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Ion Mobility Spectrometry Towards Environmental Volatile Organic Compounds Identification and Quantification: a Comparative Overview over Infrared Spectroscopy

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Abstract
Volatile organic compounds (VOCs) can be extremely toxic and hazardous to expose humans in both indoor and outdoor environments; thus, their detection, correct identification, and accurate quantification are relevant and demanding tasks that need to be addressed. Fortunately, several known analytical techniques allow the qualitative and quantitative assessment of these compounds. This review paper stresses on two independent spectroscopic techniques, infrared spectroscopy and ion mobility spectrometry, both suitable for the detection of very small concentration levels of VOCs in gaseous samples. Infrared spectroscopy is a well-known technique that has been largely applied per se or combined with additional methodologies, to study VOCs at both high and low concentration levels. On the other hand, ion mobility spectrometry gained relevance in this field, due to its capability to measure trace concentration levels, namely ppb_v and even ppt_v. For this review paper, several scientific papers were analyzed, and the most relevant were addressed throughout the text. The working principles of both techniques are carefully addressed, and updated data is provided for highlighting the advantages and disadvantages of both techniques for the environmental VOCs assessment in air quality control.

Keywords Infrared spectroscopy · Ion mobility spectrometry · Volatile organic compounds · Air quality assessment

1 Introduction

Air quality control and toxicity assessment are two of the most addressed issues in contemporary society. Volatile organic compounds (VOCs) can have a preponderant contribution to both these topics. Their presence and concentration levels in indoor and outdoor environments can directly influence air quality and affect the exposed population, causing several known pathologies. VOCs detection, identification, and quantification are, for these reasons, mandatory tasks that require analytical techniques to be accomplished.

In this work, an overview is given on the detection of VOCs through two spectrometric techniques: infrared (IR) spectroscopy and ion mobility spectrometry (IMS). The main goal of this review is to compare two analytical spectrometric techniques: IR, a very common and widely applied technique, and IMS, a more recent technique with proven results. It is intended to assess which analytical technique among the two mentioned is the most suitable for both qualitative and quantitative assessment of environmental VOCs in air samples. Relevant scientific papers are addressed and reviewed in each chapter along with an overview of the working principles of each technique. Two VOCs glossaries in the form of tables are also included as a way of easing the consultation of papers that address a specific analyte.

1.1 Volatile Organic Compounds

Volatile organic compounds are analytes whose chemical structure is mainly composed of carbon atoms that are volatile at room temperature. The European Union directive on the limitation of emissions of volatile organic compounds defines VOCs as "any organic compound …, having at 293.15 K a vapour pressure of 0.01 kPa or more, or having a corresponding volatility under the particular conditions of use" [1–5]. In this way, an organic compound with

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such an elevated vapor pressure will present a low boiling point, meaning that it will be volatile at room temperature (20 °C). Owing to this feature, VOCs can spread through the air effortlessly, rapidly, and imperceptibly to human beings [6–8].

As already mentioned, many daily use objects and activities contain or involve exposure to VOCs. In fact, emission sources of VOCs not only fill indoor environments, such as private houses, vehicles, or workplaces, but also public spaces such as shopping centers, hospitals, or schools, among many more different places [9–17]. They can be emanated from construction materials like paintings or varnishes, clothes, furniture, cleaning products like detergents, pesticides, perfumes, personal care products, and many other distinct but very common sources [7, 18–21].

Varying from almost inert to extremely reactive, VOCs have the capability of passing through biological membranes like pulmonary tissue, specifically alveolar membranes, but also through ocular or cutaneous tissues in such a way that their presence can represent a risk to human health even at trace concentration levels [22]. Eyes allergies and skin pruritus are some of the most common VOCs-provoked pathologies. Inflammatory and respiratory health conditions such as asthma and chronic obstructive pulmonary disease are also common pathologies caused by prolonged exposure to hazardous VOCs. Among other compounds, formaldehyde and benzene have been identified as carcinogenic and are directly responsible for some severe forms of cancer [23–29]. Under these facts, correct identification and quantification of VOCs are of great relevance for controlling air quality, maintaining the safety of human-use spaces, avoiding pathological health conditions, and preventing large-scale risks and hazards.

2 Analytical Techniques for VOCs Assessment

Considering the main analytical techniques that can be adequate for VOC assessment in a gas sample, one will certainly be led to elect chromatographic and spectrometric methods as the most relevant due to their intrinsic specificity and sensitivity to molecular species. Each one of these techniques can even be improved by means of dedicated procedures for specific situations or be enhanced by combining them into a new technique. Ultraviolet, visible, and infrared spectroscopy, for instance, are three possible specializations of spectrometric methods. The same applies to mass and ion mobility spectrometry, which are also spectrometry-based techniques. On the other hand, combined techniques such as gas chromatography-mass spectrometry (GC–MS) and gas chromatography-ion mobility spectrometry (GC-IMS) exemplify enhanced methodologies that provide the best characteristics of several techniques by coupling them into a single device [30, 31].

In this work, the detection and quantification of VOCs through infrared spectroscopy and ion mobility spectrometry were investigated and collated.

2.1 Infrared Spectroscopy

Infrared (IR) spectroscopy is a widely used analytical technique which started as the first structural spectroscopic technique available for organic compounds assessment. As a specific technique of vibrational spectroscopy, infrared spectroscopy has gained relevance for both qualitative and quantitative analyses of different types of samples, such as gases, liquids, solutions, powders, and even surfaces [30, 31]. IR spectroscopy allows the classification and quantification of samples through its infrared spectra in the electromagnetic spectrum region, between 700 nm and 1 mm of wavelength, or 430 THz and 300 GHz of frequency, the region where most of the vibrational resonances of chemical bonds occur [32].

From a simplified perspective, the application, and specifically, the absorption of infrared radiation by the molecules of a sample is associated with the vibration of molecular bonds. Absorption takes place for different molecular bonds at specific values of energy, and the infrared spectrum represents the fraction of the incident radiation that is absorbed at a specific energy value. Energy values correspond to certain frequencies of vibration and, complementarily, to particular wavelengths or wavenumbers [30, 31]. The majority of organic compounds, like alcohols, ketones, ethers, and VOCs in specific, absorb radiation in the infrared region of the electromagnetic spectrum. Consequently, infrared spectroscopy is one of the most effective analytical techniques for VOC identification and quantification [31]. The group of all the absorption bands observed in a spectrum can be used as a pattern or fingerprint of a molecule or sample. The intensity can be represented in the form of absorbance, transmittance, or reflectance as a function of the wavenumber, which is proportional to the energy change between the initial and final vibrational states of the molecular species [30–33].

Earliest infrared dispersive instruments have been replaced by Fourier-transform infrared devices, which are more adequate apparatus for solid, liquid, and gaseous compound analysis and spectral characterization [34–36]. From a more detailed perspective, the basis of the spectrometer optical bench corresponds to a scanning Michelson-like interferometer configuration and the spectrum is obtained by applying the Fourier transform to the interferogram signal [31–33]. Usually, the radiation source of an FTIR spectrometer is chosen according to the specific electromagnetic spectrum section to be investigated. The most common ones are high-pressure mercury lamps

and tungsten-halogen lamps, which are used as sources for the far-infrared and near-infrared regions, respectively [34, 35].

When the incident radiation reaches the sample, it can be reflected, absorbed, transmitted, or even scattered. Admitting I_0 as the intensity of the incident infrared radiation, it is possible to relate all these quantities using the following equation [32, 34]:

$$I_0 = I_r + I_a + I_t + I_s \tag{1}$$

where I_r, I_a, I_t, and I_s are the reflected, absorbed, transmitted, and scattered radiation intensities. In practical terms, the reflected, absorbed, transmitted, or scattered radiation intensities are dependent on the specificities of the sample or the surrounding conditions [32, 34].

For measuring the IR radiation, it is common to use pyroelectric detector devices that incorporate deuterium triglycine sulfate in a temperature-resistant alkali halide window. Besides the widespread utilization of these devices, other types of detectors can be used. Once detected, the signal undergoes a process of amplification and filtering in which the high frequencies are eliminated. Then, the signal is converted from analogic to digital, and the Fourier transform is mathematically applied to the resultant signal [32, 35]. The Fourier transformation of the signal is carried out through the application of two interconvertible equations, known as the Fourier-transform pair. This pair relates the signal intensity, $I(\delta)$, measured by the detector, and the spectral power density, $B(\overline{v})$, at a specific wavenumber, $\overline{v}$. Equation 2 represents the variation in power density as a function of the difference in path length, which is an interference pattern. Equation 3 demonstrates the intensity variation as a function of the wavenumber [34].

$$I(\delta) = \int_{-\infty}^{+\infty} B(\overline{v})\cos(2\pi\overline{v}\delta)d\overline{v} \tag{2}$$

$$B(\overline{v}) = \int_{-\infty}^{+\infty} I(\delta)\cos(2\pi\overline{v}\delta)d\delta \tag{3}$$

To calculate a spectrum, two interferograms need to be acquired. These interferograms are obtained from the source with and without sample absorptions. The ratio between them corresponds to what is known as a double-beam dispersive spectrum [34]. Nonetheless, the detection limits of the Fourier transform infrared spectroscopy are not low enough to detect VOCs in indoor and ambient air, so the detection and measurement of VOCs emitted by different materials through infrared spectroscopy remain an unsolved challenge until today. Multiple independent studies and approaches have been undertaken to help solving this issue.

2.1.1 VOCs Identification Through IR Spectroscopy

Regarding the addressed features of infrared spectroscopy, the identification and quantification of volatile analytes through this analytical technique cannot be directly done and require additional procedures or, at least, some kind of sample preparation. Kutsanedzie et al. aiming to evaluate the suitability of near-infrared spectroscopy for pure VOCs rapid detection and quantification [37], used chemo-responsive dyes as capture probes for studying the samples. The analytes targeted during this study were ethanol, ethyl acetate, and acetic acid. When exposed to the targeted analytes, the chemo-responsive dyes change their characteristics, namely the binding energies, energy levels, and dipole moments. These alterations can be easily observed through infrared spectroscopy, allowing to infer about the identification and quantification of VOCs. The use of a diamond-like carbon-coated silicon waveguide combined with hydrophobic polymer films is another approach for VOC identification, namely in water [38]. The target analytes can easily diffuse to the hydrophobic polymer, and once removed the water from the system, it is possible to directly detect VOCs. VOCs like ethylbenzene, p-xylene, o-xylene, toluene, and benzene have been successfully assessed using this procedure, proving the suitability of this approach. The use of polymers is somehow relevant to several independent studies. For example, filter paper and a polydimethylsiloxane polymer coating solution has been used for the preparation of a cost-effective preconcentrate sample of VOCs [39]. The procedure enabled to successfully quantify analytes in the ppb_v range of concentration. In order to address the suitability of a specific infrared spectroscopy technique, infrared attenuated total reflection spectroscopy (IR-ATR), for in-situ detection of VOCs in aqueous environments, a preliminary study for establishing the measuring protocol was developed by Lu et al. To do so, a polymer coating that traps VOCs and excludes water molecules was used to ease the analyses. The established protocol proved to be efficient in detecting at least some organic compounds, namely, p-, m-, o-xylene, toluene, and benzene; however, the VOC concentration values were not addressed in this work [40].

Coupling additional techniques to the IR spectrometer is very usual in the VOC assessment field as a way of improving the infrared spectroscopy performance. A photo-ionization detector (PID), for example, is frequently coupled to the infrared spectrometer. This sensor enables the detection of specific volatiles with an accuracy of 1 ppm_v if no other gases are present. The use of PID was successfully applied for the detection and quantification of styrene, toluene, isopropanol, acetone, and other VOCs. The results of these in-situ measurements of environmental samples proved the suitability of such methodology [41]. As mentioned, complementary detection techniques

have also been used to certify IR results. Kohl et al. and Formela et al. used, respectively, a proton transfer reaction quadrupole mass spectrometer (PTRQ-MS) and gas chromatography with a flame ionization detector (FID-GC), to complement the results obtained by IR spectroscopy. Having the goal of evaluating the interference caused by VOCs in the measurements of other not necessarily organic compounds, the total quantity of VOCs in the overall sample was assessed by the above-mentioned methodologies. Even being independent studies, coincident analytes were detected by the two distinct approaches, namely methanol, limonene, α- and β-pinenes, and hexenal [42, 43].

For situations where the sample to be analyzed requires to be collected and transported for subsequent analysis, sealed containers are the typical choice. These containers are normally used for the transportation of VOCs emitted, for example, from wildland fires. Scharko et al. collected volatile analytes with an extractive probe, during controlled fires, and stored them in 3 L capacity containers to be analyzed by FTIR. Acetaldehyde, naphthalene, and methyl nitrite were some of the organic compounds identified by the authors [44]. Similarly, 4 L capacity sealed containers with air samples were used for infrared analysis by Ju et al. Their main goal was to study the characteristic wavelength of VOCs like ethanol, ethyl acetate, and ethylene, in regard to their similar emission sources [45]. Also, a 2 L capacity homemade cylindrical chamber was developed by Gao et al. to store and then measure volatile compounds like methanol, formaldehyde, acetone, ethane, ethylene, toluene, and even mixtures of some of these VOCs, by IR spectroscopy [46]. As a remark, the main disadvantage related to the use of gas-storing containers is the possible contamination by exogenous and unwanted VOCs that may change the infrared spectra and respective sample assessment results. The aging of the containers may also represent a factor of adulteration of the results. Successive utilizations of the same container over a large period of time may lead to degradation of the isolation capacity, loss of its inert features, and consequently, lack of suitability for collecting and transporting samples. Nonetheless, containers still are one of the best options for sampling purposes.

Sorbent tubes have also been used for sample preparation and analysis of VOCs. This procedure was applied by Lampert et al. for analyzing low molecular weight VOCs with infrared spectroscopy [47]. As mentioned before, FTIR spectroscopy is not capable of providing particularly low detection limits for analytes identification of volatile samples, and the spectra are often too similar to be distinguishable. Sorbent tubes enable to overcome these issues through the preparation of samples with known concentration levels. The method revealed itself to be particularly advantageous for the VOCs assessment in industrial environments, where the emitted concentrations are considerably higher than those in ambient air [47].

