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## Terahertz Time-Domain Spectroscopy of Vitamin C and Lecithin

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**Abstract:** THz time-domain spectroscopy has recently emerged as an extremely useful and powerful probe of charge transport in materials, owing to the fact that it provides a probe of the complex conductivity over a wide frequency range, with sub-picosecond time resolution. Herein, time-domain and absorption spectra of two kind of organic molecules Vitamin C and lecithin were obtained, respectively. With analysis for the mechanism and their spectrum structures of the two molecules, it is concluded that the THz spectroscopy can be also available in applying for non-destructive inspection and identification of Vitamin C and lecithin. Never the less, it was found that between the peaks there presents nearly the same intervals, representing an ordered uniformly increasing with wavelength. We infer that this may suggest and reflect the intervals of some vibrational or rotational energy levels.

**Key words:** THz, time-domain spectroscopy, Vitamin C, lecithin

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### INTRODUCTION

The terahertz (THz) waves which categorized between millimeter radio waves and far infrared light waves, with frequencies of 0.1-10 THz, exhibit properties for both sides of the electromagnetic spectra. The THz wave band was ever named as 'lacuna' for lack of effective technique of generating and detecting (Mickan *et al.*, 2002). It was not until late 1980s when comes the ultra-fast laser light which brings forth a new effective hand for the pulse THz wave that more and more investigators begin to throw eyes on the study of THz theory and its application. The fields include THz emission (Wei-Wei *et al.*, 2005), THz spectral analysis and THz imaging (Shaohong *et al.*, 2003). The interdisciplinary collaborating investigation has come to being a new research field named as THz technique (Kawase *et al.*, 2003; Cao *et al.*, 2000; Cao and Lei, 2003; Cao *et al.*, 2003).

Like radio waves, THz can be transmitted through a wide variety of substances such as paper, cloth, ceramics, plastics, wood, bone, fat, various powders, dried food and so on. In addition, like light waves, they can easily be propagated through space, reflected, focused and refracted using THz optics. Furthermore, the short wavelength which is much shorter than that of usual radio waves allows for a spatial resolution which is sufficient in many imaging applications (Shen *et al.*, 2004; Dorney *et al.*, 2001; Miyamaru *et al.*, 2003; Yu and Zeng, 2004). The range of potential application is probably to expand even further with the increased availability of many absorption spectra peculiar to specific chemicals.

Materials research is an essential component of modern THz systems; novel, higher- power THz sources rely heavily on new materials such as quantum cascade structures. At the same time, THz technique provides a powerful tool for the characterization of a broad range of materials, including semiconductors and biomaterials. THz wave is also suitable for drug detection purposes, being able

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to screen the contents of envelopes and measurement results having proven the existence of fingerprint spectra peculiar to illicit drugs in the THz region.

In this study, organic molecules were taken as examples of the application of THz spectra; as a result, remarkable time-domain spectra of Vitamin C and lecithin were obtained. With analysis for the mechanism and their spectrum structures of the two molecules, it is found that the THz spectroscopy can be available in applying for non-destructive inspection and identification of Vitamin C and lecithin.

## MATERIALS AND METHODS

The samples, Vitamin C, lecithin in the form of powders, were carefully mixed with polyethylene (PE) powder with varying weight ratios about 1:2, depending on the absorption strength of the sample material and pressed (400 kg) into about 1 mm thick pellets. PE has low absorption ( $<5\text{ cm}^{-1}$  below 4 THz) and constant index of refraction in the range between 0.1 and 4 THz (Markelz and Roitberg, 2000), slightly depending on the pressure applied during sample preparation. The environmental temperature is  $26^\circ\text{C}$  and relative humidity is 39%.

A THz time-domain spectrometer setup (Walther *et al.*, 2000) with an optical layout used in this experiment is shown in Fig. 1. The photoconductive antennas are driven by pulses of 30 fs duration from a Ti:sapphire oscillator. One of the antennas is used as a THz pulse emitter and the other one as a field-sensitive THz detector, gated by a second portion of the fs beam. The emitter consists of 10  $\mu\text{m}$  wide metallic electrodes lithographically deposited on a semi-insulating InAs wafer. Charge carriers excited to the conduction band of the InAs substrate by the laser pulse are accelerated by the strong bias field, thereby emitting a short burst of electromagnetic radiation.

