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ΠΑΝΕΠΙΣΤΗΜΙΟ ΙΩΑΝΝΙΝΩΝ
Εργαστήριο Φυσικοχημείας

ΙΝΣΤΙΤΟΥΤΟ
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ΚΑΙ ΥΠΟΛΟΓΙΣΜΩΝ

Vibrational and Ultrasonic Broadband Spectroscopies: Research Tools in Pure and Applied Chemistry and Chemical Physics

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https://chem.uoi.gr/meli-dep/angelos-kalampounias

Current research activities

Structure and Dynamics of Condensed Matter

- High-temperature Vibrational (Raman & IR) Spectroscopy:

i. *Correlations* between spectral intensity data and stoichiometry, equilibrium constants and thermodynamics of reaction equilibria in solutions and melts

ii. Inorganic coordination *complexes* in glassy, supercooled and molten state. Structural studies of inorganic molten salts at high temperatures by Raman spectroscopy and UV/VIS spectrophotometry

iii. *Structure and dynamics* of the *fluids confined in nanopores*, nanoconfined chalcogens

iv. Studies for the fundamental understating of *structure and dynamics* of a diverse family of *glasses, supercooled liquids and melts* (halide, oxide, and chalcogenide glasses)

- Acoustic spectroscopies: Ultrasonic relaxation spectroscopy & Ultrasonically-induced birefringence

i. *Thermo–reversible aggregation* phenomena

ii. *Proton-transfer* reactions

iii. *Conformational* changes

iv. *Complexation* and *kinetics* (inclusion complexes, micellization)

v. *Relaxation mechanisms* of polymeric chains in solutions

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Simulations & Theoretical Calculations:

- **COMSOL Multiphysics®** modeling (general-purpose simulation software for modeling of the acoustic processes)

- **Gaussian 09**

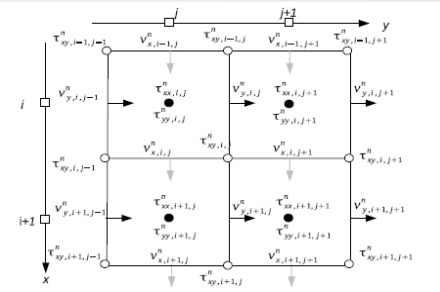
Expanding the limits of computational chemistry

(Quantum chemistry calculations for the calculation of: Vibrational spectra, thermodynamic properties & energetics, interaction sites, conformations, optimized structures, etc.)

- **PSpice®** simulation software (circuit simulations using circuit electronics)

PSpice Systems

- **Homemade FEM software** developed in MATLAB for calculations in the field of acoustics (FEM: finite element method)



Computational facilities

- Server HP ProLiant DL580 Generation 5 (G5)

(four Quad-Core Intel® Xeon® Processors)

- (hexa core i5 -9500)

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Experimental facilities

- Glassware, Stirrers & hot plates
- Drying ovens
- Chemicals/Reagents/solvents/gases
- Water and oil baths
- Desiccators
- Balances
- Pumps
- Centrifuge

- **Oscilloscopes**
- **Electric pulse & Function generators**
- **pW Power meters (CW)**
- **Fast Photodiodes**
- **Conductivity meter**
- **T-controlled Density meters (DMA)**
- **T-controlled Viscosimeters**
- **Digital Refractometer**
- **pH-meters**
- **Vacuum lines**
- **Glove-bags**
- **Optical microscope**
- **UV/Vis**
- **×2 homemade high-temperature furnaces 1100°C(3-zones, inert atmosphere)**

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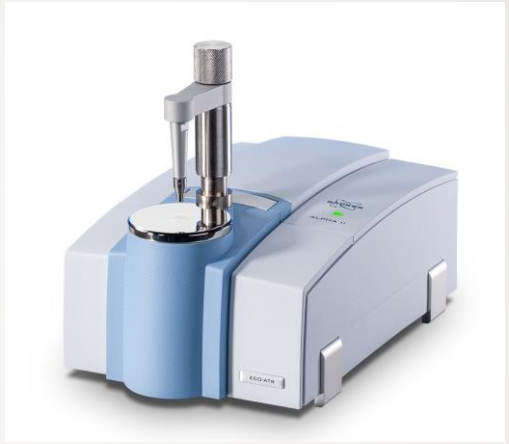
IR/NIR spectroscopy



Vibrational spectroscopy - IR

- **FTIR (Bruker-Alpha) 400-4000 cm^{-1}**
- **ATR (Attenuated Total Reflectance, ZnSe)**
- **DRIFT (Diffuse Reflectance Infrared Fourier Transform)**

(liquid cells, homemade high-T cells)

