEA}} \qquad (13)$$

3. Results and discussion

MIR as a characterization technique is important because it provides information about different vibrational modes of molecules present in a system. The position of the spectral bands associated with each of these depends on the set of atoms involved and in the type of vibrational mode (stretching, bending, etc.) used [1, 14]. For this reason, when characterizing a complex system by MIR, it seeks the spectral bands associated with vibrational modes of the different system components.

For this case, in the mid-infrared spectrum of acetone (Figure 1), spectral bands associated to the stretch of the carbonyl group (C=O) at about 1700 cm^{-1}, symmetric and asymmetric stretch of C-H bonds in the region of 3000-2850 cm^{-1}, bend of the C-H bonds of methyl groups (-CH$_3$) between 1500-1400 cm^{-1} and asymmetric and symmetrical stretches of C-C bonds of its carbon skeleton at 1350 and 1220 cm^{-1}, respectively, were identified. On the other hand, in the mid-infrared spectrum of triethylamine (Figure 2) spectral bands were assigned to stretches and bends of the C-H bonds of methyl and methylene groups (-CH$_2$-), in regions of 3000-2800 and 1500-1300 cm^{-1}, respectively. In addition, the characteristic C-N stretch was identified near 1200 cm^{-1}.

In the ATR-FTIR spectra of TEA/Acet system (Figure 3), it was observed that spectral bands associated with C-H bonds, carbonyl group and C-C bonds of acetone. Unfortunately, it was not possible to identify the spectral band associated with C-N bond of triethylamine. This was due to the proximity of the spectral band associated with the stretch of C-C bonds of the acetone and that of C-N stretch, since both usually appear in the range of 1250-1150 cm^{-1} [1, 4-17], which gave an indication of an SBO phenomenon.

Therefore, this phenomenon was studied by FEDS, using a window of analysis in the range 1260-1160 cm^{-1} and the TEA/Acet system 0.2/0.8 (v/v), since it showed a greater SBO.

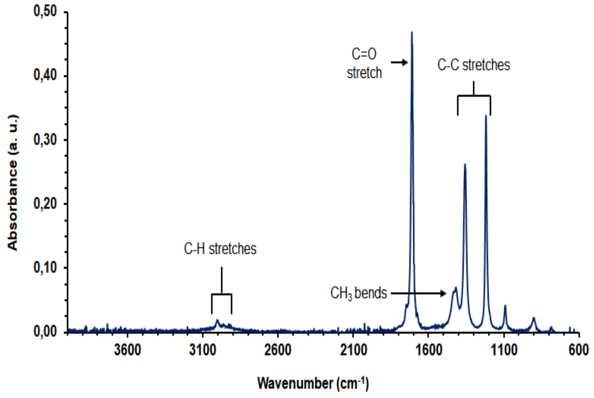

Figure 1. ATR-FTIR spectrum of acetone

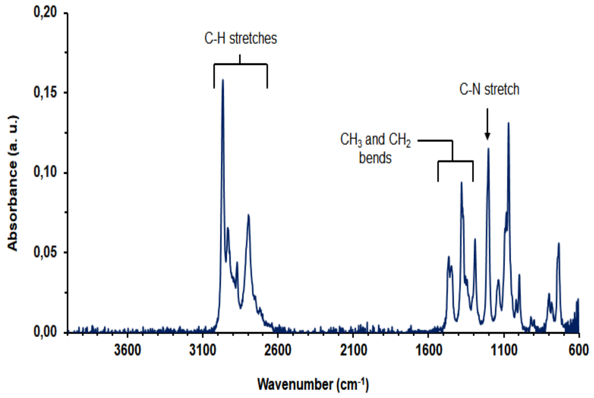

Figure 2. ATR-FTIR spectrum of trimethylamine.

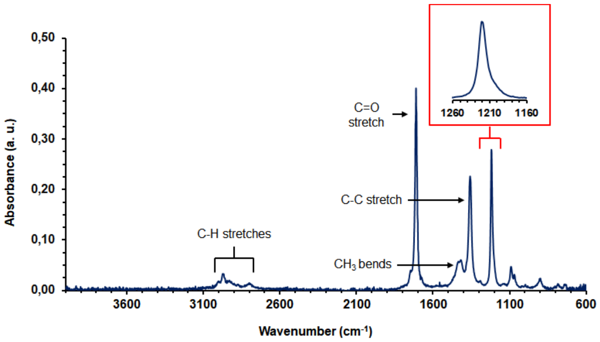

Figure 3. ATR-FTIR spectrum of TEA/Acet system 0.2/0.8 (v/v).