A technique of water suppression was implemented by Maiti et al. as a way of identifying and quantifying several endogenous compounds exhaled in the breath. The suppression of water is a relevant procedure often used in aqueous samples since water IR fingerprint covers a considerably wide spectra region which conceals the target VOCs peaks. As mentioned, VOCs can permeate through biological membranes and tissues in both directions. In this way, the human exhaled breath, which is also rich in VOCs, represents a source of information about the health condition. Isoprene, limonene, acetone, 2-propanol, and 2-hexanone were the main analytes identified by the authors through IR spectroscopy. By reducing or even eliminating water vapor from breath samples, VOC concentration is not affected, enabling not only, their correct identification, but also proper quantification. Even with hundreds of different analytes that can be present in an exhaled breath sample, this methodology proved to be suitable for the analysis of complex matrices with an infrared spectrometer [48].

A practical application of the previously described procedure and, generally, of IR spectroscopy is the open-path FTIR. Figure 1 illustrates the main steps of a complete analysis with an open-path FTIR spectrometer. As mentioned, there are several options for IR radiation sources. Once emitted, this radiation undergoes a division process into two beams of equal intensity, by the Michelson interferometer, due to a set of mirrors used to reflect and refract the light. Thereafter, the radiation beams are expanded in order to enable the analysis of a large volume of interest. The radiation passes, then, through the target volume and returns to the spectrometer along an optical path, after suffering reflection on a retroreflector placed on the other extremity of the volume of interest. Once reaching the spectrometer, the beams undergo the inverse procedure by being contracted by the same beam expander and by being added to a single radiation beam, generating constructive and destructive interferences among them. Finally, the radiation is captured by the detector, and an IR spectrum including information on the analyzed analytes is created.

The open-path Fourier-transform infrared spectrometer enables the measurement of volatiles in air samples for indoor or even outdoor environments. It can be used for the detection and quantification of volatile analytes from distances of a few meters to several kilometers; in this way, its applications are wide and diverse. To evaluate the VOCs emitted by food samples, namely spirits, vinegar, and grapes, during their spoilage, an open-path FTIR spectrometer device has been used [49]. The analysis was carried out in different laboratory rooms having a $12 \times 8 \times 3$ m^3 volumetry, under the same conditions of temperature, ventilation, and humidity, for all the distinct food samples. This protocol

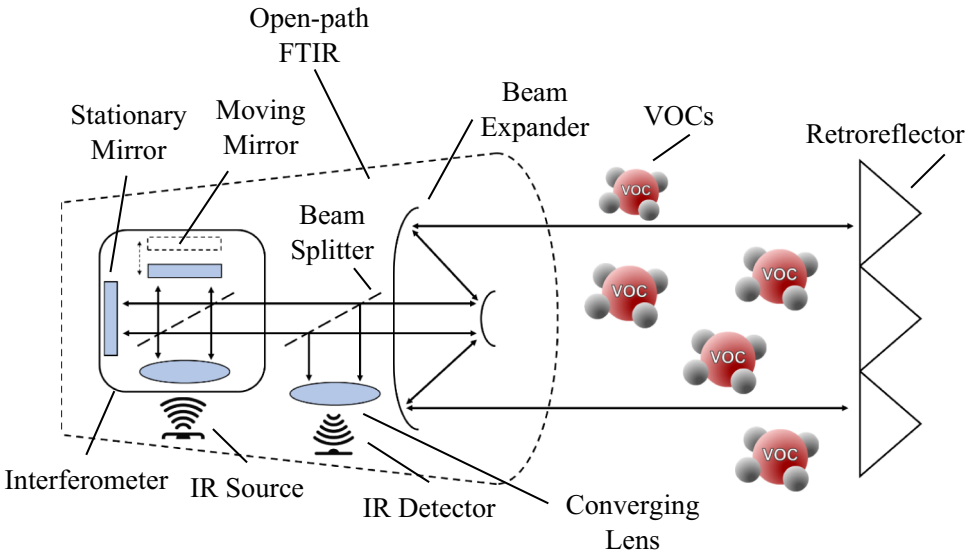

Fig. 1 Schematic of an open-path FTIR spectrometer. The main steps of a complete analysis are included, namely, the emission of IR radiation, the division, reflection, refraction and expansion of the beam, the interaction with the analytes of interest, and, finally, the radiation detection for spectra creation

prevents eventual cross-contamination of different volatile compound sources. Ethanol and ethyl acetate have been successfully detected during the measurements; however, these compounds are a common presence in indoor air environments. In this way, open-path FTIR spectroscopy suitability for such a purpose cannot be assured. The same approach was used for dynamic real-time monitoring of chloroform emitted by an indoor swimming pool [50]. Considering the measurements performed every 15 min during a complete week, results showed that open-path FTIR spectroscopy was able to, not only identify but also quantify the chloroform emitted by the swimming pool water, in the range of 13 to 182 $\mu g/m^3$ [50]. With the main goal of measuring VOCs escaping from large petrochemical tanks, target samples were diluted in a large volume of air and analyzed with an open-path Fourier-transform infrared spectrometer device. Five main VOCs have been successfully identified, namely p-, m-, o-xylene, toluene, and benzene; all of them are known for being emitted by petrochemical mixtures [51]. All the addressed studies are useful to understand the suitability of open-path FTIR spectroscopy in the field of VOCs assessment.

Another variant of the IR spectroscopy that has gained relevance for the analysis of gases and, specifically of VOCs, over the past years is the cavity ring-down spectroscopy (CRDS) [52]. The CRDS is a direct quantitative absorption-based analytical technique setting its working principle on the assessment of the variations in the rate of decay of light when projected into a high-finesse optical resonator. To briefly describe the measuring procedure, it is relevant to enumerate a few of the main steps.

The target gaseous sample is prepared and positioned in the interior of an optical cavity, commonly known as a ring-down cavity that consists of highly reflective mirrors, with reflectance above 99.9%. A laser pulse is projected into the ring-down cavity; and because of the mirrors' high reflectance, continuous reflections will take place. At each reflection, a small fraction of the incident light is lost via transmission, leading to an intensity decay. This light-intensity decay is known for presenting an exponential behavior [53, 54].

In an empty ring-down cavity, the ratio of intensity loss is solely dependent on the fraction of transmitted light during each reflection; however, in a scenario in which the cavity contains a target sample, the ratio of intensity loss depends equally on the interactions between the light and the absorbing sample. During the analysis, the decay of light intensity is measured as a function of time. From this feature, the cavity ring-down time or decay time can be calculated, which basically is the time required for the light intensity to reach $^1/_e$ of its initial intensity [53, 55]. It can be represented as t:

$$t = \frac{d}{c\left((1-R)+\alpha l_s\right)} \tag{4}$$

In Eq. 4, d corresponds to the distance between the mirrors, c is the light velocity, $(1-R)$ represents the decay in the light intensity due to the successive reflections at the cavity mirrors of reflectance R, α is the absorption coefficient of the target sample, and l_s is the length of the ring-down cavity [56, 57]. Once registered, the decay time can be used for identification purposes. The suitability of CRDS for ambient air analyses was addressed by Pradhan et al. The study aimed to assess the presence of acetylene in samples of ambient air through cavity ring-down spectroscopy. Nonetheless, for the successful qualification and quantification of the target analyte, the authors had to implement a pre-concentration process to prepare the samples for the analysis. This process consisted of using a trap holding an adsorbent material that

retained the target molecules [58]. As seen, the necessity of employing pre-processing methodologies before the measurements with the spectrometer is one of the main limitations of CRDS. The suitability of CRDS for VOCs detection and identification was equally demonstrated by Zhou et al. To do so, the authors prepared volatile samples of ethanol, ether, and acetone mixed in high-purity nitrogen at known concentrations. Then, the ternary samples were positioned in the ring-down cavity and analyzed with the spectrometer. The authors were able to successfully identify and quantify the analytes in the ppb_v range of concentration proving the capacities of CRDS for environmental monitoring applications [59]. Larracy et al. were able of using CRDS to detect and identify VOCs in one of the most complex matrices, the human exhaled breath. Once collected, the breath samples of a cohort of 158 volunteers (96 healthy individuals and 62 non-small cell lung cancer patients) were tested with the spectrometer. The CDRS technique enabled to differentiate both groups with sensitivity and specificity levels up to 80 and 90%. In addition, authors could identify isopropanol, dimethyl sulfide, and butyric acid as potential lung cancer biomarkers in the breath [60]. These results prove the suitability of CRDS for detecting and identifying VOCs even in complex matrices.

Considering the characteristic decay time t, one can plot $1/t$ as a function of the laser light frequency, which basically represents the relationship between the absorption coefficient as a function of frequency. Considering the absorption cross-section of the sample, the plotted spectrum can be used to calculate the concentration of the sample [57]. Quantification limits ranging from 10^{-6} to $10^{-13} cm^{-1}$ respectively for traditional or high-resolution systems have been reported. Consequently, the CRDS variant of IR spectroscopy has gained relevance in the assessment of gaseous and volatile samples in fields like environment, chemistry, and health [54, 55]. Huang et al., for example, dedicated their work to the detection and identification of VOCs, in specific biogenic VOCs emitted by the flora, responsible for relevant environmental and climatic alterations. To do so, the authors used a cavity ring-down spectroscopy device that enabled them to identify a direct dependence of the emissions of VOCs like acetone, methanol, and monoterpenes, on the concentration levels of CO_2 and the temperature. The identification of the analytes was achieved in ppm_v levels of concentration [52]. Schmidt et al. claim to have reached detection limits down to ppb_v levels during CRDS measurements. These detection limits were achieved during the assessment of acetylene, a common anthropogenic analyte, in both indoor and outdoor air samples [61]. The addressed results show the high-resolution capacities of the cavity ring-down spectroscopy not only for the identification of VOCs but also for their quantification. The described working principle of the CRDS is schematized in Fig. 2.

Throughout the manuscript, the most relevant studies are addressed. Table S1, in the Supplementary Materials, summarizes the VOCs analyzed by infrared spectroscopy in most of these studies. Concerning this information, it is worth noticing that m-xylene [39–41, 51, 62, 63] and toluene [38–41, 46, 51, 62–65] are some of the most common compounds in all the studies. Some other papers focus

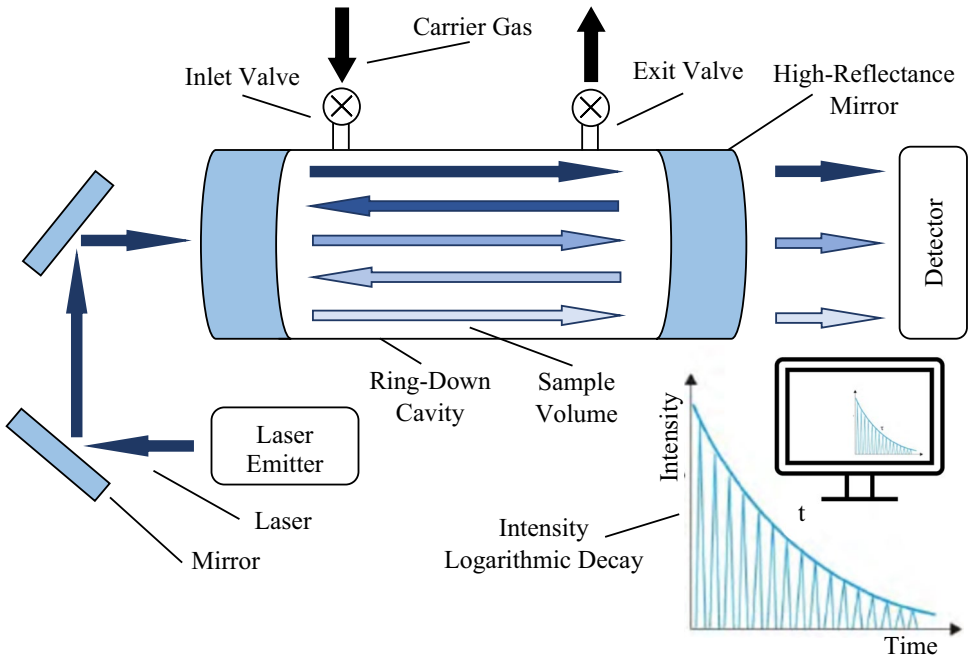

Fig. 2 Schematic of the cavity ring-down spectroscopy experimental setup and working principle. The main steps of a complete analysis are included, namely, the emission of a laser pulse, the logarithmic decay of the pulse intensity, and the data collection and processing

their results on one single or in a specific group of analytes, for example, chloroform [50], limonene [66], and volatile organic acids [67].

2.1.2 VOCs Quantification Through IR Spectroscopy

To address the VOCs quantification with IR spectroscopy, it is necessary to understand how the final spectrum is produced. The output of a Fourier-transform infrared spectrometer is a two-dimensional spectrum in which, the abscissas axis is given in terms of wavenumber, $\overline{\nu}\left(cm^{-1}\right)$ and the ordinates axis represents two possible quantities: transmittance (%) or absorbance (%). Scaled in the decreasing direction of wavenumber, the x-axis is normally distinguished into three main sections: far-infrared, mid-infrared, and near-infrared. These three regions correspond, respectively, to $< 400cm^{-1}$, $4000 - 400cm^{-1}$, and $13000 - 4000cm^{-1}$. The bands that appear along the spectrum have a direct relation to specific molecule vibration modes and are known as group frequencies. Following the presence of different functional groups, such as alcohol or ketone, specific vibrational frequencies arise and their corresponding positions appear in the spectrum. For example, molecules with alcohol as a functional group have a specific spectrum band of over 3000 cm^{-1} wavenumber, due to the O–H bond stretching. For 2000–1500 cm^{-1} interval, the main bands arising are related to the bond stretching of C = C and C = O, as happens for ketone and ester functional groups. Although a molecule can have several different bands in its spectrum, it is unnecessary to acknowledge most of them. A specific group of absorption bands, known as a fingerprint, is enough to identify the target molecule [32, 34, 35].

Transmittance and absorbance, represented from 0 to 100%, are complementary quantities typically used for the infrared spectrum y-axis. Transmittance and absorbance are a sample's capacity to transmit or absorb radiation, and while transmittance is normally chosen for spectrum interpretation, absorbance is preferred for quantitative analysis. The ratio of transmitted or absorbed radiation is proportional to the molecular species concentration, meaning that a higher concentration corresponds to a larger radiation absorption [32, 34, 68].

