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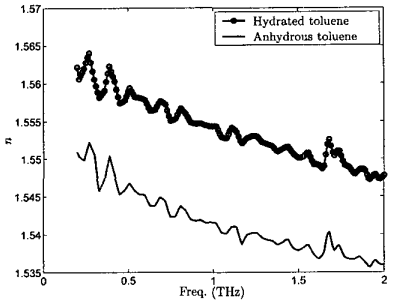

CFD6 Fig. 1. Comparison between the FIR refractive indicies of hydrated and anhydrous toluene.

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CFD6 **9:15 am**

Pulsed THz Protein Spectroscopy in Organic Solvents

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Pulsed THz spectroscopy provides a new method for probing the tertiary structure and hydration of biomolecules. In proteomics applications, the response of a protein-protein structure must be probed quickly and non-invasively. THz-frequency radiation lies in the far infrared, a region associated with structural motion modes of large molecules. The THz region has been difficult to probe in the past with Fourier Transform Infrared (FTIR) techniques, but recently the advent of pulsed THz spectroscopy (PTS) has enabled the study of molecular denaturation and hydration.[1] We are interested in using PTS to characterize the conformation and hydration of enzymatic proteins for biochip analysis.

We present measurements of the refractive index and extinction coefficient of organic solvents commonly used in studying protein activity. Our spectroscopic instrument is a pulsed THz system, based on a 100-fs Ti:Sapphire laser, surface current generation and electro-optic detection. We measure directly the refractive index, n, and extinction coefficient, k, of common organic solvents. The THz-domain n and k for three of our organic solvents are shown in Table 1. The refractive indicies of the solvents at optical frequencies are included for reference. n and k are given over a range, 0.2 to 2 THz, which approximately spans the bandwidth of our THz system. Table 1 shows that the organic solvents have very low absorption in the THz range. Low THz absorption is a property of non-polar solvents that makes them ideal media for TPS.[2]

We mount the samples in disposable cuvettes. The cuvettes have 1-mm-thick walls, n of 1.525 and k of 0.002, and a 4-mm path length. We estimate the material parameters for our samples using an iterative technique. We test both anhydrous solvents, dehydrated over molecular sieves, and solvents mixed with water before phase separation. In iso-octane and hexane, n and k are largely the same for hydrated and anhydrous solvents. This is to be expected considering they have low water miscibility. The last column in Table 1 shows the maximum weight percent [w/w] solubility of water in each solvent at 20°C. Controlling the water content of the solvents is critical in protein spectroscopy.

Figure 1 compares the refractive indicies of hydrated and anhydrous toluene. Toluene has a higher solubility of water than hexane and iso-octane and the refractive index shows a marked increase with hydration. Water content is an important parameter in studying proteins in organic solvents. The hydration of enzymatic proteins has a profound effect on their conformation and reactivity and is difficult to measure non-invasively with other techniques.[3] Preliminary results for iso-octane, toluene and cyclohexane show that the protein refractive index is profoundly affected by even small amounts of water present in the solvents.

We will present a detailed study of the hydration of protein in the non-polar hydrophilic solvent 1,4-dioxane.

CFD6 **Table 1** Table of estimated THz optical constants of organic solvents used in studying protein suspensions. The measurement accuracy of n and k is better than ± 0.005.

Solvent	Freq (THz)	n	k	$n_{optical}$	[w/w]% H_2O
iso-octane	0.2	1.421	0.003	1.3914	0.006
	2	1.415	0.003		
n-hexane	0.2	1.408	0.008	1.3749	0.01
	2	1.404	0.002		
toluene	0.2	1.555	0.015	1.4969	0.03
	2	1.540	0.008		

CFD7 **9:30 am**

Characterization of Liquid Crystals 5CB in Terahertz Frequency

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1. Introduction

The birefringence behavior of liquid crystals (LCs) is well known and extensive utilized for the modulation of visible and infrared beams. However, knowledge of the dielectric and electro-optic properties of the LCs in millimeter and submillimeter frequency region of has remained incomplete. Terahertz (THz) time-domain spectroscopy, together with its unique time-resolved feature and high signal-to-noise ratio, has become a powerful tool for studying the electromagnetic properties of materials in the millimeter and submillimeter frequency region.[1,2] In this paper, we present the experimental results of the refractive indices of nematic LCs 5 CB and a preliminary result of electrically controlled birefringence.

2. Results and discussions

A reference of temporal THz waveform is first obtained by introducing a vacant cell between the THz transmitter and the receiver. Subsequently, a LC cell is introduced in the path of the THz beam and a second set of waveform is taken. The spectra of THz transient can be obtained by applying a fast Fourier transform (FFT) to the time domain waveform. Dividing the spectra obtained with a sample by the spectra obtained without a sample yields the transmission function of the sample. The refractive indices of sample can be obtained by solving the transmission function of the sample. Since a nematic LC is a uniaxial crystal,[3] the information for n_e and n_0 of LC can be obtained by adjusting the director of LC parallel and perpendicular to the direction of polarization of THz wave, respectively. In our case, it's easy to achieve by rotating the LC cell. Figure 1 shows the n_e and n_0 of 5 CB in ~0.2–1.4 THz regime. There is no sharp resonance in this frequency range. Both Re(n_e) and Re(n_0) increase