3.1 Application of FEDS methodology

Figure 4 shows FEDS transformation of the spectral signal. Qualitatively, it can be seen that FEDS transformation narrows the spectral signal to some degree and predicts a greater number of signals from the original signal. The first fact is related to FEDS methodology, which seeks to narrow the spectral bands and preserve their

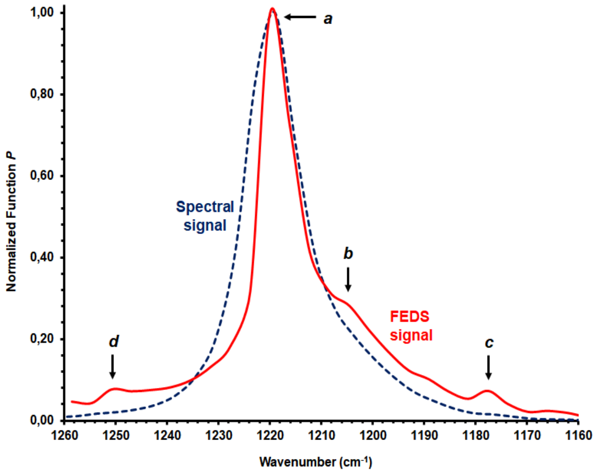

Figure 4. FEDS transformation of spectral signal.

relative positions. In this case, the narrowing is not generated largely due to the small window of analysis and its amount of data, as will be discussed below. The second fact is because of the sensitivity of its response to the spectrum form (or signal form). The narrowing is given based on the critical points of the signal [5]; any sufficiently remarkable variation (for FEDS) in its form will be translate into a FEDS signal, thus, in this case it was obtained a greater number of signals from the original signal.

The first FEDS signal identified is the one with highest intensity (***a*** in Figure 4), corresponding to maximum absorbance of the original signal. In addition, it can be observed signals of lower intensity at the end of the analysis window (***c*** and ***d*** in Figure 4), which were designed as artifacts resulting from the application of the P function in the regions of minimum absorbance, as will be discussed.

Interestingly, a "shoulder" style signal of the strongest FEDS signal (***b*** in Figure 4), assigned to a possible overlapping band in the original signal, is also seen. At this point, the FEDS transformation already gives an indication of the existence of an SBO phenomenon. However, only this analysis does not allow a good degree of certainty of the existence of an overlapping second band and an appropriate allocation of it in the original signal, since the second FEDS signal is not intense and, as mentioned above, FEDS may be susceptible to small variations in the signal form, attributed in the first instance to noise.

3.2 Effect of final spectrum noise and signal-to-noise ratio

The spectral bands have different forms, these depend on the physical state of the system, the intensity of the absorption process, temperature, pressure and other phenomena that can occur in the system as the measurement process [18]. Although, the natural form of a spectral band can be described from several "line functions", such as Gaussian, Lorentzian, Voight functions, among others [19, 20]. Variations in the shape of the spectral bands with respect to their line function are primarily due to noise, a fact that becomes more noticeable in low intensity spectral bands. In this sense, both the noise distribution in the spectral signal and the effect of this on the FEDS response were calculated and analyzed, in the same way it was done with the signal-to-noise ratio.

Commonly, the concept of noise is associated with the instrumental measurement process and can be classified depending on its source [21]. When looking to study the noise in a spectrum, that is, without deepening its source (here called "final spectrum noise"), it is considered a probabilistic definition of noise and the standard deviation is taken as a quantitative measure of it [22, 23]. In contrast, in this work the distribution of the final spectrum noise was calculated from a geometric definition of it, in which noise is considered as small variations of the signal with respect to its spectral line function and it was calculated with the equation 5.

Figure 5 and 6 show the distribution of the final spectrum noise (r) and signal-to-noise ratio (R) in the spectral signal within the analysis window and another region of the spectrum, respectively.