Being I_0 the intensity of the incident radiation and I the intensity of the radiation transmitted by the sample, transmittance, T, is given by their ratio:

$$T = \frac{I}{I_0} \tag{5}$$

As mentioned, the transmittance is vulgarly used as a percentage value, and it can be related with the absorbance. It is also common to express absorbance by the difference between the logarithms of the incident and transmitted radiation intensities:

$$A = \log I_0 - \log I = \log\left(\frac{I}{I_0}\right) = -\log T \tag{6}$$

Quantitative analysis can be carried out by using the Beer-Lambert law, which defines a linear relation between absorbance and the component of concentration. For the case in which it is intended to analyze a gaseous sample concentration, gas properties and the ideal gas law need to be considered. In this way, the concentration of an element in a sample can be obtained through a calibration curve, specifically, an absorbance versus concentration curve which allows one to determine the molar absorptivity [34, 35]. The absorbance, A, for a volatile compound can be written as:

$$A = \frac{alP}{RT} \tag{7}$$

P corresponds to the pressure, R to the universal gas constant, and T to the temperature, the same variables used in the ideal gas law. The optical path through the sample is represented by l, and a represents the component of absorptivity at the considered wavelength [32, 68].

As an elucidative example, Fig. 3 represents a spectrum of absorbance versus wavenumber for several VOCs detected and identified by infrared spectroscopy. This kind of spectrum corresponds to the outcome of an IR spectroscopy analysis as described above, in which the respective values of absorbance and wavenumber of each VOC are represented. Further details on these results will be addressed later; however, it is worth emphasizing some issues at this point. The spectrum of the figure includes the characteristic peaks of eight VOCs identified during water sample emissions. The target analytes were benzene (BENZ), toluene (TOL), m-xylene (mXYL), o-xylene (oXYL), p-xylene (pXYL), ethylbenzene (EB), trichloroethylene (TCE), and tetrachloroethylene (TeCE). The spectrum is plotted in terms of wavenumber and absorbance [38].

A considerably high number of scientific papers have addressed the quantification of VOCs by infrared spectroscopy. As for any other analytical technique, one of the correct approaches is to generate precise concentration level standards of a specific compound, in a wide range of values, and obtain the corresponding calibration curve. This process consists of correlating the spectrum's absorbance or transmittance, at a key wavenumber, with the concentration of standard samples. Besides of being straightforward for liquid solutions samples, this approach is not so direct for gaseous or volatile samples [41]. Most of the independent studies address the mentioned procedure and the related issues. For instance, Dettenrieder et al. [38] and Mamaghani et al. [64] plotted their respective calibration

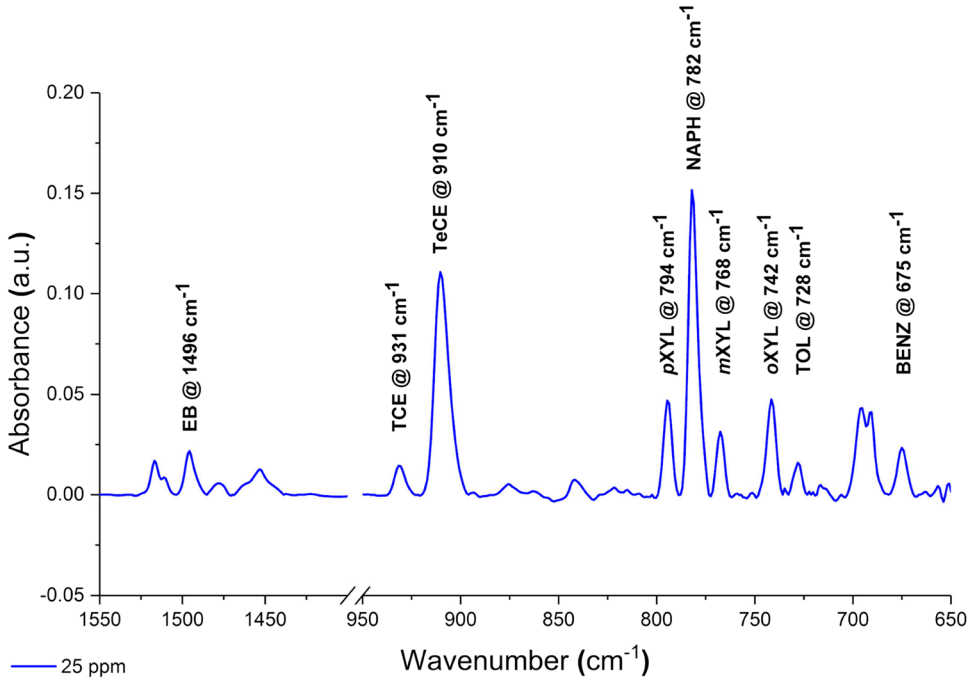

Fig. 3 Spectrum of several volatile organic compounds obtained from water samples emissions [38]

curves having into consideration the proper parameters for Eq. 7. To plot the mathematical model of the calibration curve, the computational process typically used is the prediction model based on the partial least squares (PLS) regression. This covariance-based method enables the achievement of calibration curves for any type of VOCs [37, 38, 45, 69].

As mentioned, coupling infrared spectroscopy with other techniques is one of the most common approaches for sample preparation. In the same way, other analytical techniques can be used for concentration calibration. For example, Kim et al. [39] used a hydrophobic polydimethylsiloxane polymer solution for the coating filter paper, as a procedure for the preparation of known pre-concentration headspace samples from water-emitted VOCs. Concentration values were assessed using gas chromatography-mass spectrometry (GC–MS) reference values [39]. GC–MS was also the technique used by Garde-Cerdán et al. to calibrate the concentration of VOCs emitted by aged red wines [69]. Nespeca et al., in their turn, used a gas chromatography–flame ionization detector for concentration reference values assessment [67], and Kohl et al. preferred to use the proton-transfer-reaction—mass spectrometry technique for the same purpose [42].

Regarding the concentration range detected along some of the mentioned works, parts-per-million (ppm_v) and parts-per-billion (ppb_v) are the lowest concentration levels that infrared spectroscopy, with or without additional techniques and methodologies, could quantify [38, 44, 45]. Taking into consideration all the independent studies and respective results included in this chapter, infrared spectroscopy seems to be a good option regarding the detection, identification, and quantification of VOCs.

2.2 Ion Mobility Spectrometry

Initially developed for military purposes, ion mobility spectrometry (IMS) has recently gathered interest for a large range of civil applications [70]. The range of applications extends from simpler topics like food quality/spoilage evaluation, product categorization, and fraud detection [71–73], to more complex ones, such as security purposes, health pathologies detection, and air quality assessment [10, 74, 75]. Ion mobility spectrometers have a set of specificities that enable the detection of VOCs, and VOCs only, in terms that no other analytical techniques allow. Their real-time monitoring capacity, analytical flexibility and simplicity, and high sensitivity make IMS one of the most widespread techniques nowadays. In addition, it can be used in distinct versions such as differential IMS (DIMS) and field asymmetric IMS (FAIMS) or be coupled with additional techniques like mass spectrometry (MS) or gas chromatography (GC). In those cases, the coupling gathers in a single device the advantages of each technique and creates an extremely sensitive and selective new technique. The improved devices have the remarkable capacity of identifying and quantifying VOCs in concentration ranges down to parts-per-billion (ppb_v, 10^{-9}) and parts-per-trillion (ppt_v, 10^{-12}). Even being only capable of detecting and quantifying VOCs, since it is completely blind to any other type of analytes, IMS permits to achieve outstanding results in VOCs characterization based on their size, weight, and shape, making it one of

the most suitable techniques for air quality assessment and control [76–78].

A complete procedure sequence using the IMS device starts with the injection of a gaseous sample into the apparatus, a procedure that does not require the employment of vacuum systems. The injection of the sample into the spectrometer is usually preceded by some type of sample collection or procedure to promote compounds volatilization, which in the case of IMS normally involves the creation of headspace. Since this technique only allows to measure volatile samples, it is common that volatile compounds are volatilized inside a glass vial or even in a sampling Teflon bag at room temperatures. Once reached the thermodynamic equilibrium between the liquid and the gaseous fractions of the sample, the created headspace can be analyzed in the spectrometer. The VOCs can be measured from pure samples, a mixture of distinct analytes, or even from a VOC-emitting solid or liquid sample. For instance, to identify VOCs by their respective retention time obtained in ion mobility spectrometry measurements, pure samples of each analyte were used by Levin et al. to create headspace which was then injected into a GC-IMS device [79]. Yokoshiki et al., in their turn, prepared a ternary mixture of VOCs for quantification purposes. The mixture consisting of acetone, ethanol, and diethyl ether was prepared inside a sampling Teflon bag. For the analyses, flow rates of 0.05 L/min, 0.1 L/min, 0.15 L/min, 0.20 L/min, and 0.25 L/min were used for carrying the samples into the spectrometer, with ambient air used as carrier gas [80]. Headspace formation was also the procedure selected by Jurado-Campos et al. during their qualitative study. The authors prepared complex mixtures of analytes at known concentrations in 20 mL glass vials. The vials were then isolated to reach the thermodynamic equilibrium between the liquid and gaseous portions of the sample. Once completed the process, the volatilized analytes were analyzed with the spectrometer [81]. As seen, headspace formation prior to the analysis by ion mobility spectrometry is a very common and with the proven-results procedure to measure VOCs. Figure S1, available in the Supplementary Materials, exemplifies the headspace formation procedure. In (a) the glass vial containing the compound is closed with an aluminum cap with a septum and sealed with parafilm to avoid eventual contaminations. In (b) two needles are used to collect a portion of the headspace with a syringe or into the spectrometer, for analysis.

The headspace created from VOCs can be categorized into two main groups: static headspace and dynamic headspace. For the static headspace, the sample is prepared, isolated from exogenous contaminations, and left for a predefined amount of time. During this period, the liquid and gaseous portions of the sample interact, the analytes volatilize, and a thermodynamic equilibrium is reached. Once attained the equilibrium in the interior of the container, a portion of the headspace is collected and transferred to the device, usually with the help of a syringe and two needles. This procedure is commonly employed when the study aims to qualify or quantify a large number of discrete samples, at a specific temperature, instead of evaluating continuously their evolution or alteration over time, as for dynamic headspace. Rodríguez-Maecker et al., with the purpose of identifying terpenes by IMS, opted for the static headspace to prepare the samples. As in previously mentioned works, the samples were prepared in 20 mL glass vials and isolated for the headspace formation. In this study, however, the process of volatilization was accelerated by subjecting the vials to a temperature of 35 °C and agitation of 500 rpm for 5 min. The described protocol enabled the successful identification of more than two dozen analytes [82]. Vautz et al. adopted a similar procedure to the one described above. Here, the authors applied a temperature of 40 °C, for 10 min, to 20 mL vials containing counterfeit money samples. Their main goal was to test the suitability of several techniques for data-processing the analytes existent in the emissions of the money [83]. The increasing temperatures and vial stirring enable faster volatilization of compounds that are already able to become gaseous almost effortlessly at room temperatures.

Static headspace proved to be a suitable approach to analyze VOCs by IMS if the headspace is given proper time to reach the equilibrium or if the volatilization process is instigated under known and controlled parameters. Static headspace is equally suitable for cases in which the evolution of the characteristics of the samples over time is negligible. In order to not affect the outcomes and to prevent eventual exogenous contaminations, inert vials and adequate sealing conditions should be ensured during the entire procedure.

For the dynamic headspace procedure, in opposition to the static headspace, a continuous carrier gas flow passes through the vial containing the VOCs-emitting sample and then, is directed into the spectrometer. For example, to measure VOCs emitted by plants and assess their impacts on humans, Vautz et al. placed 3 g of leaves inside 20 mL vials and heated them at 60 °C. As mentioned, this procedure accelerates the volatilization process. Leaves from nine different common herbaceous plants were analyzed. A continuous flow of carrier gas was flushed through the vial and directed into the spectrometer. The used carrier gas was nitrogen with a flow of 100 mL/min [84]. Similarly, a continuous airflow of 1 L/min was inserted into vials with samples of carbon disulphide and uninterruptedly transferred to the ion mobility spectrometer. This study aimed to study possibly toxic chemicals in an industrial context. To do so, the authors selected the static headspace as the most adequate sampling procedure [85]. This dynamic approach is often employed when the authors aim to include the temporal variable in the study. Whenever the alterations of the presence of VOCS or the variation of their concentration levels through time is a relevant issue, the dynamic headspace

is the procedure commonly selected for sampling preparation. In summary, dynamic headspace allows a continuous analysis rather than a discrete one as it occurs with the static headspace technique.

2.2.1 VOCs Identification Through IMS

Once prepared and introduced into the IMS device, the sample will suffer ionization by a radioactive (tritium or nickel) or by a photonic source (X-ray ionization, for example). One of the most common radioactive ionization sources is Tritium ($_1{}^3H$) ($300MBq$). Tritium spontaneously emits a high-energy particle, β^-, as described in Eq. 8 [86]:

$$_1{}^3H \rightarrow {}_2{}^3He + \beta^- \tag{8}$$

The emitted β^- particle reacts with nitrogen, the inert gas present inside the ionization chamber, to create background ions from nitrogen. Background ions are equally known as primary ions:

$$N_2 + \beta^- \rightarrow N_2^+ + \beta'^- + e^- \tag{9}$$

The emission of both β^- particles and primary ions occurs through multiple and continuous reactions. Nitrogen primary ions will then react with molecules of H_2O, NH_3, or NO present inside the ion mobility tube and create new ions. These new ions, $(H_2O)_nH^+$, $(H_2O)_nNH_4^+$, or $(H_2O)_nNO^+$, are called reactant ions, and unlike primary ions, they are visible in the final spectrum. Reactant ions form an intense peak visible along the entire spectrum and named reactant ion peak (RIP) [76, 87, 88].

All VOCs of a sample react, in the next step, with the reactant ions. In a scenario in which the sample is composed of a single volatile analyte, M, the reaction between this generic compound and the reactant ions occurs according to the reaction:

$$M + (H_2O)_nH^+ \leftrightarrow M(H_2O)_{n-x}H^+ + xH_2O \tag{10}$$

, in which the x value is, of course, dependent on humidity levels. Being a chemical bounding between protons and molecules, the product ions of this reaction are protonated monomers of the compound M. If the concentration of the analyte is sufficiently high, the monomer can continue to react with the remaining M molecules, giving rise to the formation of protonated dimers. There is even the possibility of larger clusters being formed, as follows [76, 87, 89–91]:

$$M + (H_2O)_{n-x}H^+ \leftrightarrow M_2(H_2O)_{n-(x+i)}H^+ + iH_2O \tag{11}$$

IMS is able of working in two different modes, positive and negative. The previous reactions exemplify the positive mode procedure. For the negative mode, the reactant ions are formed due to the reaction of the primary ions with O_2 molecules instead of H_2O, NH_3, or NO molecules. Having MX as a generic compound, its product ions can be created, in negative mode, by associative or dissociative electron attachments. Those reactions are represented in Eqs. 12 and 13, respectively [76].

$$\boldsymbol{MX + (H_2O)_nO_2^- \leftrightarrow M + X^- + nH_2O + O_2} \tag{12}$$

$$\boldsymbol{MX + (H_2O)_nO_2^- \leftrightarrow (MX)O_2^- + nH_2O} \tag{13}$$

Once created, the product ions are exposed to a homogeneous and weak electric field ($500V/cm$) that accelerates the ions through the IMS tube. Figure 4 represents the action of this field in the interior of the IMS tube during a complete analysis.

