

Characterization of Absorption Spectrum of Ethanol Gas for Use as Terahertz Alcohol Sensor

Junichi Hamazaki, Shingo Saito, and Iwao Hosako

National Institute of Information and Communications Technology, Tokyo 184-8795, Japan.

Abstract—The absorption spectra of pure ethanol gas and ethanol gas mixed with air were characterized for examining the use of ethanol gas as a terahertz alcohol sensor. A comparison of the spectra of both gases showed that the absorbance of the latter was ~ 1.3 times greater than that of the former.

I. INTRODUCTION AND BACKGROUND

At parties and bars, many people drink alcohol to relax, relieve tension, and enjoy themselves. This leads to a decrease in their attentiveness and reaction time. Moreover, they lose their power of judgment. Indeed, drunk driving is known to cause serious traffic accidents^{1, 2}. As a means of preventing this outcome, we suggest installation of alcohol detection sensors in automobiles.

Ethanol gas molecules have a broad optical absorption spectrum in the terahertz (THz) region^{3, 4}. The spectrum is believed to correspond to a torsional mode with large coupling between the molecules' internal and overall rotations. Some organic molecules show absorption spectra in the THz region, with the shape of the spectrum varying among different molecules. THz molecular sensor is a strong candidate for use as alcohol sensors in automobiles. For examining their suitability, detailed characterization of the ethanol absorption spectrum in the THz region is required.

In this study, we investigated the absorption spectra of pure ethanol gas and ethanol gas mixed with air in the THz region. We obtained the absolute calibration curve of the absorption intensity for both gases. We found that ethanol gas mixed with air had greater absorption than pure ethanol gas. We inferred this difference as resulting from the interaction between ethanol gas and air in the former gas.

II. RESULT AND DISCUSSION

Experiments were performed at room temperature. An 18-cm-long stainless steel gas cell was mounted in an FT-IR spectrometer (BOMEM, DA8). To characterize the ethanol absorption spectrum in detail, the absorption spectra of three types of gas—(A) pure ethanol gas, (B) ethanol gas mixed with air, and (C) air—were determined.

Figure 1 shows the absorption spectra of (A), (B), and (C). In this case, the partial pressures of ethanol gases of (A) and (B) were set at 3 kPa, and those of air of (B) and (C) were set at atmosphere. We found that the absorbance of (B) was larger than the sum of the absorbances of (A) and (C). (For example, at 6.2 THz, the absorbances of (A), (B), and (C) were 42 dB/m, 65 dB/m, and 10 dB/m, respectively.)

Figure 2 shows the absorption intensities of (A) and (B) at 6.2 THz as a function of the partial pressure of ethanol gas. The

partial pressure of air was set at atmosphere. We observed that the absorption intensity of both gases linearly increased with the partial pressure. The rate of increase of (B) was also ~ 1.3 times greater than that of (A); an observation valid throughout the absorbance range.

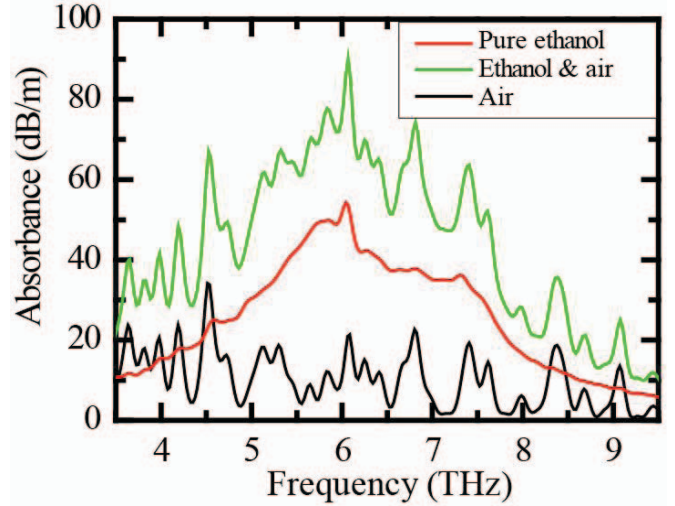


Fig. 1. Absorption spectra of pure ethanol gas at 3 kPa (red line), ethanol gas at 3 kPa mixed with air at atmosphere (green line), and air at atmosphere (black line).

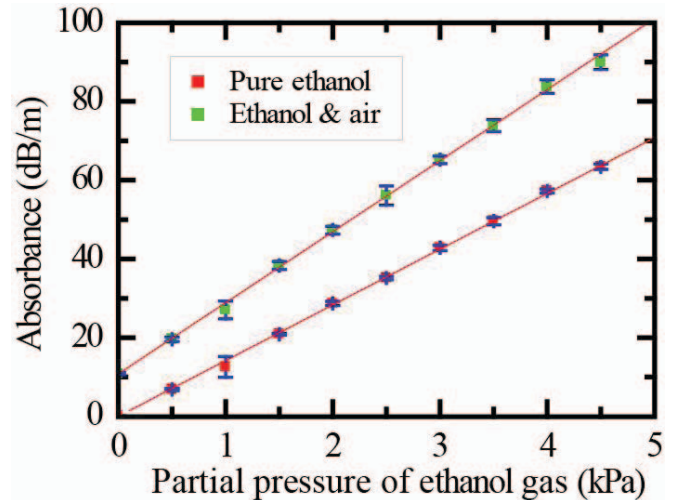


Fig. 2. Absorption intensities of pure ethanol gas (red) and ethanol gas mixed with air at atmosphere (green) as a function of the partial pressure of ethanol gas. Red lines indicate absolute calibration curves.