Vibrational spectroscopy - IR

- **FTIR (Jasco 4700) 400-7800 cm^{-1}**
- **ATR (Attenuated Total Reflectance, Diamond)**

- **Specac Pearl (Liquid FTIR transmittance accessory)**

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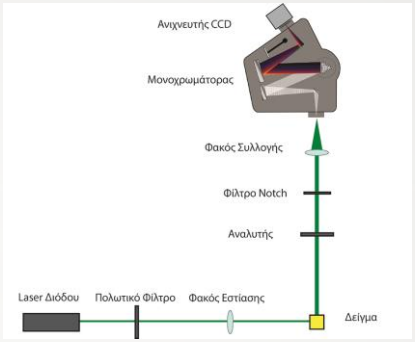
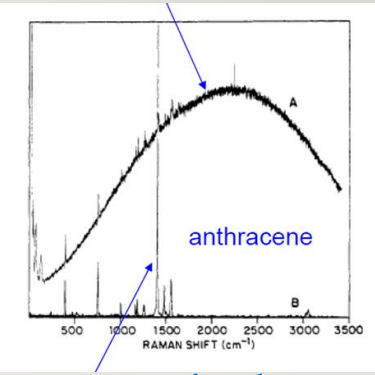
In-situ High-temperature Raman spectroscopy

Vibrational spectroscopy – macro-Raman (In collaboration with Assist. Professor S. Kaziannis, Department of Physics, UoI)

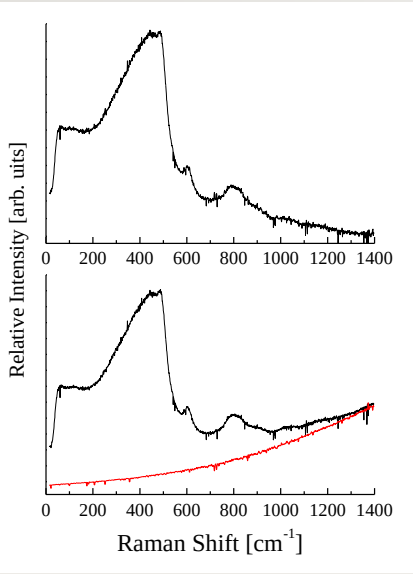
- Scattering angle 90° or 180° (backscattering) utilizing optical fibers
- CCD detector
- High-Temperature optical furnace
- Polarization dependent measurements (VV, VH)
- **Continuous-mode operation:** continuous-wave lasers (He-Ne @ 632.8nm, diode-pumped solid-state laser @ 532 nm)
- **Pulsed-mode gated-operation:** pulsed lasers (Nd:YAG Laser, ns duration, @ 532 nm)

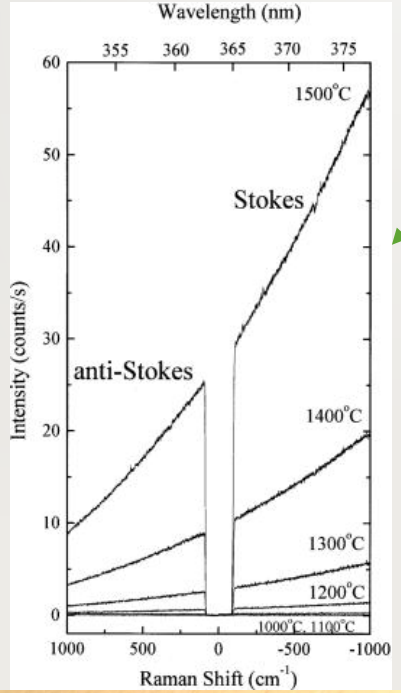


Raman signal + Fluorescence



Raman signal





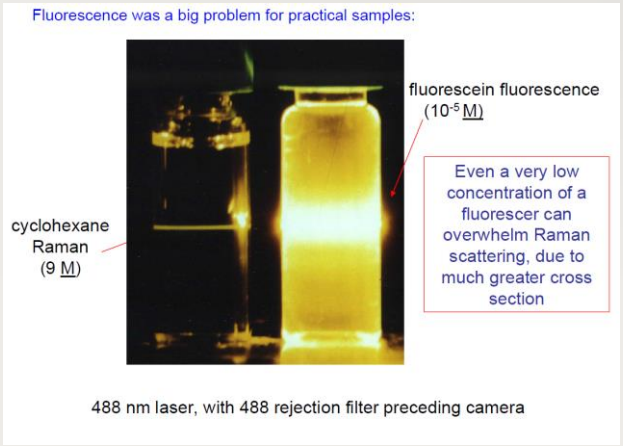
Thermal radiation of furnace and material in the recording range of the Raman spectrum