For both cases the results were similar. First, it was observed that noise is greater in areas of signal with greater slope and, conversely, it is lower in areas with less slope, such as regions of maximum and minimum absorbance, in which signals tend to have small changes. This fact has a direct relationship with the geometric definition of noise taken, in which the final spectrum noise was considered as small variations of the signal with respect to a spectral line function, calculated by the distance between adjacent points and associated with the signal geometry or form. According to this, areas with greater slope those variations or distances will be greater, than in areas with less

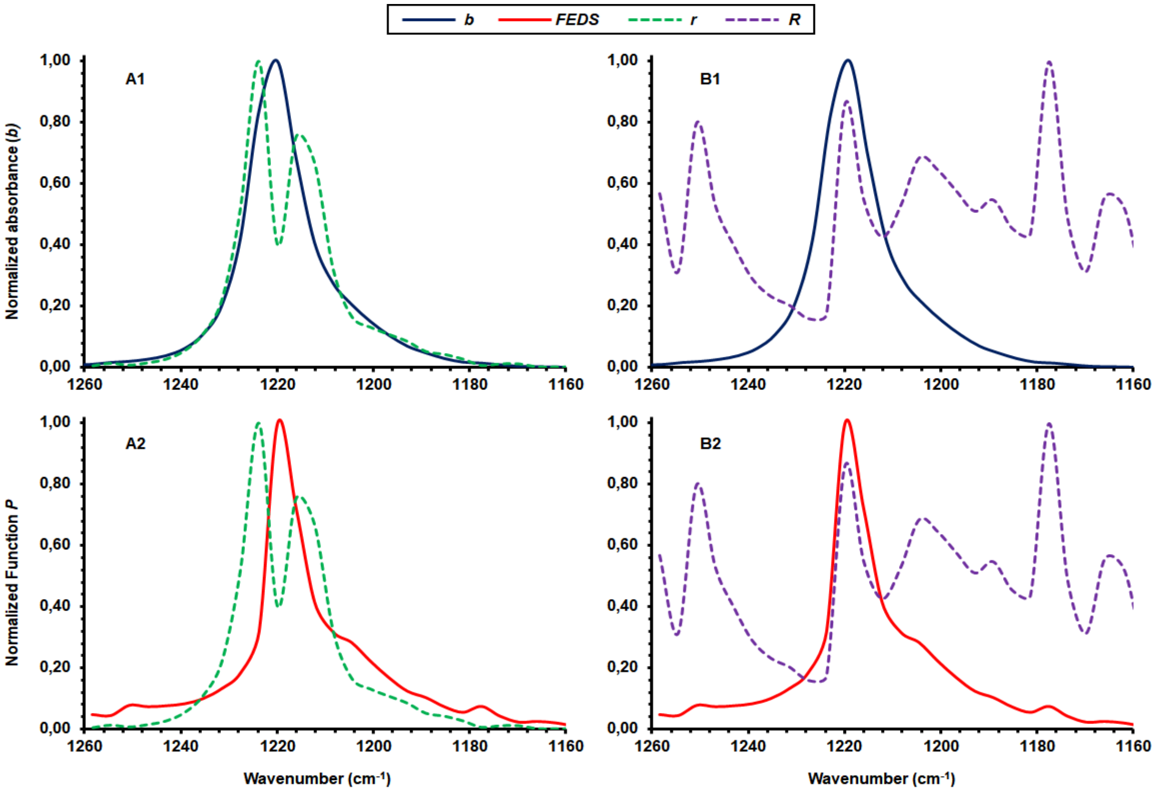

Figure 5. Distribution of r (**A1**) and R (**B1**) in the analysis window; comparison of FEDS response (**A2** and **B2**, respectively).

