

# Terahertz Pulsed Spectroscopy as a new tool for measuring the structuring effect of Solutes on Water

Nina Kaun<sup>1</sup>, Josefa R. Baena<sup>2</sup>, David A. Newnham<sup>3</sup> and Bernhard Lendl<sup>1</sup>

<sup>1</sup>Inst. of Chemical Technologies and Analytics, Vienna University of Technology, A-1060 Vienna, Austria, <http://www.iac.tuwien.ac.at/cavs>

<sup>2</sup>Dep. Of Anal. Chem. University of Cordoba, Campus de Rabanales, E-14071, Cordoba, Spain

<sup>3</sup>TeraView Limited, Platinum Building, St John's Innovation Park, Cambridge, CB4 0WS UK, [www.teraview.com](http://www.teraview.com)



## ABSTRACT

Absorption spectra of aqueous solutions of “chaotropes” (structure-breakers) and “kosmotropes” (structure makers) have been recorded in the mid-IR and terahertz spectral region. A different impact of the two groups of solutes on the absorption spectrum of water was found in the recorded THz spectra. A concentration dependent increased absorption across the investigated terahertz spectral region (0.04 - 2 THz, 1,3 - 66 cm<sup>-1</sup> respectively) has been recorded for all studied chaotropic solutions, whereas the opposite has been obtained for kosmotrope-containing solutions. In the case of ionic solutes a further increase in absorption towards higher wavenumbers was measured.

## THE INSTRUMENT

TPI spectra 1000  
(TeraView Limited, UK)

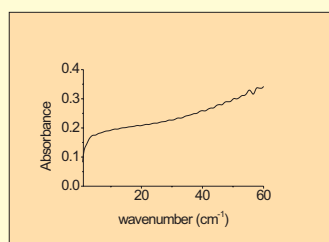


The nitrogen-purged TPI spectra 1000 sample compartment was equipped with a conventional flow cell connected to a peristaltic pump. As windows two 4 mm thick Polyethylene plates were used with a 50 μm thick spacer forming the cuvette.

## AQUEOUS SOLUTIONS

Solutions of various concentrations, water as background

## SPECTRUM OF PURE WATER

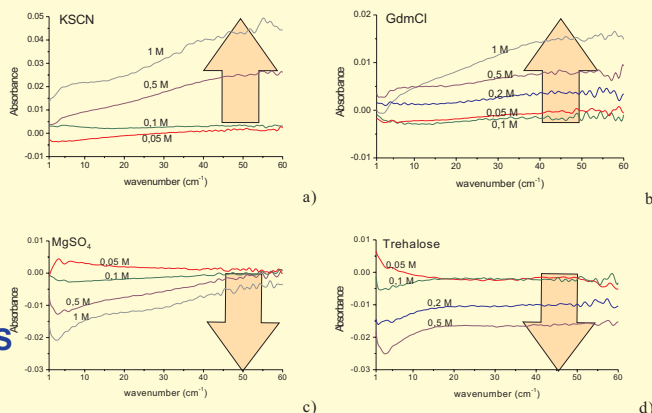


Absorbance spectrum of pure water with air filled flow cell as background at 295 K

## CHAOTROPES “Disorder makers”

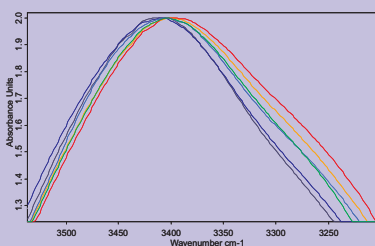
ADDING  
SOLUTES

## KOSMOTROPES “Order makers”



The terahertz spectra of aqueous solution of different solutes can thus be viewed as a combination of two different effects, which are reflected in the slope and intercept of the simplified spectrum respectively. We propose that from the sign of the intercept this being positive or negative a distinction between chaotrope and kosmotrope can be made. A significant slope is only observed for ionic substances.

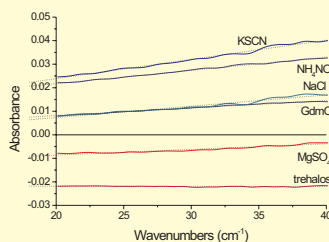
## COMPARISON TO THE MID-IR



The red line gives the kosmotropes trehalose (0.5 M) and MgSO<sub>4</sub> (1 M). The blue ones are the KSCN (0.5 M), GdmCl (0.5 M), NH<sub>4</sub>NO<sub>3</sub> (1 M) and NaCl (1 M). The green one refers to water of HPLC grade.

Compared to the terahertz region the effect of the solutes is here less pronounced.

## EVALUATION



	Slope (m)	Intercept (b)
MgSO <sub>4</sub>	2.4e-4	-1.3e-2
trehalose	2.5e-6	-2.1e-2
KSCN	8.2e-4	7.6e-3
GdmCl	3.2e-4	1.9e-3
NH <sub>4</sub> NO <sub>3</sub>	5.6e-4	1.1e-2
NaCl	4.8e-4	-2.3e-3



Financial support by the Austrian Science Foundation within the project P13350 ÖCH is gratefully acknowledged.