The power of fs laser pulse used in our experiment is 400 mW and the available frequency range is 0.2-2.5 THz. Detect method adopt the electrical optical sampling technique with the ZnTe wafer as field-sensitive detector ( $<110>$  ZnTe) (Taday *et al.*, 2003; Liu Rui *et al.*, 2004). The Reference pulse and sample pulse spectra are all carried in nitrogen environment.

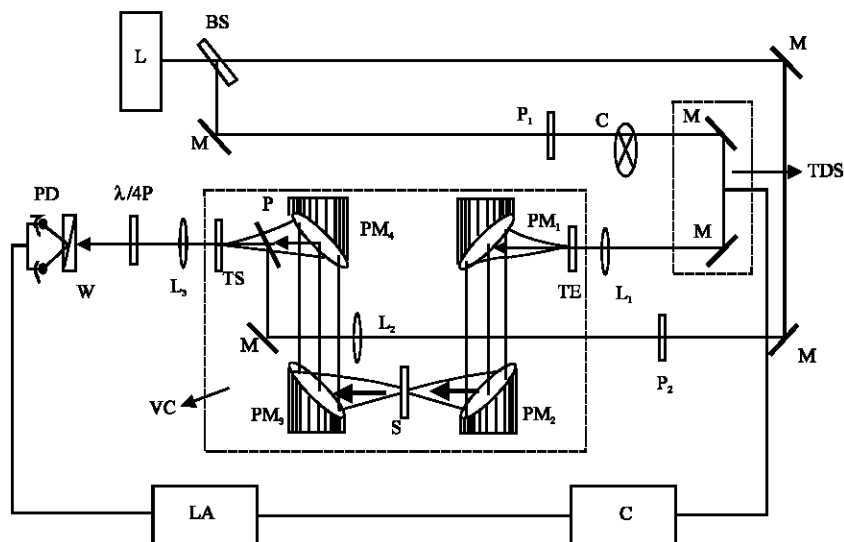


Fig. 1: Schematic setup of THz time-domain spectrometer

### RESULTS AND DISCUSSION

Figure 2a shows the reference pulse and sample pulse propagated through a 1 mm thick lecithin pill in nitrogen environment at temperature of about 295 K. As we can see, there is obvious time-delay between the two pulses. This is due to the lecithin pill sample whose refractive index is bigger than that of nitrogen itself. Figure 2b presents the Fourier spectra of them, respectively. As we can see,