To clarify the absorbance change by mixing with air, we measured the absorbance of (B) as a function of partial pressure of air. The inset of Fig. 3 shows absorbance change at 6.2 THz. It is found that the change can be described by two parts: a drastically increased region (0-1 kPa) and slowly increased region (3-100 kPa). We claimed that the drastic increment owes to interaction between ethanol gas and air. The slow increment is considered as trivial air absorbance, since its slope corresponds to the absorbance slope of air (blue line in inset of Fig. 3).

Fig. 3 shows a close-up of the inset. Note that the vertical axis is converted to absorbance change. To characterize the change, we fitted our data using a function given by,

$$\delta\alpha = A_1x + A_2\{1 - \exp(-x/\tau)\} \quad (1)$$

where x [kPa] denotes partial pressure of air, and τ indicates the relaxation coefficient of the absorption increment. The first term denotes air absorbance and the second denotes absorbance change due to the interaction. This term describes linear increase in a small x region ($x < \tau$) and saturation in a large x region ($x > \tau$). As a result, we estimated A_1 , A_2 , and τ as 0.07, 14, and 0.8, respectively. The estimation of τ at 0.8 (near 1) indicates that ethanol molecules interact with a similar number of air molecules. Therefore, we suggested the origin of the increment is a chemical reaction between ethanol and air.

The qualitative trend of the absorbance change can be explained as follows. In the case of the rarefied air region (< 1 kPa), the reaction occurs actively. This is because almost all ethanol molecules are unreacted; therefore absorbance increased drastically. On the other hand, almost all ethanol molecules are reacted in the thick air (> 2 kPa); thus the absorbance increment becomes saturated. However, the origin of why absorbance increased due to the reaction throughout the absorbance range was not clarified, nor was the type of reaction that occurred.

We also considered “collision-induced absorption” to be the origin of the absorbance increment, though it is known that such absorption increases superlinearly in relation to additional gas⁵; thus this was neglected.

III. CONCLUSION

We investigated the absorbance spectrum of ethanol gas mixed with air in the THz region. We found that an absorbance increment of ethanol gas by increasing the partial pressure of air. The absorbance mixed with air was eventually ~ 1.3 times greater than that of pure ethanol gas. By characterizing the absorbance change, we considered that the absorbance increment was due to a chemical reaction between ethanol and air. We claim that nitrogen, oxygen, and water molecules are the candidate components in relation to the chemical reaction; though this is not yet clarified. Details will be discussed by identifying the components.

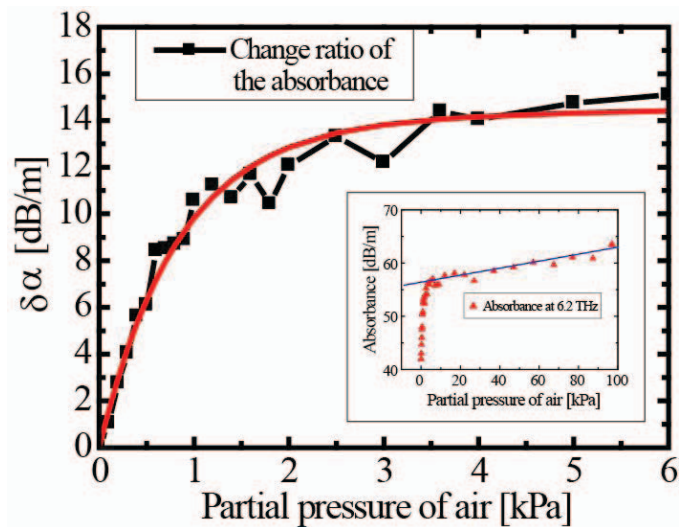


Fig. 3. Changes of ethanol absorbance as a function of partial pressure of air in the range of 0-6 kPa. The partial pressure of ethanol was set 3 kPa. Red line denotes fitting curve. Inset shows experimental data as a function absorbance change as a function of partial pressure of air, from 0 kPa to atmosphere. The blue line denotes the slope of air absorbance.

REFERENCES

- [1] L. J. Horwood and D. M. Fergusson, *Accident Analysis & Prevention*, **32**, 805-814 (2000).
- [2] E.A. Maylor, P.M. Rabbitt, *Br. J. Psychol.* **84**, 301-317 (1993).
- [3] J. R. Durig and R. A. Larsen, *J. Mol. Str.* **238**, 195-222 (1989).
- [4] M. L. Senent, Y. G. Smeyers, R. Dominuez-Gomez, and M. Villa, *J. Chem. Phys.* **112**, 5809-5819 (2000).
- [5] L. Frommhold, “Collision-induced Absorption in Gases,” *Cambridge University Press*, (2006).