The electric field acts along the tube and is provided by equally spaced guard rings spread through the drift tube and connected through a chain of resistors. Eventually, ions collide with the inert neutral gas molecules causing them to decelerate. Still, under the electric field effect, product ions gain velocity until undergoing a new collision [76, 88]. The sequence of collisions will make the ion velocity tend to an ion-specific value, denominated ion drift velocity, v_d. Drift velocity, as mentioned, is different for distinct compounds,

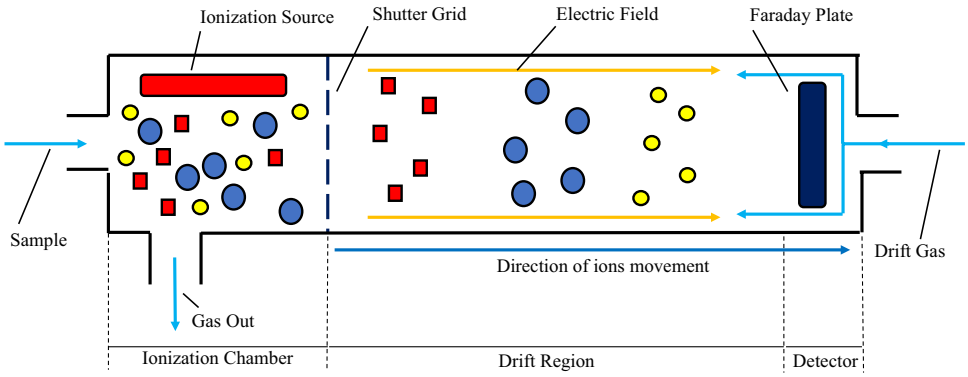

Fig. 4 Schematic of a complete measurement by IMS. The sample is ionized in the ionization chamber, and the formed ions are exposed to an electric field that will enable the detection of each VOC at their specific drift and retention times

and it can be related to the electric field magnitude, E, through the ion mobility constant of the analyte, K, [76, 92]:

$$K = \frac{v_d}{E} \tag{14}$$

Additionally, drift velocity can be calculated by the ratio between the IMS tube length, L (around $98mm$), and the time that product ions take to cross that same length.

$$v_d = \frac{L}{t_d} \tag{15}$$

The drift time, t_d, corresponds to the time each ion takes to go through the entire IMS tube, and it enables a new formulation for the ion mobility constant, K, [87, 93]:

$$K = \frac{L}{Et_d} \tag{16}$$

Ion mobility constant, however, may depend on pressure, P, and temperature, T, conditions. To circumvent this effect, it is common to normalize its value to standard environmental pressure, $P_0 = 760Torr$, and temperature, $T_0 = 273.15Kelvin$. With this calculation, the so-called normalized ion mobility constant, K_0, arises [88, 94]:

$$K_0 = K\left(\frac{P}{P_0}\right)\left(\frac{T_0}{T}\right) \tag{17}$$

As mentioned, both ion mobility constant and drift time are constant and sample-specific values; in this way, the ratio between K and t_d is also a parameter that can be used for VOCs' differentiation. It is worth reinforcing that the entire described procedure occurs at both atmospheric pressure and room temperature and does not require the utilization of vacuum systems to operate.

When the product ions reach the IMS tube end, they are detected through a Faraday plate at their specific drift times. In this way, two coordinates are achieved by the IMS measurement: the drift time (ms) and the ions' intensity level (V). Considering the distinct techniques that can be coupled to the IMS, the final spectrum of each variation presents differences. For the scenario where the IMS is coupled to a gas chromatography column, for example, a third coordinate is also represented in the plotted spectrum, defined as retention time, r_t, (s). This temporal value corresponds to the time each compound needs to go through the entire chromatographic column and is directly related to the compounds' capability of adsorbing to the column walls [77, 78, 95]. A GC-IMS three-dimensional spectrum is, thus, generated as follows: the x and y-axis represent drift (ms) and retention (s) times, respectively; a third coordinate, typically represented by a color scale in a two-dimensional view, corresponds to the components' intensity (V). The intensity is directly related to the concentration of each compound presented in the analyzed sample. In other to quantify all the analytes, a calibration protocol must be applied to obtain a calibration curve which, in turn, is used to convert intensity values to concentration values [76, 96]. Figure 5 represents an ion mobility spectrometry spectrum, from a room air sample, in its two- and three-dimensional views, in which some of the represented VOCs are identified (1: monomer of ethanol, 2: monomer of 2-propanol, 3: dimer of ethanol, 4: monomer of acetone, and 5: dimer of 2-propanol, among many others) [97].

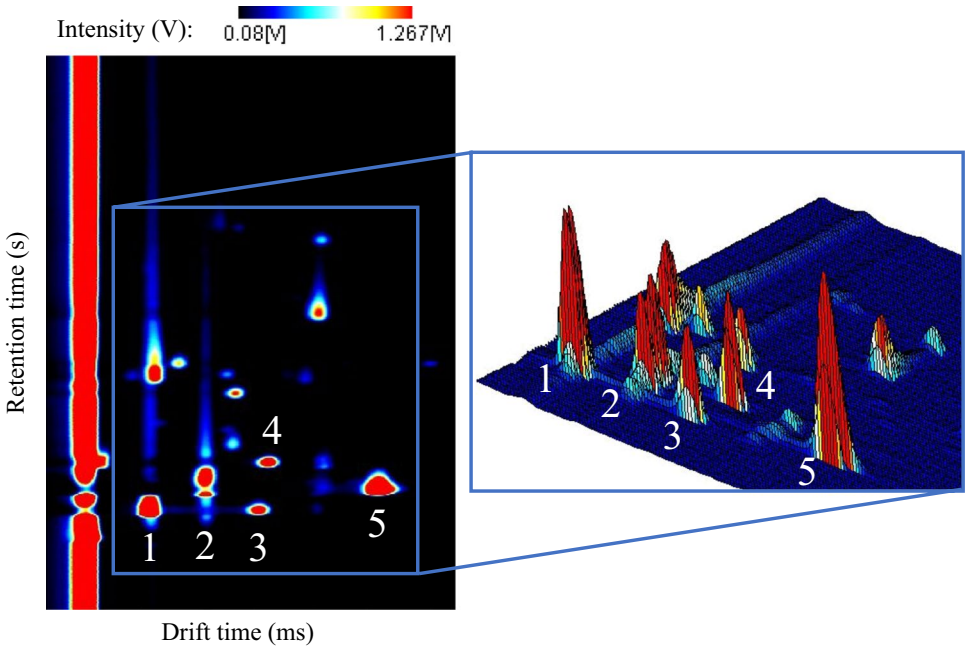

Fig. 5 Example of a three-dimensional spectrum plotted after an ion mobility spectrometry analysis, in which some VOCs are identified (1: monomer of ethanol, 2: monomer of 2-propanol, 3: dimer of ethanol, 4: monomer of acetone, and 5: dimer of 2-propanol)

Considering the capacities and measurement procedures of the IMS, considerable studies have been undertaken around the identification of VOCs. For example, Szczurek et al. used IMS to identify three VOCs in humid air samples. Known as BTX, benzene, toluene, and xylene are commonly described as hazardous VOCs for both environment and human beings. To identify these compounds through IMS, a distinct sampling dynamic procedure, known as permeation tubes, was used by the authors [98]. A permeation tube consisting of a PTFE or other inert material manufactured tube was filled with the compound intended to be analyzed. The analytes were set to permeate through the tube's wall, and a carrier gas with a pre-defined flow was used to drag the VOCs into de spectrometer. Regarding this sampling procedure, permeation tubes enable easy control of temperature and control of the VOCs permeation rate through the tube walls. Such characteristics favor the assessing of the analyzed concentration levels; in this way, permeation tubes are one of the most frequently used sampling procedures for identification and quantification purposes. An exemplificative schematic of a permeation tube is included in Figure S2, in the Supplementary Materials.

Ruzsanyi et al. also used a system of permeation tubes for calibration of the results obtained by ion mobility spectrometry regarding human-emitted VOCs, such as acetaldehyde, acetone, hexanal, and others [75]. In their turn, Fernandes et al. having in view the development of a calibration methodology assembled Teflon permeation tubes with 0.2 mL samples of pure 2-hexanone. These 5 cm length tubes were maintained in a thermogravimetric device for an accurate control of temperature (40, 60, and 85 °C) and flow (25, 50, 100, 150, and 200 mL/min). VOCs were, then, analyzed by GC-IMS [99].

For some situations, it is not intended to analyze specific compounds but rather a group of VOCs emitted by some sample. Biological samples are an example of those situations. For instance, the identification and quantification of analytes emitted by the human body are a way of assessing eventual pathologies or even inferring about exposure to hazardous compounds. For such scenarios, distinct sampling techniques can be applied. As an example, a body plethysmography chamber was successfully used by Mochalski et al., for monitoring VOCs released by the human body, namely, via skin and exhaled breath [24]. Under this situation, the human body is the VOCs-emitting sample, and the chamber works as a vial of large dimensions in which the headspace reaches stability for analyzing all human-emitted volatile compounds. If the goal is to collect and evaluate VOCs from specific locations or sources, more specific techniques are usually the proper choice. For specific compound collection, but still in human body sampling, Vautz et al. designed and manufactured a 5 mL sampling Teflon chamber for a local collection of skin-emitted VOCs. A humidity-temperature sensor was implemented in the interior of the chamber for accurate control of these two quantities. A carrier gas at the constant flow of 1 mL/min passed through the chamber to transport the emitted VOCs into de GC-IMS. This procedure enabled to successful detect 15 VOCs, and 9 of these, like 3-octanol, benzaldehyde, decanal, or propionic acid, were identified [100]. A similar setup has also been developed by Ruzsanyi et al. [101]; however, the selected material for chamber manufacturing was stainless steel. A constant airflow of 3 mL/min was used for dragging the VOCs into the spectrometer. Since they are inert, i.e., they do not emit contaminant analytes, both Teflon and stainless stell are good options for chamber manufacturing. In addition, they enable effortless sterilization after each use, which constitutes another advantage. Having the goal of investigating the variation of the concentration of several analytes in human breath over a specific amount of time, Bunkowski et al. collected samples of exhaled air using sample loops of 10 mL. After the collection, the samples were transferred to the spectrometer inlet for analysis. This procedure enabled the identification of VOCs like decanal, 1-hexanol, and d-limonene, among other human-borne analytes [102].

Sample loops, typically made of stainless steel, are another ordinary technique used for collecting and transporting analytes. They are commonly used for human breath collection since they enable to maintain the sample at homogeneous conditions of temperature and humidity during the process, which extends from the collection to the analysis, preserving its metabolomic characteristics. In these cases, the extremities of the sample loops are usually connected to a mouthpiece for exhaled breath collection and to the spectrometer. This exact method was used by Bessa et al. to collect breath samples of patients with chronic obstructive pulmonary disease. After collection into a 10 mL sample loop, samples were analyzed by ion mobility spectrometry, and as happened in the previously addressed work, typical exhaled breath analytes, like acetone or decanal, were successfully identified [103]. The main limitation of using any kind of technique for exhaled breath sample collection is the eventual accumulation of liquid-phase droplets, which may cause drawbacks during ion mobility spectrometry analysis.

As seen from Eq. 10, the humidity present in the IMS analysis directly affects the results, in such a way that, the eventual accumulation of liquids from breath will alter the obtained results; however, if the analysis is done under optimal conditions, IMS even enables pattern recognition. For example, Santos et al. were able to use IMS for the differentiation of two portions of the exhaled breath, the alveolar portion and the oesophageal portion. A cohort of 31 healthy volunteers was used for exhaled breath analysis through IMS. To do so, a prototype for collecting exhaled breath samples was developed by the authors and utilized during

this work. Once collected, the samples were injected into an IMS device, and the results were statistically processed through partial-least square discrimination (PLSDA) and principal component analyses (PCA). The main goal of the authors was to assess the suitability of IMS to differentiate both portions of exhaled breath. The outstanding sensitivity of ion mobility spectrometry enabled the authors to achieve an almost perfect classification of both groups from the cohort. The principal components calculated during the principal component analysis enabled a distinction of both groups of almost 100%. To be more specific, the sum of all the components, also known as the total explained variance, reached levels of 97.9%. If IMS proved to be capable of distinguishing such complex samples almost perfectly, then, its suitability for overall VOCs detection is evident [104].

Ion mobility spectrometers allow, not only, measurements from sampling reservoirs, but also in-situ measurements. Air samples in these scenarios can be collected directly from the air by the device or collected by some inert material pump and transported to the spectrometer. If the goal is to investigate the exogenous factors that may eventually influence exhaled breath analysis, IMS devices enable to automatic measure room air samples at regular time intervals for continuous analysis of, not only, the presence, but also, the concentration variation of VOCs [105]. This automatic capability of measuring in-situ air samples also enables IMS to continuously control all the VOCs emitted during industrial processes. Yang et al. used GC-IMS and other techniques to evaluate the VOCs responsible for the strong odor felt during industrial fermentation processes, and they were able to successfully detect and identify the main sources of the compounds 2-methyllisoborneol and geosmin, and even some aldehydes like hexanal, octanal and decanal [106]. Factories, public spaces, workshops, and other public spaces with a high influx of people or continuously exposed to chemical compounds emission require careful and permanent control. Due to their in-situ measuring capability, ion mobility spectrometers are among the most suitable analytical techniques for such studies. In scenarios where the device cannot be placed exactly at the target location, it can be assembled in a nearby location, and a reservoir can be used for the collection and subsequent sample transportation. In fact, this limitation was faced by Moura et al. Due to the impracticability of placing the GC-IMS in all the target locations and performing in-situ measurements, a 1 L capacity inert Teflon pump was used for collecting and transporting the air samples to be analyzed. This procedure prevented eventual contaminations by exogenous compounds or exposition to environmental conditions that could lead to sample degradation. Even not consisting of in-situ measurements, the authors' approach was considerably similar as samples were collected and almost immediately inserted into the ion mobility spectrometer for analysis [10].