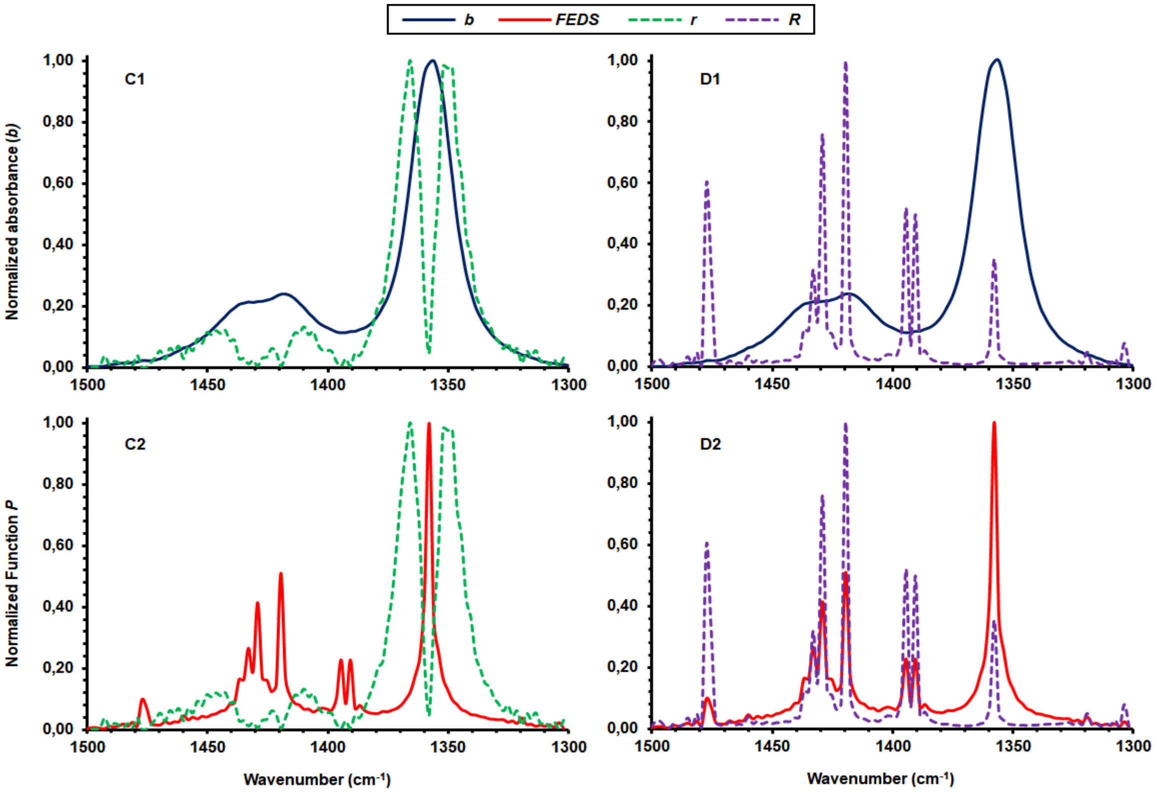

Figure 6. Distribution of r (**C1**) and R (**D1**) in another spectral region; comparison of FEDS response (**C2** and **D2**, respectively).

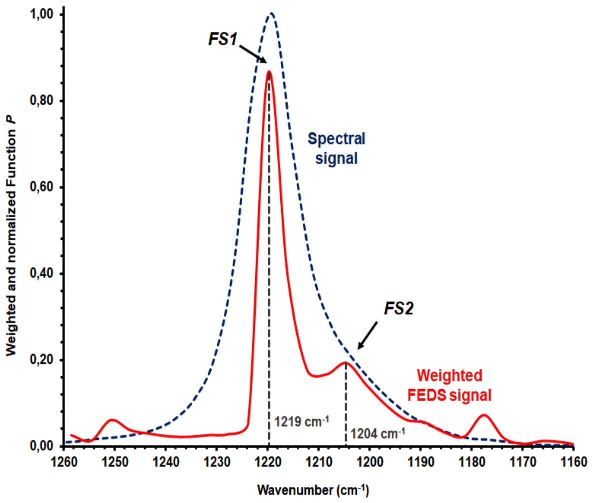

Figure 7. Weighing of FEDS response based on *R* in the analysis window.

