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Dehydration Process of the Monohydrates of Asparagine Enantiomers Observed by Terahertz Spectroscopy

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ABSTRACT

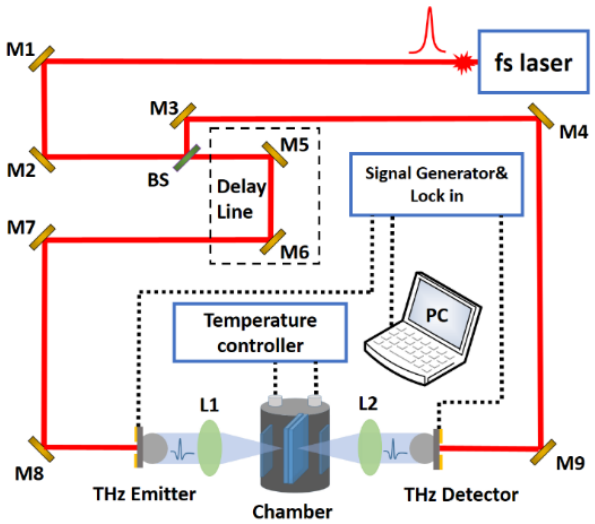
Terahertz time-domain spectroscopy (THz-TDS) has been used to investigate the absorption spectra of L-, D-, and DL-asparagine in the frequency range of 0.3-2.4 THz, as well as their monohydrates. The spectra exhibit distinct differences in peak frequencies among the three enantiomers and three monohydrates. The observed results show that the chirality and the presence of crystallization water both lead to spectral differences, which are attributed to the intermolecular interactions. In addition, the monohydrates can be converted into asparagine enantiomers under heating.

INTRODUCTION

Asparagine is one of the 20 amino acids that make up organic proteins. It is mainly used to treat bronchiectasis, anti-peptic ulcer and gastric dysfunction. Asparagine is a chiral molecule with a pair of enantiomers. It also has two stable states: anhydrous form and monohydrate form.

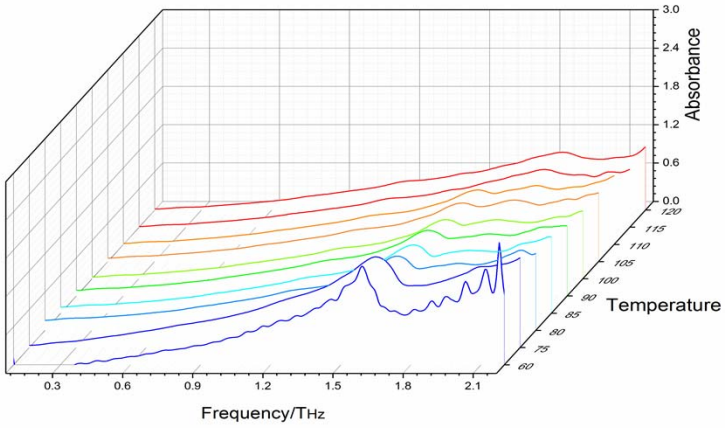
In this paper, THz time-domain spectroscopy (THz-TDS) has been used to determine the difference in absorption spectra of L-type, D-type, DL-type of asparagine and their monohydrates, as well as the dehydration process. It is significant for further substance identification and analysis.

METHOD

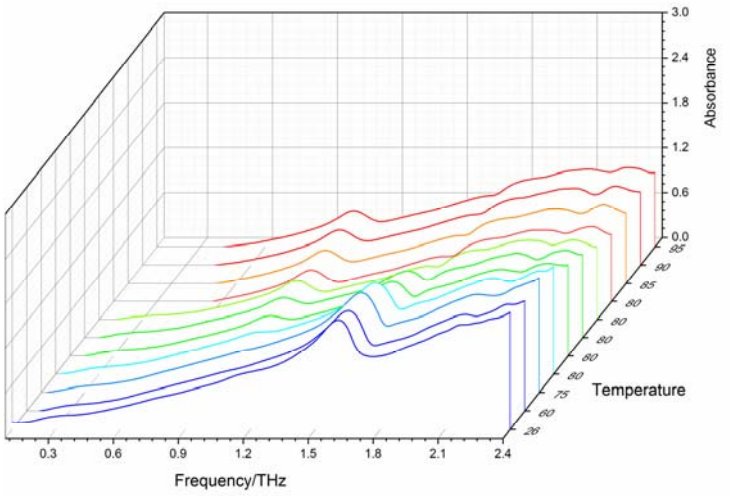


THz-TDS is equipped with a high stability temperature controller and a temperature-variable chamber with a cell holder. The sample holder is specially designed for mounting the sample cell with a cooling structure. The sample cell is connected to a thermostat and the cooling system filled with liquid nitrogen. The room temperature is maintained at 295 K in the laboratory.

RESULTS



The dehydration process of L-asparagine monohydrate. There is no change under 60 ℃, so we only show the spectrum above 60 ℃. In order to clearly observe the change, the spectrum above 60 ℃ was smoothed by a digital filter. The absorption peak at 1.638 THz get weaker and shows a blue shift when the temperature increase. At about 90 ℃, there are two peaks, which means dehydration process is undergoing. At about 120 ℃, the monohydrate lost all the crystallization water and totally convert into L-asparagine.



The dehydration process of D-asparagine monohydrate. Under 75 ℃, the monohydrate is very stable. Above 75 ℃, the dehydration process is getting more obvious with the increase of temperature. At about 90 ℃, the monohydrate is totally converted into D-asparagine.

References

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