Independently of the selected method among all the aforementioned ones, each study has its own target compounds for identification. In general and independent of the type of procedures, all the addressed works provide a list of the identified or analyzed VOCs. Acetone, being one of the most common VOCs in room air, was identified in several independent studies [10, 24, 75, 79, 80, 106–108]. Similarly, ethanol is also a very common analyte, being identified in [10, 79–81, 106]. Among all the addressed works underlying this review, hexanal is the most common analyte to be identified [10, 24, 75, 79, 105, 106, 108, 109]. On the other hand, some volatile compounds were only identified in a small number of papers. Ammonia and acetophenone, for example, were only found by Vautz et al. [108]; 2-propanol was identified by Ireland et al. [110]; ethyl acetate was only detected by Moura et al. [10], and terpenes have been addressed by Rodríguez-Maecker et al. [82], with a large group of specific analytes, such as limonene, α-pinene, and β-pinene being identified in this work. Atrazine and simazine have been stressed in the work by Kalhor et al. [111]. Generally speaking, it is possible to see identical results in independent studies with a similar goal, which gives consistency to the IMS technique. For instance, being the detection of human metabolites as the main goal, some VOCs were found to be characteristic of human presence, namely, nonanal, octanal, and acetone, all detected in four of the addressed studies [24, 75, 108, 109]. As mentioned, acetone is a common air compound; however, nonanal and octanal seem to be human-characteristic. Benzaldehyde, heptanal, acetic acid, 2-pentanone, and decanal were identified in at least two independent studies on human emanated analytes, [24, 75, 105, 108, 109], proving that they should be targeted with a more profound study and, again, showing the IMS results consistency. Not being able to exhaustively analyze all the addressed works, Table S2 in the Supplementary Materials, summarizes all the identified VOCs by ion mobility spectrometry, enabling a direct comparison among independent works.

2.2.2 VOCs Quantification Through IMS

Moving from the sampling procedures and VOCs identification to their quantification, some scientific work has been done regarding the issue of the establishment of calibration protocols for IMS. Unfortunately, the relation between the VOCs concentration and the signal measured at the Faraday plate is a rather complex topic, which involves kinetics and thermodynamics. At this point, it should be considered that, as mentioned, one of the main limitations for the quantification through IMS is the humidity present in the drift tube, which can affect the IMS sensitivity [112]. Another issue that should be considered is that IMS presents some limitations regarding the analysis of

high-concentration compounds due to the saturation of the ionization source and the depletion of reactant ions. IMS devices that use radioactive ionization sources, like tritium or nickel sources, present a linear behavior for concentration versus intensity but solely for very low concentration levels. However, when the concentration is seen to increase, the calibration curve exhibits a plateau, limiting the concentration range of analysis. In this way, a typical calibration curve for this type of IMS has a logarithmic behavior [113]. For IMS devices that do not use radioactive ionization sources, like the ultraviolet (UV)—IMS, the calibration models for the concentration/intensity relationship have been reported as linear [114].

The VOCs quantification through IMS is a rather complex process with several variables to be considered; nonetheless, Puton et al. described pretty well the theory behind the relation of a VOC concentration and the magnitude of the detected signal, with detailed information and a careful approach, for the scenario of a spectrum presenting contributions from the RIP (r) signal and stable monomer (m) and dimer (m2) signals, without any analyte decomposition during the periods of ionization and drift [115]. Considering v_i the drift velocity for ion of a given kind i of ions, and t the time, the ion concentration n_i in the reaction region is obtained by the following balance equation:

$$\frac{\partial n_i}{\partial t} = div\left(n_i v_i\right) + D_i \Delta n_i + P_i - L_i = 0 \tag{18}$$

In Eq. 18, D_i represents the diffusion coefficient, P_i is the component representing the resulting ions from the ionization, and L_i corresponds to the rate of ions loss due to recombination between them.

Considering k_{rM} and k_{mM}, the constant rates of monomer and dimer formation, respectively represented by Eqs. 10 and 11, and since the signals in consideration are just the RIP (r), the monomer (m), and the dimer (m2) of a single analyte M, Eq. 18 can be solved for each of these ions, as follows:

$$\frac{\partial n_r}{\partial x} = -\frac{k_{rM} n_M}{K_r E} + \frac{N_0}{K_r E}; n_r(0) = 0 \tag{19a}$$

$$\frac{\partial n_m}{\partial x} = \left(\frac{k_{rM} n_M}{K_r E}\right) n_r - \left(\frac{k_{mM} n_M}{K_m E}\right) n_m; n_m(0) = 0 \tag{19b}$$

$$\frac{\partial n_{m2}}{\partial x} = \left(\frac{k_{mM} n_M}{K_{m2} E}\right) n_m; n_{m2}(0) = 0 \tag{19c}$$

In the set of Eq. 19, x is the drift tube length, the electric field is represented by E, K_i is the ion mobility constant of the type I of ions, and N_0 corresponds to the rate of reactant ions production. By solving this set of equations, it is possible to obtain the expression for the concentration of RIP (n_r), monomer (n_m), and dimer (n_{m2}), as follows:

$$n_r = \frac{N_0}{k_{rM} n_M}\left(1 - exp\left(-a_r n_M x\right)\right) \tag{20a}$$

$$n_m = \frac{N_0}{k_{nM} n_M}\left(1 - \frac{a_m exp\left(-a_r x n_m\right) - a_r exp\left(-a_m x n_m\right)}{a_m - a_r}\right) \tag{20b}$$

$$n_{m2} = \frac{N_0 a_{m2}}{k_{mM} n_M}\left(x n_M - \frac{a_r + a_m}{a_r a_m} + \frac{a_m^2 exp\left(-a_r x n_M\right) - a_r^2 exp\left(-a_m x n_M\right)}{a_r a_m\left(a_m - a_r\right)}\right) \tag{20c}$$

where a_r, a_m and a_{m2} are constants given by:

$$a_r = \frac{k_{rM}}{K_r E} \tag{21a}$$

$$a_m = \frac{k_{mM}}{K_m E} \tag{21b}$$

$$a_{m2} = \frac{k_{mM}}{K_{m2} E} \tag{21c}$$

Once theoretically defined the concentration values, their relationship with the signal detected at the Faraday plate is then given by:

$$S_i = \gamma K_i n_i\left(x_{RR}\right) \tag{22}$$

where γ is a proportionality constant, and x_{RR} is the length of the reaction section inside the ionization chamber. The set of Eq. 19 and Eq. 20 shows that a calibration curve relating the concentration, and the signal intensity values is rather complex and not straightforward to deal with. By analyzing each contribution individually, it is expected that the intensity of the detected signal from RIP decreases with concentration since the reactant ions are being used for monomers and dimers formation. Regarding the monomer and dimer behaviors, it is expected the monomer intensity to increase with the increase of concentration, but due to the increase of dimer intensity, the monomer intensity starts decreasing after a certain limit. Figure 6 sketches the characteristic behavior of RIP (blue line), monomer (red line), and dimer (black line) for the relationship between their respective concentration and intensity, for a generic scenario with arbitrary units [115].

The dimer behavior is the more complex one. Considering Eqs. 20c and 22, the relationship between the concentration and the dimer relative intensity can be expressed by the equation.

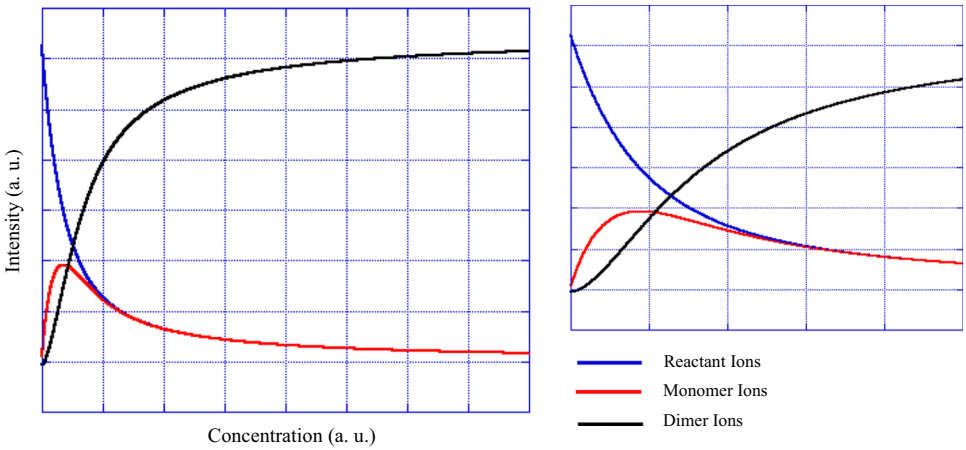

Fig. 6 Curves of the relationship between concentration and intensity for RIP, monomer, and dimer signals

$$S_{m2} = \gamma K_{m2} n_{m2}(x_{RR}) = \gamma K_{m2}(x_{RR})\left(\frac{N_0 a_{m2}}{k_{mM} n_M}\left(x n_M - \frac{a_r + a_m}{a_r a_m} + \frac{a_m^2 exp(-a_r x n_M) - a_r^2 exp(-a_m x n_M)}{a_r a_m (a_m - a_r)}\right)\right) \quad (23)$$

For better analysis, Eq. 23 can be further simplified and represented by:

$$S_{m2} = A1 - \frac{A2}{n_M} + \frac{A3}{n_M} exp(-A4 * n_M) - \frac{A5}{n_M} exp(-A6 * n_M) \quad (24)$$

where:

$$A1 = \frac{\gamma K_{m2}(x_{RR}) N_0 a_{m2} x}{k_{mM}} \quad (25a)$$

$$A2 = \frac{\gamma K_{m2}(x_{RR}) N_0 a_{m2}(a_r + a_m)}{k_{mM} a_r a_m} \quad (25b)$$

$$A3 = \frac{\gamma K_{m2}(x_{RR}) N_0 a_{m2} a_m^2}{k_{mM}(a_r a_m (a_m - a_r))} \quad (25c)$$

$$A4 = a_r x \quad (25d)$$

$$A5 = \frac{\gamma K_{m2}(x_{RR}) N_0 a_{m2} a_r^2}{k_{mM}(a_r a_m (a_m - a_r))} \quad (25e)$$

$$A6 = a_m x \quad (25f)$$

In this way, it is clear that the dimer behavior is composed of three main parcels which have been plotted in the graph in Fig. 7. Essentially, it represents the three parcels: a hyperbola (red line), two exponential-like functions (blue and green lines), and the complete dimer curve (black line).

Considering the several procedures for VOC calibration through IMS, the most commonly found approach in scientific works consists of the acquisition and analysis of predeveloped multi-compound calibration mixtures. In such a procedure, a mixture of several liquid compounds with their respective concentration values is created by certified manufacturers. The intensity values measured from such mixtures can be directly related to the respective concentrations delivered by the manufacturer, defining a calibration equation. This was the chosen approach for the calibration process of all the identified human metabolites in Mochalski et al.'s work. With the concentration ranging from 10 ppb_v to 100 ppm_v for each analyte, the authors were able to calibrate and define concentration values for all the skin and breath VOCs. Lower concentrations were also measured by diluting the original mixtures at ratios of 1:2000 and 1:3000 [24]. Since the employed mixtures are developed by certified companies that comply with all the scientific regulations, they tend to be among the most accurate ways of calibrating one or several analytes, which describes a major advantage for these procedures. Besides the mentioned advantages, the standards of analytes should not be blindly trusted. As with any other process, the production of analyte mixtures is not invulnerable to inaccuracies, so they must be previously checked and, if possible, tested against previously certified samples. The mixtures' prices, typically in the range of some hundreds, represent an equally relevant disadvantage of this procedure.

The exponential dilution method is another common approach for attaining different concentration values in a sample. This process consists of inserting a very small but known amount of compound in a much large container and leaving it for headspace equilibrium, enabling the obtention of the desired concentration value. Successive dilutions of the same sample, using a gas blending device, lead the concentration to exponentially decrease, enabling the plotting of the calibration curve. Bocos-Bintintan et al. used this methodology for carbon disulfide

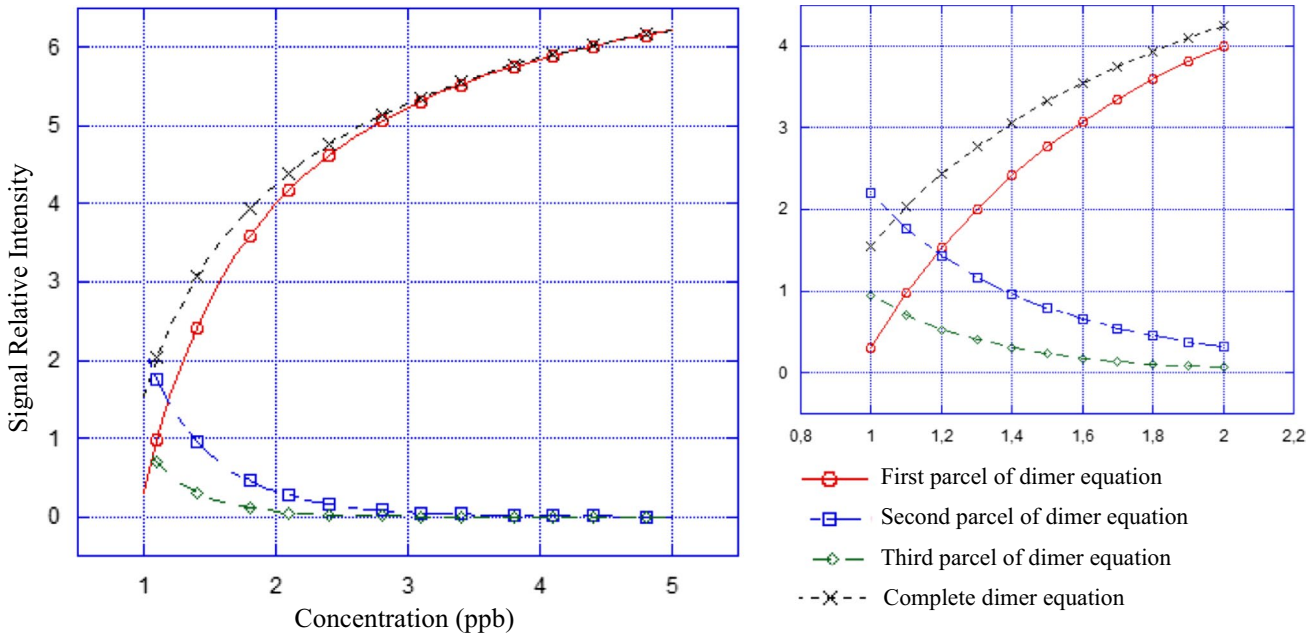

Fig. 7 Representation of the three main parcels, hyperbola (red line) and two exponential-like functions (blue and green line) that comprise the dimer equation (black line) for concentration vs. relative intensity

calibration [85]. Having ppm_v as target levels, the authors achieved concentration values between 0.10 ppm_v and 15 ppm_v by diluting, for example, 10 µL of carbon disulfide in a 10.6 L container filled with air. During the quantitative analysis of Gao et al.' work, the desired calibration standards of 50, 100, 200, 500, and 1000 ng/L were achieved by diluting pre-prepared mixtures with known concentrations, in ultrapure deionized water, which was later volatilized. A calibration curve was plotted for the five mentioned points, to represent intensity against concentration values [107]. One of the main limitations of sample preparation and respective dilutions is the volatilization process; however, some gas generator devices can simplify this procedure. In fact, for such a goal, a vaporizer was used by Ruzsanyi et al., which enabled the diluted samples' volatilization and analyses within the concentration range of 0.2–30 ppb_v [101].

