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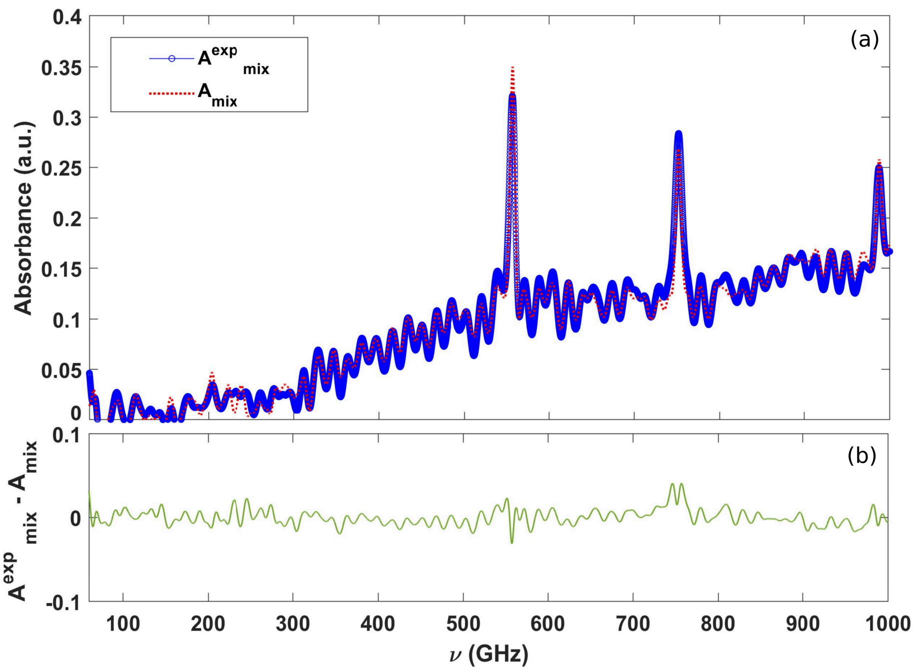

Fig. 5. (a) Comparison of the experimental absorbance of BuOH-1/EtOH mixture at 15 mbar total pressure with the weighted sum of measured absorbances for pure BuOH-1 and EtOH at the same pressure and temperature. (b) residual difference between the experimental absorbance vs. the calculated one. The root-mean-square (RMS) deviation is 0.007.

4. Conclusions

In this work, we experimentally explored the spectral characteristics of five alcohols in the frequency range (60-1200) GHz by using high-resolution THz-FDS spectroscopy. The spectral characterization of these selected VOCs, under controlled conditions of pressure, temperature and RH, allowed the quantitative evaluation of their molar absorption coefficients and the recognition of specific spectral features for each compound. Our attention has been particularly focused on the two isomeric forms of butanol, BuOH-1 and BuOH-2, which to our knowledge, have never been characterized in the THz spectrum in the gaseous phase. For them, we were also able to identify spectral differences for the intense main peak at 0.5 GHz between BuOH-1 and BuOH-2, attributable to the arrangement of the methyl groups with respect to the carbon attached to the hydroxyl group. Moreover, we studied the spectral absorption measurements for the mixtures alcohol/air and alcohol/alcohol. In particular, the BuOH-2/air mixture absorbances, compared to the pure BuOH-2 one, increase in all the spectral region as the air content grows. At lower frequencies, we noticed a modification of the spectral pattern. Finally, we studied the optical response in the THz regime for the alcohol-mixture (BuOH-1/EtOH). The spectral absorption measurement for the BuOH-1/EtOH mixture was compared with the weighted linear combination of independently acquired pure compound spectra, achieving a good agreement.

Our results prove that THz-FDS is a reliable methodological high-resolution approach in the gas sensing, for applications in human breath analysis and environmental/occupational monitoring [60] and corroborate the great potentiality of THz-FDS for the quantitative evaluation of VOCs contents in the multiple-component mixtures. In addition, the assembled measurement unit adopted for this work is compact, light and does not require high power consumption. For these reasons it can be easily adopted for *in situ* measurements and implementable for remote-distance monitoring. In order to increase the selectivity and sensitivity of the THz-FDS sensing system, it is possible to implement a platform to collect and accumulate large amounts of chemicals that are diluted in the air [10,11,61–63]. Furthermore, the data analysis of this spectroscopic methodology can be equipped with advanced computational analyses: network analysis, machine learning, and principal components analysis algorithms [64] allowing for a back-door robust post-processing for the spectral interpretation and pattern recognition necessary for fast detection of gaseous chemicals [60].

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Data availability. Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.

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