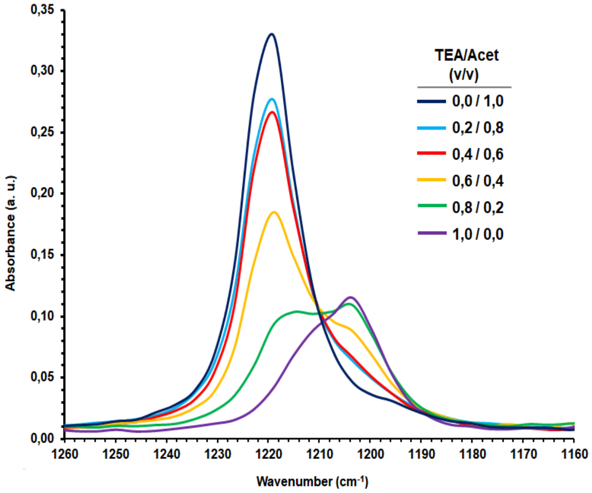

Figure 8. ATR-FTIR spectra of various TEA/Acet mixtures in 1260-1160 cm^{-1} region.

slope or smaller distances between adjacent points. It was observed that this fact has a connection with the distribution of the signal-to-noise ratio obtained. This is greater in regions where the noise is lower, a result of its definition. It was also evidenced that this fact has a connection with the higher intensity FEDS signals, since the regions of maximum signal-noise ratio coincide with the higher intensity FEDS signals.

The above can be understood if it is considered that FEDS causes a narrowing of the spectral bands based on their critical points. In the case of a spectrum interval, the critical points correspond to both maximum and minimum absorbance values, in which the slope or the change ratio of the value of the spectral function is minimum. It is at these points that r is also minimal and, therefore, R is maximum, coinciding with the most intense FEDS signals. This observation made it possible to define a criterion for weighting FEDS signals from the value of the signal-to-noise ratio, with the aim of using it as a tool to better differentiate the response signals in the case of interest. Figure 7 shows the result after applying equation 7 in the analysis window.

When applying the weighting criterion of the FEDS response based on R, the presence of two main FEDS signals, ***FS1*** and ***FS2*** at 1219 and 1204 cm^{-1}, respectively, was clearly observed. At this point, it can be affirmed with a good degree of certainty that FEDS predicts an SBO phenomenon between two bands and the position of its maximum absorbance values is associated with the position of ***FS1*** and ***FS2***. To verify this prediction, the ATR-FTIR spectra of the different TEA/Acet mixtures were superimposed on the analysis window, the result is shown in Figure 8.

In this figure, it is evident that as the amount of triethylamine in the mixture increases, a second band appears near 1204 cm^{-1}, this is corresponding to the stretch of C-N bond, which is clearly seen when there is only triethylamine in the medium. Therefore, it was proved experimentally that in this region there is an SBO phenomenon for TEA/Acet mixtures, as predicted by FEDS.

3.3 Effect of data number and spectral smoothing

The previous analysis was performed in the interval from 1260 to 1160 cm^{-1}, the amount of data within this analysis window was small and, therefore, the FEDS response on the spectral signal was wide compared to FEDS response in larger analysis windows [5], this fact decreases the accuracy of the assignment of the FEDS signals in the original signal. For this reason, it was evaluated the effect of the number of data within the analysis window in the FEDS response, for this, a process of simulation of intermediate data for each two consecutive data was carried out from the equation 8. Since this method presents a simple alternative to increase the amount of data within the analysis window in comparison with the recording of ATR-FTIR spectra with higher resolution, which means