Advantages of a time-resolved macro Raman setup

1) Reduces Blackbody radiation interference

2) Overcomes Fluorescence

(Raman measurement faster than the slower fluorescence mechanism)



Acoustic spectroscopy – Ultrasonic relaxation spectroscopy

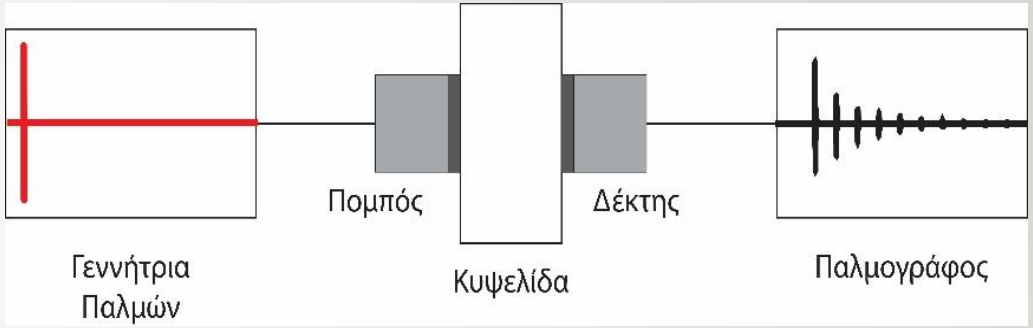
A Pulse-Echo setup :

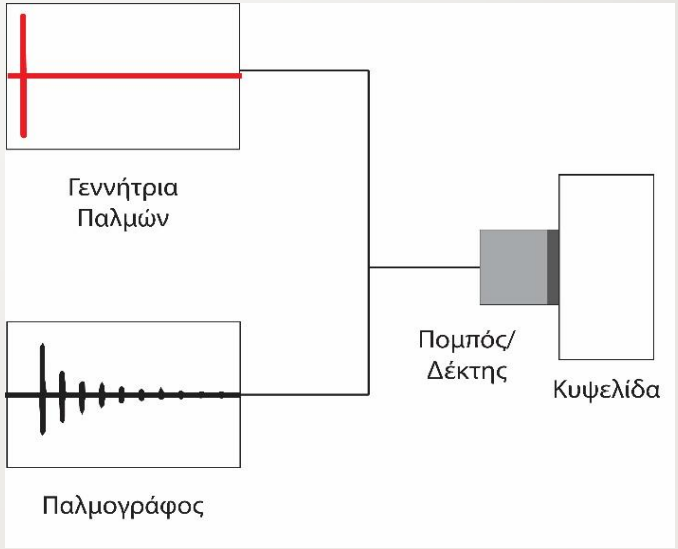
Short-duration RF electric pulses trigger the ultrasonic waves that propagate through the sample

For a fixed pathlength one is able to estimate:

- the speed of sound u_s (u_s = pathlength / time between neighboring echoes)
- the sound attenuation a (exponential decay of the signal)

u_s, a **versus** *frequency*





- ✓ Non-destructive technique
- ✓ Required sample volume < 2 ml
- ✓ Low-ultrasonic intensity (no sono-chemistry effects)
- ✓ Low-repetition rate of the ultrasonic pulses to avoid heating and streaming effects
- ✓ Frequency range: MHz region
- ✓ Temperature range: -15^o έως +60^{o}C

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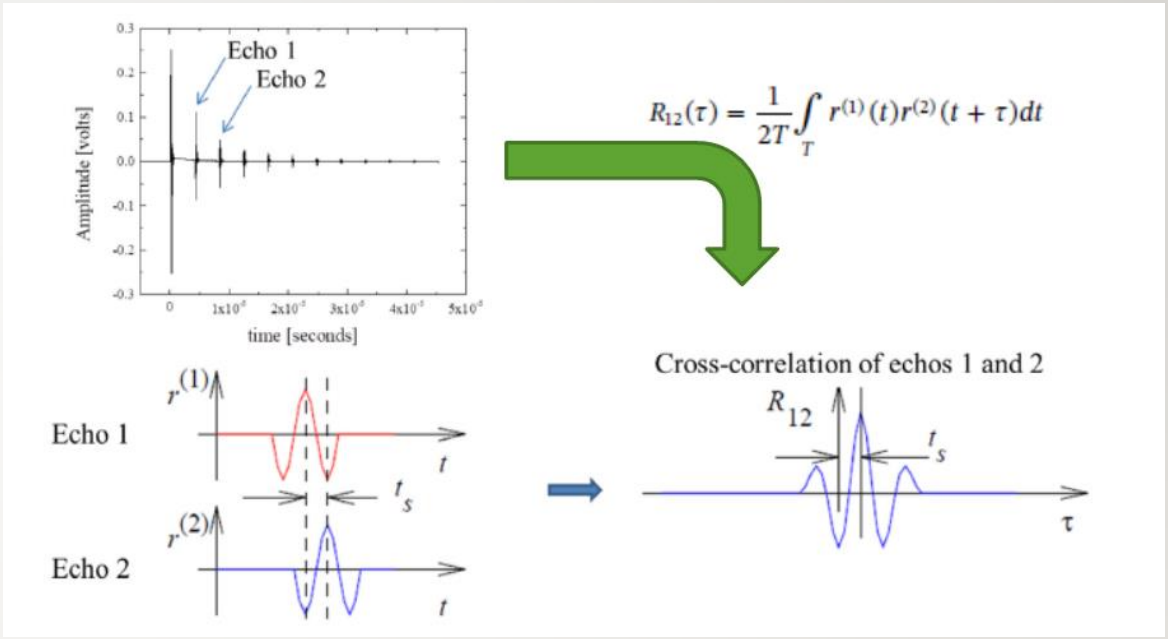
Sound speed and attenuation estimation