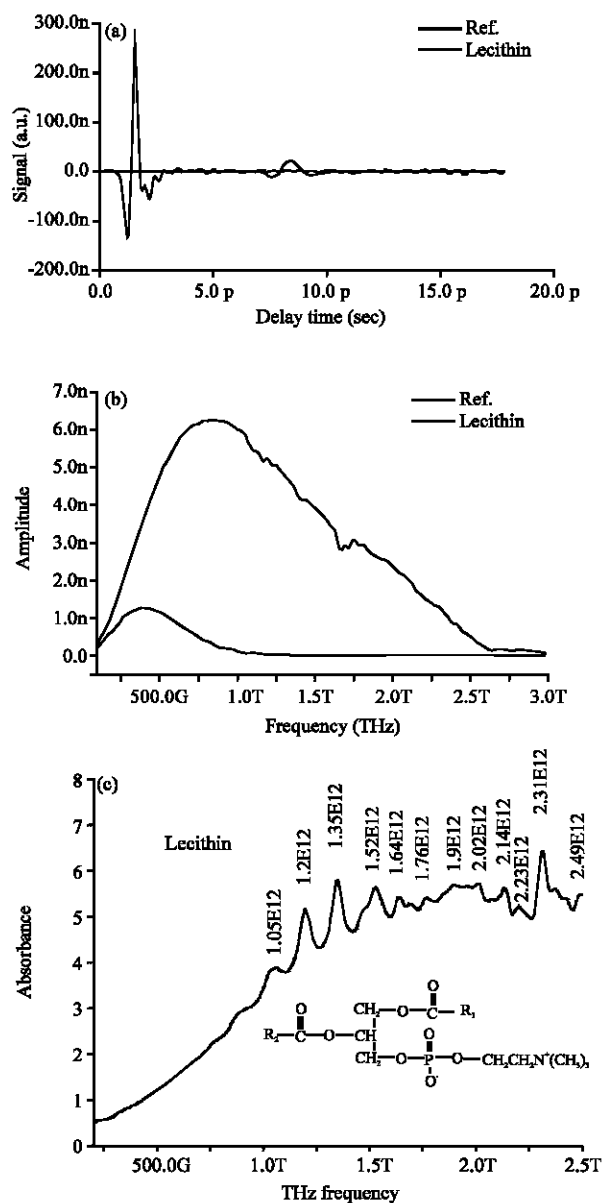


Fig. 2: Reference pulse and sample pulse propagated through a 1 mm thick lecithin pill (a); Fourier spectra (b); Absorption coefficient of Lecithin from 0.2 to 2.5 THz at temperature of 295 K. (c)

Table 1: Absorption peaks of lecithin in THz region

Fre.(THz)	1.05	1.2	1.35	1.52	1.64	1.76
Abs.	m	s	s	s	m	w
Fre.	1.9	2.02	2.14	2.23	2.31	
Abs.	w	w	m	m	s	

s: strong, w: weak, m: medium

there is a big ‘crawl down’ band for the sample spectrum but reference spectrum, which suggests a big absorption band in the corresponding frequency region.

Figure 2c presents the absorbance spectrum of Lecithin from 0.2 to 2.5 THz where it presents a big absorption band at the whole. In addition, a number of peaks in the spectrum are presented, especially in the high frequency side. These peaks, as laid out in Table 1, such as the 1.2, 1.35, 1.52 and 2.31 THz, are remarkably sharp which means strong absorption for the right frequency. It aims at absorption coefficient of Lecithin at different frequencies.

There is an interesting thing in the spectra of sample absorption in THz wave band, as shown in Fig. 2c. Between these peaks they show nearly the same intervals, representing an ordered uniformly increasing with wavelength. We infer that this may suggest and reflect the intervals of some vibrational or rotational energy levels.

Similarly, Fig. 3a refers to the corresponding time-domain signal of reference pulse and sample pulse propagated through a vitamin-C pill. Figure 3b aims at their FT spectra and Fig. 3c represents for absorbance frequency spectra of the vitamin-C sample. The main peaks are laid out in Table 2.

It is notable that there are almost no so many peaks in the spectra for vitamin-C. On the contrary, only a few obvious and strong peaks can be seen in Fig. 3c. For example, at the frequency region of 1.73, 2.02 and 2.25 THz, the main peaks even bring forth some weak shoulder peaks. It may result from some small rotational energy levels based on some vibrational level, where the energy intervals widened with the quantum number J increasing. According to the calculation of result based on DFT arithmetic theory, the absorption at THz wave band mainly results from the molecular rotation and twisting. While the frequency of molecular rotation and twisting is correlated with molecular structure, so the different absorption peaks at THz wave band may essentially reflect their different structures.

It is similarly interesting that, in Fig. 3c, the peaks also distribute nearly according to the same interval of wavelength. What’s more, each has one or two shoulder peaks presented in left or right also with the similar interval of wavelength. This may suggest and reflect the same interval of rotational energy levels based on some vibrational energy. And on the other hand, since these are condensed phase measurements and there are few rotations detected, it also may result from Fringing (an etalon), as the far infrared or THz literature is fraught with etalon artifacts (fringing) being incorrectly assigned to molecular vibrations. The periodic spacings seen in the lecithin and vitamin C spectra are possibly etalon effects. Indeed, if the sample is about 0.5 mm thick, the fringing effect (~15 cm<sup>-1</sup>) jives well with the sample thickness.

According to the physical model for THz optics parameter by Dorney *et al.* (2001), after simple deducing, we can obtain the refraction index  $n_s$ , extinction coefficient  $k_s$  and absorption coefficient  $\alpha_s$ :

$$n_s(\omega) = \phi(\omega) \cdot \frac{c}{\omega d} + 1 \tag{1}$$

$$k_s(\omega) = \ln\left(\frac{4n_s(\omega)}{\rho(\omega) \cdot (n_s(\omega) + 1)^2}\right) \cdot \frac{c}{\omega d} \tag{2}$$