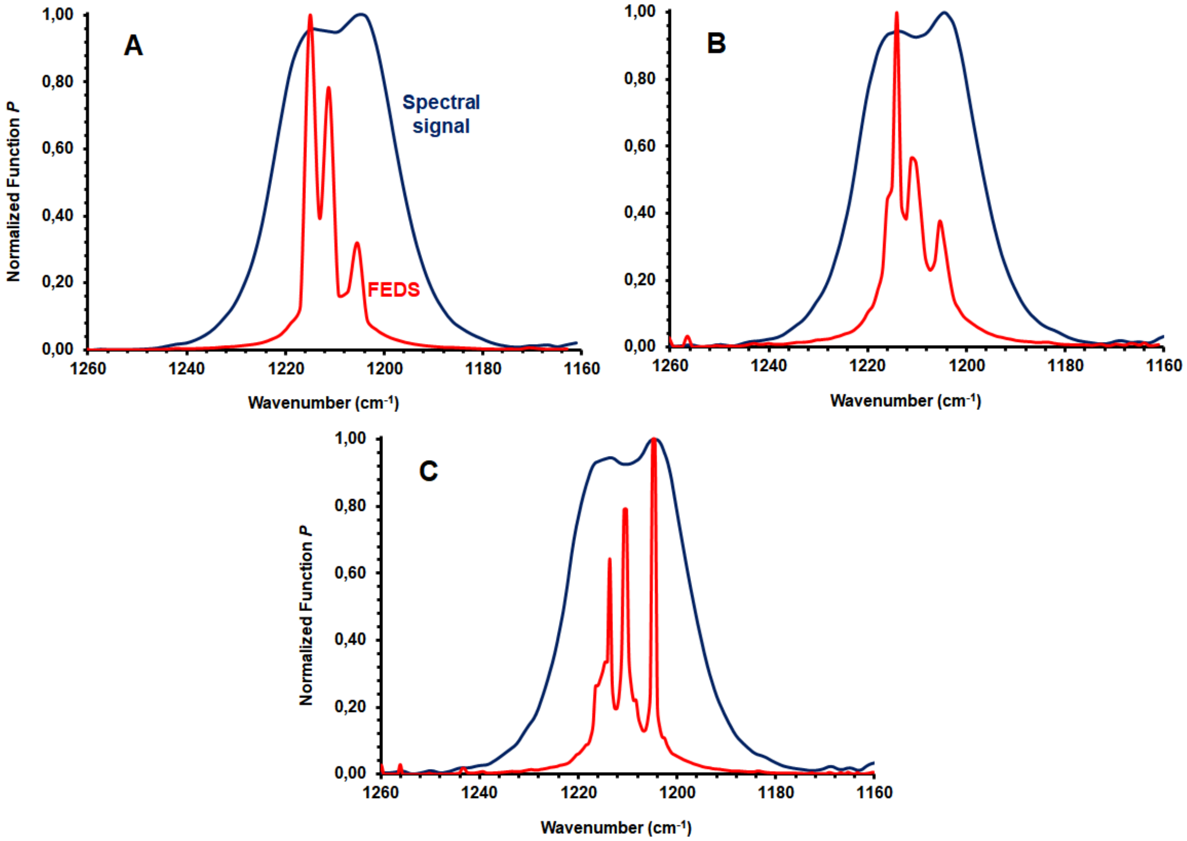

Figure 9. Effect of the data number in the FEDS response. Original signal in (**A**), simulation of 1 and 3 intermediate data for every two consecutive ones in (**B**) and (**C**), respectively.

a higher sample cost, or regression methods from the initial data, which can be rather tedious. Figure 9 shows the results in a specific analysis window of an ATR-FTIR spectrum for a TEA/Acet system. There is a clear dependence on the shape of FEDS signals with number of data within the analysis window. More data implies narrower FEDS signals, but more intense. This dependence is due to working with a set of discrete data, since a smaller available amount of data, the construction of a continuous function from these will differ to a greater degree than desired. In this case, a wide FEDS signal was obtained instead of a narrow one. Additionally, a greater number of points improves the FEDS response because its methodology is based on measuring variations or fluctuations in the signal with respect to its spectral line function, as mentioned above. These fluctuations and the distance between the adjacent points will be greater if there is a smaller number of points, therefore, the FEDS response will be wide. By increasing the number of points, the fluctuations will be subtle throughout the signal due to their proximity, however, they will be more pronounced at their critical points. Therefore, the FEDS response will be narrower and more intense at these points, which improves the assignment of highest contribution signals.

Additionally, the effect of the spectral smoothing process as a data processing tool was studied, since it is a method commonly applied in the spectral analysis to reduce noise [11, 24]. In this case, smoothing was evaluated by a moving average with a 3 data window, equation (2), because this algorithm is easy to apply and provides good results [24, 25]. Figure 10 shows the effect of smoothing on the FEDS response. It was observed that as the amount of smoothing increases, the intensity of some FEDS signals decreases. While others increase in intensity and become more acute or narrower, these being the main ones, assigned to maximum absorbance values in the original signal.