Being one of the addressed sample preparation techniques, PTFE permeation tubes are also frequently used for calibration purposes. As already mentioned, these tubes are typically filled with pure compounds, and then, by controlling temperature and flow, it is possible to calibrate their emission rates and respective concentrations. For example, permeation tubes have been used by Ruzsanyi et al. not only for VOC identification but also for quantification [75]. This procedure allowed authors to attain a concentration range of 50–200 ppb_v for target compounds, such as acetaldehyde, propanol, acetone, or isoprene. Similarly, Ireland et al. described a complete experiment for 2-propanol calibration with 14 cm length PTFE permeation tubes filled with approximately 3–4 mL [110]. Reyes-Garcés et al., in their turn, also used permeation tubes to plot calibration curves for α-pinene ($y(x) = 251.8x + 186.3$, $R^2 = 0.9962$), limonene ($y(x) = 318.4x + 15.7$, $R^2 = 0.9973$), and acetone ($y(x) = 484.7x + 100.2$, $R^2 = 0.9962$). These linear calibration curves equations were attained because authors only considered the linear section of the data; in other words, they are only suitable for the lower values of concentration (linear section of the graph) considered in the study and not for the overall dataset [113]. Fernandes et al. filled 2 cm long PTFE permeation tubes with 0.2 mL of 2-hexanone having as the main goal, the plot of the respective calibration curve. The tubes were kept inside a thermogravimetric device to be continuously controlled regarding temperature, weight, and flow. The authors identified a monomer and a dimer of the 2-hexanone in the three-dimensional IMS spectrum. For the specific case of 2-hexanone, the random M compound in Eqs. 10 (monomer) and 11 (dimer) is now substituted by the compound under analysis, 2-hexanone, leading to the formation equation of the 2-hexanone monomer, Eq. 26, and to the formation equation of the 2-hexanone dimer, Eq. 27 [99].

$$C_6H_{12}O + \left(H_2O\right)_n H^+ \leftrightarrow C_6H_{12}O\left(H_2O\right)_{n-x} H^+ + xH_2O \tag{26}$$

$$C_6H_{12}O + \left(H_2O\right)_{n-x}H^+ \leftrightarrow \left(C_6H_{12}O\right)_2\left(H_2O\right)_{n-(x+i)}H^+ + iH_2O \quad (27)$$

As mentioned, IMS devices that use a radioactive ionization source have a limitation in analyzing higher concentrations. In these scenarios, the calibration curve obtained for the relationship between concentration and intensity tends to a plateau and is expressed in logarithmic terms. Figure S3 of the Supplementary Materials represents the calibration curve achieved for 2-hexanone by Fernandes et al., whose data was fitted with a logarithmic equation. The intensity values correspond to the sum of the IMS signal volumes of both the monomer and dimer of the 2-hexanone. The formation of protonated dimers and even larger clusters are typical in IMS measurements, and this is the scenario for 2-hexanone. In this way, the total concentration emitted by the permeation tubes has to be related to the sum of intensities and, specifically, peak volumes, of both monomer and dimer of 2-hexanone. The corresponding calibration equation and respective R^2 are included in the graph of Figure S3 [99]. Nonetheless, the results are debatable since the logarithmic curve has no scientific base to be suitable for IMS data modeling. The correct approach considered by the authors should have been the one addressed in Eqs. 18, 19, 20, 21, 22, 23, 24, and 25, although, as mentioned, it is not a straightforward process, and it is a rather complex fitting.

As seen, calibration procedures for VOCs quantification by IMS are still very demanding research topics; however, some work is being done about it. This might not be a major drawback as IMS is suited to detect traces (say ppt_v to ppb_v) of VOCs rather than moderate or high concentration levels, for which the device has to be adjusted. Nonetheless, the calibration procedures for IMS still require a much deeper study before being completely established and understood.

Taking into consideration all the independent studies and respective results included here, ion mobility spectrometry seems to have more advantages than disadvantages regarding the detection, identification, and quantification of VOCs.

2.3 IR Versus IMS

Taking into consideration the characteristics of each technique and all the differences between infrared spectroscopy and ion mobility spectrometry regarding VOCs detection, it is possible to confront them, in a comparative way. This comparison is summarized in Table 1.

As mentioned, infrared spectroscopy detection limits are not low enough to allow the detection of traces of VOCs in air samples; however, its use with additional techniques or methodologies, like photo-ionization detectors or chemo-responsive dyes, enables VOCs detection and quantification (quantification occurs at a minimum level of ppm_v or, rarely, at ppb_v). Ion mobility spectrometry can detect analytes at levels of ppb_v and even ppt_v; nonetheless, it only enables the analysis of volatile samples, while IR spectroscopy can analyze all kinds of samples (solids, liquids, gaseous). On the other hand, IMS can only evaluate organic compounds; however, IR spectroscopy applies to a much larger range of analytes. Regarding sample preparation, IMS does not require special preparation or additional techniques. It can even perform in-situ air samples analysis. In its turn, infrared spectroscopy generally requires a more complex sample presentation or even the use of additional methodologies. For both techniques, measurements can be carried out in an almost real-time regime, with both techniques requiring more or less complex spectra processing after the analysis, as well as trained users for both analysis and data assessment. Coincidently, the humidity levels during the analyses are a limitation and an issue for both techniques. For quantitative analysis of the compounds, infrared spectroscopy provides a well-established, direct, and linear relation between absorbance (or transmittance) and concentration levels while in IMS, calibration curves necessary to convert intensity in concentration levels still require some research and protocol development. The costs of both techniques are

Table 1 Direct comparison between infrared spectroscopy and ion mobility spectrometry

Technique characteristic	Infrared spectroscopy	Ion mobility spectrometry
Detection limits	ppm_v–ppb_v	ppb_v–ppt_v
Sample type	Solid/liquid/gaseous	Volatile
Compounds	Organic/inorganic	Organic
Sample preparation	Frequently necessary	Rarely necessary
Additional techniques	Necessary	Necessary
Real-time	Quasi	Quasi
Pattern recognition	Good	Good
Quantitative procedure	Well-established	Under development
Trained staff requirement	High	Low
Portability	Yes	Yes
Cost	High	High

Table 2 Ion mobility spectrometry SWOT analysis

Ion mobility spectrometry SWOT table	
Strengths	Weaknesses
Detection limits	Sample type
Concentration range	Lack of a library of analytes
Almost real-time	Lack of calibration procedures
In-situ measurement	Price
Adaptability to distinct scenarios	
Portability	
System's simplicity	
Opportunities	Threats
Possible coupling with additional techniques	Exposure to hazardous environments leading to the adulteration of the sample
Calibration protocol development	Possibility of device damages during in-loco measurements
Machine learning algorithm implementation	Costs of maintenance
New and distinct applications	

relatively elevated, and concerning portability and applicability to distinct scenarios, an ion mobility spectrometer can be used in practically every location for off-line or on-line analysis; however, an infrared spectrometer does not offer such ease for location-specific measurements and requires additional preparation before the analysis procedure. Even having the possibility of assembly integrated IR systems for in-loco measurements, their complexity is much higher when compared with the IMS device assembly.

To help clarify even more the most recent of the addressed techniques, ion mobility spectrometry, a SWOT analysis was carried out, and it is featured in Table 2. The SWOT analysis is an expeditious strategic technique that enables the assessment of strengths (S), weaknesses (W), opportunities (O), and threats (T) of the subject under analysis. When applied to characterize an analytical technique, it allows for portraying its main advantages (strengths), disadvantages (weaknesses), issues requiring development (opportunities), and topics that may negatively influence or affect both the measurements/results and the device itself (threats).

3 Conclusions

Anthropogenic volatile organic compounds, if present in a location at toxic concentration levels, may represent a threat to the environment and all living beings. Their presence in both indoor and outdoor environments can be equally hazardous to people due to their capability of passing through biological tissues; in this way, the detection, identification, and quantification of VOCs is a mandatory issue that must be carefully addressed.

In this work, both advantages and disadvantages of infrared spectroscopy and ion mobility spectrometry as suitable techniques for VOC analysis and assessment have been addressed. A deep search of the literature was carried out on each technique having in view the practical applications. Relevant scientific studies were selected for a careful serialization, and the most pertinent were reviewed in this paper. Different methods of sample preparation were included, as well as tables summarizing the VOCs studied in each paper, for both techniques. The quantitative analysis approached by the main works was also referred to and included in the respective sections. A final chapter summarizing the general comparison of both infrared spectroscopy and ion mobility spectrometry was included in the review.

The addressed techniques revealed positive and negative points concerning VOC assessment. To decide which one is the most suitable, you need a deeper knowledge of the scenario in which the technique is going to operate, the sample's state of matter and type of compounds that are intended to be measured, and what are the main goals of the study in question. Regarding IR spectroscopy, due to its poorer detection limits than the IMS limits, the necessity of sample preparation, and the requirement of additional techniques or procedures, this analytical technique seems to have several limitations concerning VOCs detection, identification, and quantification. Nonetheless, IMS detection limits of ppb_v-ppt_v, portability, analytical simplicity, and high sensitivity, among all the mentioned features, largely outweigh the maintenance costs and the lack of solutions for non-volatile sample analysis. In this way, IMS seems to be the best choice, instead of IR, for most of the scenarios.

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References

1. Solomons, T.W., Fryhle, C.: Organic chemistry. John Wiley & Sons Inc, New York, United States of America (2009). (**ISBN: 9781119248972**)
2. Carey, F., Giuliano, R.: Organic chemistry. McGraw-Hill Education, New York, United States of America (2017). ISBN-10: 0073402745
3. Klein, D.: Organic chemistry. John Wiley and Sons Inc, New York, United States of America (2017). (**ISBN: 978-1-119-44425-1**)
4. Bruice, P.: Organic chemistry. Pearson Education, New York, United States of America (2017)
5. Directive 2004/42/CE of the European parliament and of the council of 21 April 2004 on the limitation of emissions of volatile organic compounds due to the use of organic solvents in certain paints and varnishes and vehicle refinishing products. Official Journal of the European Union L143/87, 87–96 (2004)
6. Cumeras, R., Correig, X.: Volatile organic compound analysis in biomedical diagnosis applications. Apple Academic Press Inc, New York, United States of America (2019). (**ISBN: 9781774634264**)
7. Hester, R., Harrison, R.: Issues in environmental science and technology - volatile organic compounds in the atmosphere. The Royal Society of Chemistry, Cambridge, United Kingdom (1995). (**ISBN: 978-0-85404-215-9**)
8. Koppmann, R.: Volatile organic compounds in the atmosphere. Blackwell Publishing, Oxford, United Kingdom (2007). (**ISBN: 978-1-405-13115-5**)
9. Montero-Montoya, R., López-Vargas, R., Arellano-Aguilar, O.: Volatile organic compounds in air: sources, distribution, exposure and associated illness in children. Ann. Glob. Health **84**, 225–238 (2018). https://doi.org/10.29024/aogh.910
10. Moura, P., Vassilenko, V., Fernandes, J., Santos, P.: Indoor and outdoor air profiling with GC-IMS. In : Technological Innovation for Life Improvement, DoCEIS 2020. IFIP Advances in Information and Communication Technology, 2020, Caparica, Portugal 577:437–444 (2020). https://doi.org/10.1007/978-3-030-45124-0_43
11. Baurès, E., Blanchard, O., Mercier, F., Surget, E., le Cann, P., Rivier, A., Gangneux, J.-P., Florentin, A.: Indoor air quality in two French hospitals: measurement of chemical and microbiological contaminants. Sci. Total Environ. **642**, 168–179 (2018). https://doi.org/10.1016/j.scitotenv.2018.06.047
12. Chan, C., Lee, S., Chan, W., Ho, K., Tian, L., Lai, S., Li, Y., Huang, Y.: Characterisation of volatile organic compounds at hotels in Southern China. Indoor Built Environ. **20**, 420–429 (2011). https://doi.org/10.1177/1420326X11409458
13. Śmiełowska, M., Marć, M., Zabiegala, B.: Indoor air quality in public utility environments - a review. Environ. Sci. Pollut. Res. **24**, 11166–11176 (2017). https://doi.org/10.1007/s11356-017-8567-7
14. Yang, W., Sohn, J., Kim, J., Son, B., Park, J.: Indoor air quality investigation according to age of the school buildings in Korea. J. Environ. Manage. **90**, 348–354 (2009). https://doi.org/10.1016/j.jenvman.2007.10.003
15. Li, J., Gutierrez-Osuna, R., Hodges, R., Luckey, G., Crowell, J., Schiffman, S., Troy Nagle, H.: Using field asymmetric ion mobility spectrometry for odor assessment of automobile interior components. IEEE Sens. J. **16**, 5747–5756 (2016). https://doi.org/10.1109/JSEN.2016.2568209
16. Ismail, A. R., Rani, M. R. A., Makhbul, Z. K. M., Usman, I. M. S., Meier, C., Rahman, M. N. A., Sopian, K., Tahir, M. M.: Assessment of environmental factors at automotive industry: a case study at car body assembly line. In: 2nd WSEAS/IASME International Conference on Energy Planning, Energy Saving, pp. 76–82. Environmental Education (EPESE'08), Corfu, Greece (2008)
17. Wah, C., Yu, F., Kim, J.: Building pathology, investigation of sick building - VOC emissions. Indoor. Built. Environ. **19**, 30–39 (2010). https://doi.org/10.1177/1420326X09358799
18. Crump, D., Squire, R., Yu, C.: Sources and concentrations of formaldehyde and other volatile organic compounds in the indoor air of four newly built unoccupied test houses. Indoor Built Environ. **6**, 45–55 (1997). https://doi.org/10.1159/000463298
19. Kagi, N., Fujii, S., Tamura, H., Namiki, N.: Secondary VOC emissions from flooring material surfaces exposed to ozone or UV irradiation. Build. Environ. **44**, 1199–1205 (2009). https://doi.org/10.1016/j.buildenv.2008.09.004
20. Yu, C., Crump, D., Brown, V.: Exposure risk assessment of the emissions of wood preservative chemicals in indoor environments. CLEAN **37**, 466–474 (2009). https://doi.org/10.1002/clen.200900046
21. Guo, H., Murray, F., Lee, S.C., Wilkinsin, S.: Evaluation of emissions of total volatile organic compounds from carpets in an environmental chamber. Build. Environ. **39**, 179–187 (2004). https://doi.org/10.1016/j.buildenv.2003.08.015
22. Costello, B. D. L., Amann, A., Alkateb, H., Flynn, C., Filipiak, W., Khalid, T., Osborne, D., Ratcliffe, N. M.: A review of the volatiles from the healthy human body. J. Breath Res. **8**, 014001 (2014). https://doi.org/10.1088/1752-7155/8/1/014001
23. Molhave, L., Bach, B., Pederson, O.F.: Human reactions to low concentrations of volatile organic compounds. Environ. Int. **12**, 167–175 (1986). https://doi.org/10.1016/0160-4120(86)90027-9
24. Mochalski, P., Wiesenhofer, H., Allers, M., Zimmermann, S., Guntner, A., Pineau, N., Lederer, W., Agapiou, A., Mayhew, C.A., Ruzsanyi, V.: Monitoring of selected skin- and breath-borne volatile organic compounds emitted from the human body using gas chromatography ion mobility spectrometry (GC-IMS).