$$\alpha_s(\omega) = \frac{2k_s(\omega) \cdot \omega}{c} \tag{3}$$

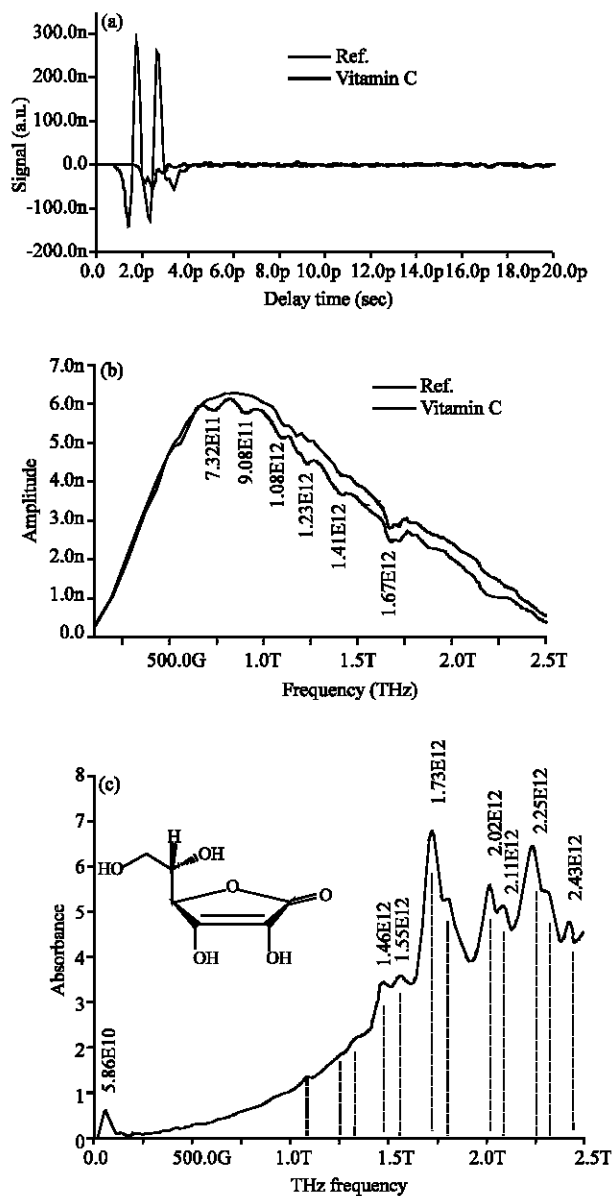


Fig. 3: Reference pulse and sample pulse propagated through a 1 mm thick vitamin C pill (a); Fourier spectra (b); Absorption coefficient of Vitamin C from 0.2 to 2.5 THz at temperature of 295 K (c)

Table 2: Absorption Peaks of Vitamin C in THz region

Fre. (THz)	1.46	1.55	1.73	1.82	2.02	2.11	2.25	2.43
Abs.	w	w	s	w	s	m	s	m

s: strong, w: weak, m: medium

Considering the total energy of molecular inside as  $E = E_e + E_v + E_r$ , where  $E_e$  is for the energy of electron movement, while  $E_v$  and  $E_r$  refer to vibrational and rotational energy of molecules. Since

every kind of movement energy is quantized, when the molecular phase jumps from  $E''$  to  $E'$  ( $<E1''$ ), it will emit electromagnetic radiation of which frequency is determined by:

$$\begin{aligned} \nu &= \frac{E'' - E'}{h} = \frac{1}{h} [(E''_e + E''_v + E''_r) - (E'_e + E'_v + E'_r)] \\ &= \frac{\Delta E_e}{h} + \frac{\Delta E_v}{h} + \frac{\Delta E_r}{h} = \nu_e + \nu_v + \nu_r \end{aligned} \quad (4)$$

Proved by theories and experiments, the energy difference of electron movement  $\Delta E_e$  is the largest, while  $\Delta E_e$  is the smallest and even usually  $\nu_e > \nu_v > \nu_r$ . This means there may be vibrational energy levels at every electron energy level, while rotational energy levels with smaller energy differences based on the vibrational energy level as well.

In fact, the response of molecules to THz radiation mainly comes from the collective vibrational mode of molecular fabrication and conformation. This collective vibrational mode mostly reflects molecular integral frame information, but not the relative localization electron structure that generally measured by optical method, nor the vibrational mode relative to single chemical bond.