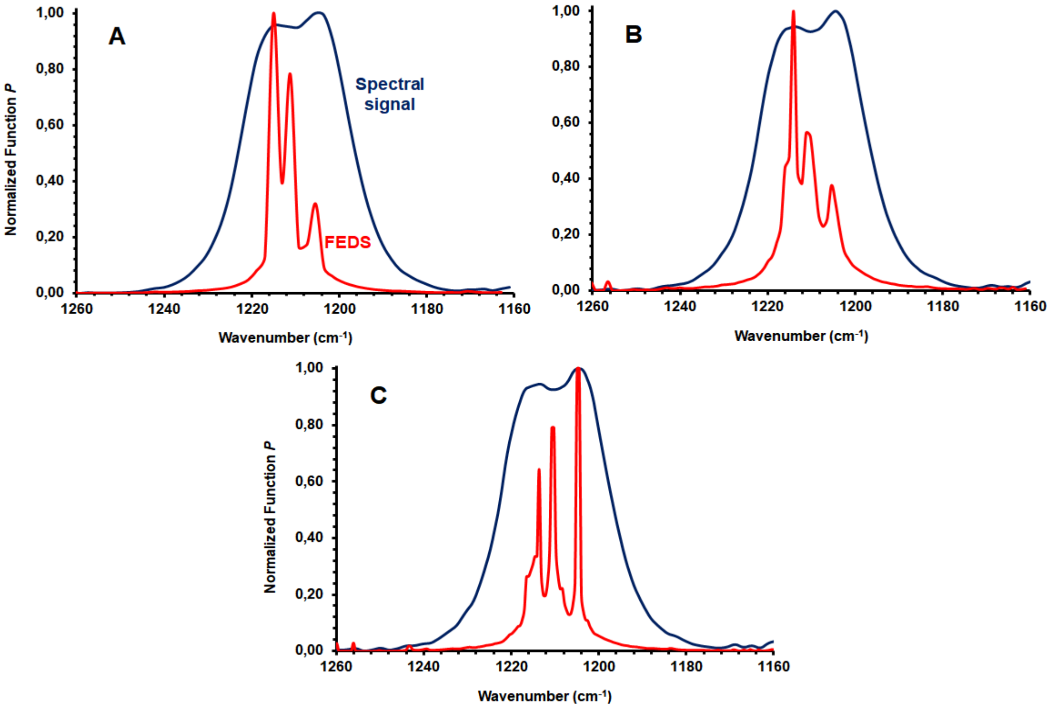

Figure 10. Effect of the smoothing process with (**A**) 5, (**B**) 10 and (**C**) 20 loops in the FEDS response.

This phenomenon is due to the fact that the averaging of a window of consecutive data, in this case 3 data, causes a reduction of the final spectrum noise and a greater approximation of the signal to its line function. As the final spectrum noise decreases, the unwanted fluctuations of the line function decrease, however, the fluctuations of the signal associated with the absorbance maxima will remain and the response of the FEDS in these regions will be more intense and narrower.

According to this, the moving-average smoothing process represents a potential tool for pre-processing data in the analysis by FEDS, since it allows directing the response signals to those of maximum intensity, thus facilitating an adequate allocation. However, it is important to take into account the amount of data within the analysis window when smoothing is carried out. Since the process of consecutive averaging the information decreases, a window of analysis with little data the loss of information could be significant.

3.4 Quantitative approximation

To evaluate the accuracy of the assignment of maximum absorbance values by FEDS to each band involved in the SPE, the calculation of the TEA/Acet molar fraction was made. The result obtained by equation 12 was 0.1471 ± 0.0002, while the value calculated from the ratio in volumes of the mixture and the concentration of each reagent, equation 13, was 0.133 ± 0.005. The percentage of absolute error was 10.6 %, explained by the approximations considered in the calculations, such as compliance with the Beer-Lambert law at work concentrations and the use of reported density values for the reagents. Despite all of this, the result shows that FEDS represent a potential tool to address the problem of the SBO and the assignment of maximum absorbance values associated with each band.

4. Conclusions

The results show that the overlap phenomenon in the mid-infrared can be addressed by FEDS. Its easy application and interpretation make these tools an important alternative to dealing with this type of problem. In addition, it was possible to establish how to enhance the response of FEDS, and guarantee a correct assignment of signals and an appropriate analysis by considering the effect of different aspects involved in the analysis of signals such as the signal-to-noise ratio, the amount of data within the analysis window, and the spectral smoothing.

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Conflicts of interest

The authors declare that they have no conflicts of interest of aby kind in relation to the publication.

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