J. Chromatogr. **1076**, 29–34 (2018). https://doi.org/10.1016/j.jchromb.2018.01.013
25 Van Berkel, J.J.B.N., Dallinga, J.W., Möller, G.M., Godschalk, R.W.L., Moonen, E.J., Wouters, E.F.M., Van Schooten, F.J.: A profile of volatile organic compounds in breath discriminates COPD patients from controls. Respir. Med. **104**(Elsevier), 557–563 (2010). https://doi.org/10.1016/j.rmed.2009.10.018
26. Haick, H., Broza, Y., Mochalski, P., Ruzsanyi, V., Amann, A.: Assessment, origin, and implementation of breath volatile cancer markers. Chem. Soc. Rev. **43**, 1423–1449 (2013). https://doi.org/10.1039/C3CS60329F
27. Di Francesco, F., Fuoco, R., Trivella, M., Ceccarini, A.: Breath analysis: trends in techniques and clinical applications. Microchem. J. **79**, 405–410 (2005). https://doi.org/10.1016/j.microc.2004.10.008
28. Miekisch, W., Schubert, J., Noeldge-Schomburg: Diagnostic potential of breath analysis - focus on volatile organic compounds. Clin. Chim. Acta **347**, 25–39 (2004). https://doi.org/10.1016/j.cccn.2004.04.023
29. Risby, T.H., Solga, S.F.: Current status of clinical breath analysis. Appl. Phys. B **85**, 421–426 (2006). https://doi.org/10.1007/s00340-006-2280-4
30. Günzler, H., Williams, A.: Handbook of analytical techniques. WILEY-VCH Verlag GmbH, Weinheim, Germany (2001). (**ISBN: 978-3-527-61832-3**)
31. Silverstein, R., Webster, F., Kiemle, D.: Spectrometric identification of organic compounds. John Wiley & Sons Inc, New York, United States of America (2005). (**ISBN: 978-0-470-61637-6**)
32. Larkin, P.: IR and Raman spectroscopy - principles and spectral interpretation. Elsevier Inc, Oxford, United Kingdom (2011). (**ISBN: 9780123869845**)
33. Thompson, J.: Infrared spectroscopy. Taylor & Francis Group, Danvers, Massachusetts, United States of America (2018). https://doi.org/10.1201/9781351206037
34. Stuart, B.: Infrared spectroscopy: fundamentals and applications. John Wiley & Sons, Ltd., New York, United States of America (2004). ISBN: 978–0–470–85428–0
35. Smith, B.: Fundamentals of fourier transform infrared spectroscopy. CRC Press, Taylor & Francis Group, Boca Raton, Florida, United States of America (2011). https://doi.org/10.1201/b10777
36. Mantsch, H., McElhaney, R.: Applications of infrared spectroscopy to biology and medicine. J. Mol. Struct. **217**, 347–362 (1990). https://doi.org/10.1016/0022-2860(90)80374-S
37. Kutsanedzie, F., Hao, L., Yan, S., Ouyang, Q., Chen, Q.: Near infrared chemo-responsive dye intermediaries spectra-based in-situ quantification of volatile organic compounds. Sens. Actuators, B Chem. **254**, 597–602 (2018). https://doi.org/10.1016/j.snb.2017.07.134
38. Dettenrieder, C., Türkmen, D., Mattson, A., Österlund, L., Karlsson, M., Mizaikoff, B.: Determination of volatile organic compounds in water by attenuated total reflection infrared spectroscopy and diamond-like carbon coated silicon wafers. Chemosensors **8**, 75 (2020). https://doi.org/10.3390/chemosensors8030075
39. Kim, E., Lim, Y.: Effective preconcentration of volatile organic compounds from aqueous solutions with polydimethylsiloxane-coated filter paper. Microchem. J. **145**, 979–987 (2019). https://doi.org/10.1016/j.microc.2018.12.010
40. Lu, R., Li, W., Mizaikoff, B., Katzir, A., Raichlin, Y., Sheng, G., Yu, H.: High-sensitivity infrared attenuated total reflectance sensors for in situ multicomponent detection of volatile organic compounds in water. Nat Protocol **11**, 377–386 (2016). https://doi.org/10.1038/nprot.2016.013
41. Radica, F., Ventura, G., Malfatti, L., Guidi, M., D'Arco, A., Grilli, A., Marcelli, A., Innocenzi, P.: Real-time quantitative detection of styrene in atmosphere in presence of other volatile organic compounds using a portable device. Talanta **233**, 122510 (2021). https://doi.org/10.1016/j.talanta.2021.122510
42. Kohl, L., Koskinen, M., Rissanen, K., Haikarainen, I., Polvinen, T., Hellén, H., Pihlatie, M.: Interferences of volatile organic compounds (VOCs) on methane concentration measurements. Biogeosciences **16**, 3319–3332 (2019). https://doi.org/10.5194/bg-16-3319-2019
43. Formela, K., Marc, M., Wang, S., Saeb, M.: Interrelationship between total volatile organic compounds emissions, structure and properties of natural rubber/polycaprolactone bio-blends cross-linked with peroxides. Polym. Testing **60**, 405–412 (2017). https://doi.org/10.1016/j.polymertesting.2017.04.024
44. Scharko, N., Oeck, A., Tonkyn, R., Baker, S., Lincoln, E., Chong, J., Corcoran, B., Burke, G., Weise, D., Myers, T., Banach, C., Griffith, D., Johnson, T.: Identification of gas-phase pyrolysis products in a prescribed fire: first detections using infrared spectroscopy for naphthalene, methyl nitrite, allene, acrolein and acetaldehyde. Atmos. Meas. Tech. **12**, 763–776 (2019). https://doi.org/10.5194/amt-12-763-2019
45. Ju, W., Lu, C., Zhang, Y., Jiang, W., Wang, J., Lu, Y., Hong, F.: Characteristic wavelength selection of volatile organic compounds infrared spectra based on improved interval partial least squares. J. Innov. Opt. Health Sci. **12**, 1950005 (2019). https://doi.org/10.1142/S1793545819500056
46. Gao, T., Andino, J., Alvarez-Idaboy, J.: Computational and experimental study of the interactions between ionic liquids and volatile organic compounds. Phys. Chem. Chem. Phys. **12**, 9830–9838 (2010). https://doi.org/10.1039/c003386c
47. Lampert, C.: Analysis of volatile organic compounds in air samples by infrared spectroscopic analysis of sorbent tube samples - Master Thesis., Middle Tennessee State University (2013). Corpus ID: 102938946
48. Maiti, K., Lewton, M., Fill, E., Apolonski, A.: Sensitive spectroscopic breath analysis by water condensation. J. Breath Res. **12**, 046003 (2018). https://doi.org/10.1088/1752-7163/aad207
49. Jiao, L., Guo, Y., Chen, J., Zhao, X., Dong, D.: Detecting volatile compounds in food by open-path Fourier-transform infrared spectroscopy. Food Res. Int. **119**, 968–973 (2019). https://doi.org/10.1016/j.foodres.2018.11.042
50. Chen, M., Duh, J., Shie, R., Weng, J., Hsu, H.: Dynamic real-time monitoring of chloroform in an indoor swimming pool air using open-path Fourier transform infrared spectroscopy. Indoor Air **26**, 457–467 (2016). https://doi.org/10.1111/ina.12215
51. Wu, C., Wu, T., Hashmonay, R., Chang, S., Wu, Y., Chao, C., Hsu, C., Chase, M., Kagann, R.: Measurement of fugitive volatile organic compound emissions from a petrochemical tank farm using open-path Fourier transform infrared spectrometry. Atmos. Environ. **82**, 335–342 (2014). https://doi.org/10.1016/j.atmosenv.2013.10.036
52. Huang, J., Hartmann, H., Hellén, H., Wisthaler, A., Perreca, E., Weinhold, A., Rücker, A., Dam, N., Gershenzon, J., Trumbore, S., Behrendt, T.: New perspectives on CO2, temperature, and light effects on BVOC emissions using online measurements by PTR-MS and cavity ring-down spectroscopy. Environ. Sci. Technol. **52**, 13811–13823 (2018). https://doi.org/10.1021/acs.est.8b01435
53. Maity, A., Maithani, S., Pradhan, M.: Chapter 3 - cavity ring-down spectroscopy: recent technological advances and applications. In: Gupta, V., Ozaki, Y. (eds.) Molecular and Laser Spectroscopy 2, pp. 83–120. Elsevier, Oxford, England, United Kingdom (2020). https://doi.org/10.1016/B978-0-12-818870-5.00003-4
54. Berden, G., Peeters, R., Meijer, G.: Cavity ring-down spectroscopy: experimental schemes and applications. Int. Rev. Phys. Chem. **19**, 565–607 (2010). https://doi.org/10.1080/014423500750040627