Owing to the sensitivity of macromolecular structure to environment, the distributing and intensity of collective vibrational mode actually includes the influence of environment. Base on this, THz spectroscopy take good advantages of studying the macromolecular structure, intermolecular action and the interaction between molecules and environment. The high relativities of spectrum at THz wave band and their overall structures, especially for Bio-molecules, is the important microcosmic foundation for the fresh THz technology applied in biomedicine systems and materials.

## CONCLUSIONS

It is very useful and powerful to apply THz technique, with its far-infrared radiation, to extract molecular spectral information in an otherwise inaccessible portion of the electromagnetic spectrum. In this study, it was found that the Vitimin C, lecithin present novel properties in THz region. And it is interesting that among the absorption peaks we find nearly the same intervals, representing an ordered uniformly increasing with wavelength. We infer that this may suggest and reflect the intervals of some vibrational or rotational energy levels. With analysis for the mechanism and their spectrum structures of the three molecules, it is concluded that, besides the non-destructive inspection and identification of druggery, the THz spectroscopy can be also available in applying for biomaterials and even it is possible that the THz time-domain spectra may provide more fine structural information of molecules.

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## REFERENCES

- Cao, J.C., H.C. Liu and X.L. Lei, 2000. Spectrum dynamics of negative-effective-mass oscillators under terahertz radiation. *J. Applied Phys.*, 87: 2867.
- Cao, J.C. and X.L. Lei, 2003. Synchronization and chaos in minibandsemiconductor superlattices. *Phys. Rev. B*, 67: 085309.
- Cao, J.C., 2003. Multiphoton process in terahertz-driven two-dimensional structures. *Phys. Rev. Lett.*, 91: 237401.

- Kawase, K., Y. Ogawa and Y. Watanabe, 2003. Non-destructive terahertz imaging of illicit drugs using spectral fingerprints. Vol. 11, No. 20/OPTICS EXPRESS 2549
- Markelz, A.G. and A. Roitberg, 2000. Pulsed terahertz spectroscopy of DNA, bovine serum albumin and collagen between 0.1 and 2.0 THz. *Chem. Phys. Lett.*, 320: 42.
- Mickan, S.P., J.S. Dordick, J. Munch, D. Abbott and X.C. Zhang, 2002. Pulsed THz protein spectroscopy in organic solvents. CFD6, the conference of laser and electro-optics (CEOL), long beach, ca, May 24.
- Miyamaru, F., M. Yamaguchi and M. Hangyo *et al.*, 2003. THz-time-domain spectroscopy of amino acids in solid phase. CLEO'03 2
- Rui, L. and G. Chunming, 2004. Generation of terahertz radiation via optical rectification and electro-optic detection in ZnTe crystal. *Acta Phys. Sin.*, 57: 1217 (In Chinese).
- Shaohong, W., B. Ferguson, Z. Cunlin and Z. Xicheng, 2003. Terahertz computer tomography. *Acta Phys. Sin.*, 52: 120 (In Chinese).
- Shen, Y.C., P.C. Upadhy, E.H. Linfield and A.G. Davies, 2004. Vibrational spectra of nucleosides studied using terahertz time-domain spectroscopy. *Vibrational Spectroscopy*, 35: 111.
- Taday, P.F., I.V. Bradley and D.D. Arnone, 2003. Terahertz pulse spectroscopy of biological materials: L-glutamic acid. *J. Biol. Phys.*, 29: 109.
- Timothy, D.D., R.G. Baraniuk and D.M. Mittleman, 2001. Material parameter estimation with terahertz time-domain spectroscopy. *J. Opt. Soc. Am. A.*, 18: 1562.
- Walther, M., B. Fischer, M. Schall, H. Helm and P. Uhd Jepsen, 2000. Far-infrared vibrational spectra of all-trans, 9-cis and 13-cis retinal measured by THz time-domain spectroscopy. *Chem. Phys. Lett.*, 332: 389.
- Wei-Wei, Y., W. Wei-Ning, Z. Guo-Zhong, Z. Cun-Lin and Y. Hai-Tao, 2005. THz spectrum of aromatic amino acid. *Acta Phys. Sinica*, 54: 3094-3099.
- Yu, B. and F. Zeng, 2004. Torsional vibrational modes of tryptophan studied by terahertz time-domain spectroscopy. *Biophys. J.*, 86: 1649.