55. Maithani, S., Pradhan, M.: Cavity ring-down spectroscopy and its applications to environmental, chemical and biomedical systems. J. Chem. Sci. **132**, 114 (2020). https://doi.org/10.1007/s12039-020-01817-x
56. Gkinis, V., Popp, T., Johnsen, S., Blunier, T.: A continuous stream flash evaporator for the calibration of an IR cavity ring-down spectrometer for the isotopic analysis of water. Isot. Environ. Health Stud. **46**, 463–475 (2010). https://doi.org/10.1080/10256016.2010.538052
57. Sahay, P., Scherrer, S., Wang, C.: Measurements of the weak UV absorptions of isoprene and acetone at 261–275 nm using cavity ringdown spectroscopy for evaluation of a potential portable ringdown breath analyzer. Sensors **13**, 8170–8187 (2013). https://doi.org/10.3390/s130708170
58. Pradhan, M., Lindley, R., Grilli, R., White, J., Martin, D., Orr-Ewing, A.: Trace detection of C2H2 in ambient air using continuous wave cavity ring-down spectroscopy combined with sample pre-concentration. Appl. Phys. B **90**, 1–9 (2008). https://doi.org/10.1007/s00340-007-2833-1
59. Zhou, S., Han, Y., Li, B.: Simultaneous detection of ethanol, ether and acetone by mid-infrared cavity ring-down spectroscopy at 3.8 µm. Appl. Phys. B **122**, 187 (2016). https://doi.org/10.1007/s00340-016-6465-1
60. Larracy, R., Phinyomark, A., Scheme, E.: Infrared cavity ring-down spectroscopy for detecting non-small cell lung cancer in exhaled breath. J. Breath Res. **16**, 026008 (2022). https://doi.org/10.1088/1752-7163/ac5e4f
61. Schmidt, F., Vaittinen, O., Metsälä, M., Kraus, P., Halonen, L.: Direct detection of acetylene in air by continuous wave cavity ring-down spectroscopy. Appl. Phys. B **101**, 671–682 (2010). https://doi.org/10.1007/s00340-010-4027-5
62. Evyapan, M., Hanoosh, W., Hassan, A.: Determination of volatile organic compounds by a novel polymer spin-coated thin film and surface plasmon resonance. Anal. Lett. **50**, 2579–2594 (2017). https://doi.org/10.1080/00032719.2017.1302463
63. Abdullahi, M., Hassan, M., Noor, Z., Ibrahim, R.: Integrated air stripping and non-thermal plasma system for the treatment of volatile organic compounds from wastewater: statistical optimization. Desalin. Water Treat. **6**, 1–12 (2015). https://doi.org/10.1080/19443994.2015.1076353
64. Mamaghani, A., Haghighat, F., Lee, C.: Gas phase adsorption of volatile organic compounds onto titanium dioxide photocatalysts. Chem. Eng. J. **337**, 60–73 (2018). https://doi.org/10.1016/j.cej.2017.12.082
65. Hong, Y., Huang, Y., Lee, I., Chiang, C., Lin, C., Jeng, H.: Assessment of volatile organic compounds and particulate matter in a dental clinic and health risks to clinical personnel. J. Environ. Sci. Health, Part A **50**, 1205–1214 (2015). https://doi.org/10.1080/10934529.2015.1055129
66. Fang, Y., Lakey, P., Riahi, S., McDonald, A., Shrestha, M., Tobias, D., Shiraiwa, M., Grassian, V.: A molecular picture of surface interactions of organic compounds on prevalent indoor surfaces: limonene adsorption on SiO2. Chem. Sci. **10**, 2906 (2019). https://doi.org/10.1039/C8SC05560B
67. Nespeca, M., Rodrigues, C., Santana, K., Maintinguer, S., Oliveira, J.: Determination of alcohols and volatile organic acids in anaerobic bioreactors for H2 production by near infrared spectroscopy. Int. J. Hydrogen Energy **42**, 20480–20493 (2017). https://doi.org/10.1016/j.ijhydene.2017.07.044
68. Owen-Reece, H., Smith, M., Elwell, C., Goldstone, J.: Near infrared spectroscopy. Br. J. Anaesth. **82**, 418–426 (1999). https://doi.org/10.1093/bja/82.3.418
69. Garde-Cerdán, T., Lorenzo, C., Alonso, G., Salinas, M.: Employment of near infrared spectroscopy to determine oak volatile compounds and ethylphenols in aged red wines. Food Chem. **119**, 823–828 (2010). https://doi.org/10.1016/j.foodchem.2009.07.026
70. Armenta, S., Alcala, M., Blanco, M.: A review of recent, unconventional applications of ion mobility spectrometry (IMS). Anal. Chim. Acta **703**, 114–123 (2011). https://doi.org/10.1016/j.aca.2011.07.021
71. Chen, T., Chen, X., Lu, D., Chen, B.: Detection of adulteration in Canola oil by using GC-IMS and chemometric analysis. Int. J. Anal. Chem. **2018**, 3160265 (2018). https://doi.org/10.1155/2018/3160265
72. Baumbach, J.I., Stach, J.: Ion mobility spectrometry - basic elements and applications. Int. J. Ion Mobil. Spectrom. **5**, 1–21 (2002)
73. Karpas, Z.: Applications of ion mobility spectrometry (IMS) in the field of foodomics. Food Res. Int. **54**, 1146–1151 (2012). https://doi.org/10.1016/j.foodres.2012.11.029
74. Romera, K., Fernandez-Maestre, R.: Ion mobility spectrometry: the diagnostic tool of third millennium medicine. Rev. Assoc. Med. Bras. **64**, 861–868 (2018). https://doi.org/10.1590/1806-9282.64.09.861
75. Ruzsanyi, V., Wiesenhofer, H., Ager, C., Herbig, J., Aumayr, G., Fischer, M., Renzler, M., Ussmueller, T., Lindner, K., Mayhew, C.: A portable sensor system for the detection of human volatile compounds against transnational crime. Sens. Actuators, B Chem. **328**, 129036 (2021). https://doi.org/10.1016/j.jchromb.2012.10.028
76. Eiceman, G., Karpas, Z., Hill, H., Jr.: Ion mobility spectrometry. CRC Press, Taylor & Francis Group, Boca Raton, FL, USA (2014). (**ISBN: 9781138199484**)
77. Santos, F. J., Galceran, M. T.: The application of gas chromatography to environmental analysis. Trends in Analytical Chemistry **21**, 672–685 (2002). https://doi.org/10.1016/S0165-9936(02)00813-0
78. Kanu, A., Hill Jr., H.: Ion mobility spectrometry detection for gas chromatography. J. Chromatogr. A **1177**, 12–27 (2008). https://doi.org/10.1016/j.chroma.2007.10.110
79. Levin, M., Lantsuzskaya, E.: Identification of volatile organic compounds by retention times and ion mobility spectra. J. Anal. Chem. **69**, 1153–1158 (2014). https://doi.org/10.1134/S1061934814120089
80. Yokoshiki, Y., Nakamoto, T.: Ternary gas mixture quantification using field asymmetric ion mobility spectrometry (FAIMS). Sensors **19**(13), 3007 (2019). https://doi.org/10.3390/s19133007
81. Jurado-Campos, N., Martín-Gómez, A., Saavedra, D., Arce, L.: Usage considerations for headspace-gas chromatography-ion mobility spectrometry as a suitable technique for qualitative analysis in a routine lab. J. Chromatogr. A **1640**, 461937 (2021). https://doi.org/10.1016/j.chroma.2021.461937
82. Rodríguez-Maecker, R., Vyhmeister, E., Meisen, S., Martinez, A., Kuklya, A., Telgheder, U.: Identification of terpenes and essentials oils by means of static headspace gas chromatography-ion mobility spectrometry. Anal. Bioanal. Chem. **409**, 6595–6603 (2017). https://doi.org/10.1007/s00216-017-0613-2
83. Vautz, W., Liedtke, S., Martin, B., Drees, C.: Data interpretation in GC-ion mobility spectrometry. Int. J. Ion Mobil. Spectrom. **21**, 97–103 (2018). https://doi.org/10.1007/s12127-018-0233-3
84 Vautz, W., Hariharan, C., Weigend, M.: Smell the change: on the potential of gas chromatography ion mobility spectrometry in ecosystem monitoring. Ecol. Evol. **9**, 4370–4377 (2019). https://doi.org/10.1002/ece3.3990
85. Bocos-Bintintan, V., Ratiu, I.: Hunting for toxic industrial chemicals: real-time detection of carbon disulfide traces by means of ion mobility spectrometry. Toxics **8**(4), 121 (2020). https://doi.org/10.3390/toxics8040121
86. Daris, R., St-Pierre, C.: Beta decay of tritium. Nucl. Phys. A **138**, 545–555 (1969). https://doi.org/10.1016/0375-9474(69)90237-1
87. Wilkins, C., Trimpin, S.: Ion mobility spectrometry - mass spectrometry. CRC Press, Taylor & Francis Group, Boca

Raton, Florida, United States of America (2011). (**ISBN: 9781138199095**)
88. Paglia, G., Astarita, G.: Ion mobility-Mass Spectrometry - Methods and Protocols. Humana Press, Springer, New York, United States of America (2020). https://doi.org/10.1007/978-1-0716-0030-6
89. Hill, H., Siems, W., Louis, R., McMinn, D.: Ion mobility spectrometry. Anal. Chem. **62**, 1201–1209 (1990). https://doi.org/10.1021/ac00222a001
90 Kaur-Atwal, G., O'Connor, G., Aksenov, A., Bocos-Bintintan, V., Thomas, P., Creaser, C.: Chemical standards for ion mobility spectrometry: a review. Int. J. Ion Mobil. Spectrom. **12**, 1–14 (2009). https://doi.org/10.1007/s12127-009-0021-1
91. Krylov, E., Nazarov, E., Miller, R., Tadjikov, B., Eiceman, G.: Field dependence of mobilities for gas-phase-protonated monomers and proton-bound dimers of ketones by planar field asymmetric waveform ion mobility spectrometer (PFAIMS). J. Phys. Chem. **106**, 5437–5444 (2002). https://doi.org/10.1021/jp020009i
92. Gabelica, V., Marklund, E.: Fundamentals of ion mobility spectrometry. Curr. Opin. Chem. Biol. **42**, 51–59 (2018). https://doi.org/10.1016/j.cbpa.2017.10.022
93 Creaser, C.S., Griffiths, J.R., Bramwell, C.J., Noreen, S., Hill, C.A., Paul Thomas, C.L.: Ion mobility spectrometry: a review. Part 1. Structural analysis by mobility measurement. Roy. Soc. Chem. **129**, 984–994 (2004). https://doi.org/10.1039/B404531A
94. Ewing, R. G., Atkinson, D. A., Eiceman, G. A., Ewing, G. J.: A critical review of ion mobility spectrometry for the detection of explosives and explosive related compounds. Talanta **54**, 515–529 (2001). https://doi.org/10.1016/s0039-9140(00)00565-8
95. Borsdorf, H., Eiceman, G.: Ion mobility spectrometry: principles and applications. Appl. Spectrosc. Rev. **41**, 323–375 (2006). https://doi.org/10.1080/05704920600663469
96. Kirk, A., Allers, M., Cochems, P., Langejuergen, J., Zimmermann, S.: A compact high resolution ion mobility spectrometry for fast trace gas analysis. Analyst **138**, 5159–5504 (2013). https://doi.org/10.1039/C3AN00231D
97. Moura, P.C., Vassilenko, V.: Gas chromatography - ion mobility spectrometry as a tool for quick detection of hazardous volatile organic compounds in indoor and ambient air: a university campus case study. Eur. J. Mass Spectrom. **28**, 113–126 (2022). https://doi.org/10.1177/14690667221130170
98. Szczurek, A., Maziejuk, M., Maciejewska, M., Pietrucha, T., Sikora, T.: BTX compounds recognition in humid air using differential ion mobility spectrometry combined with a classifier. Sens. Actuators, B Chem. **240**, 1237–1244 (2017). https://doi.org/10.1016/j.snb.2016.08.164
99. Fernandes, J., Vassilenko, V., Moura, P.C., Viktor, F.: Gas chromatography - ion mobility spectrometry instrument for medical applications: a calibration protocol for ppb and ppt concentration range. In: Technological Innovation for Applied AI Systems. IFIP International Federation for Information Processing. 12th Advanced Doctoral Conference on Computing, pp. 394–357. Electrical And Industrial Systems (DoCEIS 2021), Caparica, Portugal (2021). https://doi.org/10.1007/978-3-030-78288-7_34
100. Vautz, W., Seifert, L., Mohammadi, M., Klinkenberg, I., Liedtke, S.: Detection of axillary perspiration metabolites using ion mobility spectrometry coupled to rapid gas chromatography. Anal. Bioanal. Chem. **412**, 223–232 (2020). https://doi.org/10.1007/s00216-019-02262-7
101. Ruzsanyi, V., Mochalski, P., Schmid, A., Wiesenhofer, H., Klieber, M., Hinterhuber, H., Amann, A.: Ion mobility spectrometry for detection of skin volatiles. J. Chromatogr. B **911**, 84–92 (2012). https://doi.org/10.1016/j.jchromb.2012.10.028
102. Bunkowski, A., Maddula, S., Davies, A., Westhoff, M., Litterst, P., Bödeker, B., Baumbach, J.: One-year time series of investigations of analytes within human breath using ion mobility spectrometry. Int. J. Ion Mobil. Spectrom. **13**, 141–148 (2010). https://doi.org/10.1007/s12127-010-0052-7
103. Bessa, V., Darwiche, K., Teschler, H., Sommerwerck, U., Rabis, T., Baumbach, J., Freitag, L.: Detection of volatile organic compounds (VOCs) in exhaled breath of patients with chronic obstructive pulmonary disease (COPD) by ion mobility spectrometry. Int. J. Ion Mobil. Spectrom. **14**, 7–13 (2011). https://doi.org/10.1007/s12127-011-0060-2
104. Santos, P., Vassilenko, V., Conduto, C., Fernandes, J., Moura, P.C., Bonifácio, P.: Pilot study for validation and differentiation of alveolar and esophageal air. In: Technological Innovation for Applied AI Systems, Doctoral Conference on Computing, pp. 331–338. Electrical and Industrial Systems, DoCEIS 2021, Caparica, Portugal (2021). https://doi.org/10.1007/978-3-030-78288-7_32
105. Westhoff, M., Rickermann, M., Franieck, E., Littterst, P., Baumbach, J.: Time series of indoor analytes and influence of exogeneous factors on interpretation of breath analysis using ion mobility spectrometry (MCC/IMS). Int. J. Ion Mobil. Spectrom. **22**(3), 39–49 (2019). https://doi.org/10.1007/s12127-019-00243-1
106. Yang, X., Jiao, R., Zhu, X., Zhao, S., Liao, G., Yu, J., Wang, D.: Profiling and characterization of odorous volatile compounds from the industrial fermentation of erythromycin. Environ. Pollut. **255**, 113130 (2019). https://doi.org/10.1016/j.envpol.2019.113130
107. Gao, W., Yang, X., Zhu, X., Jiao, R., Zhao, S., Yu, J., Wang, D.: Limitations of GC-QTOF-MS technique in identification of odorous compounds from wastewater: the application of GC-IMS as supplement for odor profiling. Atmosphere **12**, 265 (2021). https://doi.org/10.3390/atmos12020265
108. Vautz, W., Slodzynski, R., Hariharan, C., Seifert, L., Nolte, J., Fobbe, R., Sielemann, S., Lao, B., Huo, R., Thomas, C.L., Hildebrand, L.: Detection of metabolites of trapped humans using ion mobility spectrometry coupled with gas chromatography. Anal. Chem. **85**, 2135–2142 (2013). https://doi.org/10.1021/ac302752f
109. Müller-Wirtz, L., Kiefer, D., Ruffing, S., Brausch, T., Hüppe, T., Sessler, D., Volk, T., Fink, T., Kreuer, S., Maurer, F.: Quantification of volatile adehydes deriving from in vitro lipid peroxidation in the breath of ventilated patients. Molecules **26**, 3089 (2021). https://doi.org/10.3390/molecules26113089
110. Ireland, C., Coto, M., Brown, L., Paris, R., Ducati, C.: Analyzing the photo-oxidation of 2-propanol at indoor air level concentrations using field asymmetric ion mobility spectrometry. J. Vis. Exp. **136**, e54209 (2018). https://doi.org/10.3791/54209
111. Kalhor, M., Hamzehpour, N., Ghashghaei, E., Faridi, M., Kalhor, H.: Ultrasound-assisted emulsification-microextraction coupled to ion mobility spectrometry for monitoring of atrazine and simazine in environmental water. Int. J. Ion Mobil. Spectrom. **19**, 139–144 (2016). https://doi.org/10.1007/s12127-016-0193-4
112. Mayer, T., Borsdorf, H.: Accuracy of ion mobility measurements dependent on the influence of humidity. Anal. Chem. **86**, 5069–5076 (2014). https://doi.org/10.1021/ac5007393
113. Reyes-Garcés, N., Gómez-Ríos, G., Silva, E.A., Pawliszyn, J.: Coupling needle trap device with gas chromatography - ion mobility spectrometry detection as a simple approach for on-site quantitative analysis. J. Chromatogr. A **1300**, 193–198 (2013). https://doi.org/10.1016/j.chroma.2013.05.042
114. Li, F., Xie, Z., Schimdt, H., Sielemann, S., Baumbach, J. I.: Ion mobility spectrometer for online monitoring of trace compounds. Spectrochimica Acta - Part B: Atomic Spectroscopy **57**, 1563–1574 (2002). https://doi.org/10.1016/S0584-8547(02)00110-6
115. Puton, J., Holopainen, S., Mäkinen, M., Sillanpää, M.: Quantitative response of IMS detector for mixtures containing two active components. Anal. Chem. **84**, 9131–9138 (2012). https://doi.org/10.1021/ac3018108