Time-domain – Velocity estimation

- ✓ The precise transit time is estimated from the **cross-correlation of two consecutive echoes** in the backwall echo train
- ✓ Pathlength is fixed
- ✓ Speed of sound u_s = pathlength / transit time



Time-domain – Attenuation estimation

the attenuation coefficient ***a*** (***exponential decay of the signal***) is calculated from the amplitudes of the echoes observed ***in the time-domain trace*** as:

$$a_f = \frac{-20}{2(m-n)d} log\left(\frac{I_m}{I_n}\right)$$

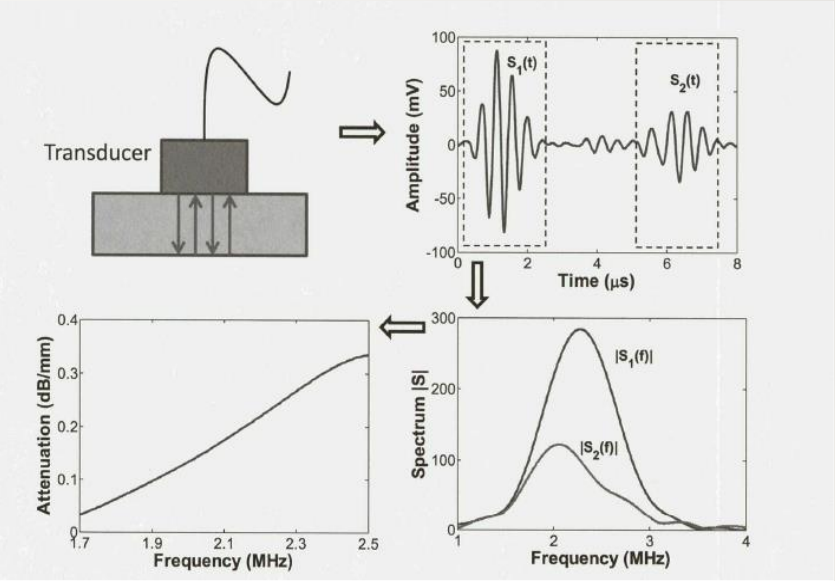
where I_m and I_n are the maximum amplitudes of the m^{th} and n^{th} pulse echoes in Volts, respectively.

Frequency-domain – Attenuation estimation

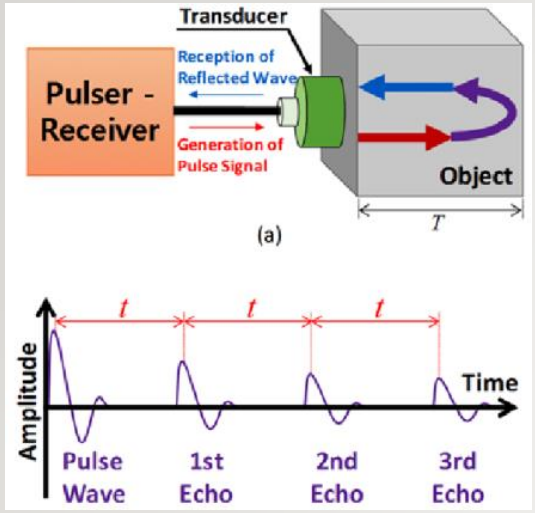
the attenuation coefficient ***a*** is calculated using **spectral ratio FFT technique *in the frequency-domain*** as:

(R_{top}, R_{bottom}: reflection coefficients)

$$\alpha(f) = \frac{1}{2d}\left[\ln\left|\frac{S_1}{S_2}\right| - \ln\left|\frac{D(f,2d)}{D(f,4d)}\right| + \ln\left|R_{top}R_{bottom}\right|\right]$$



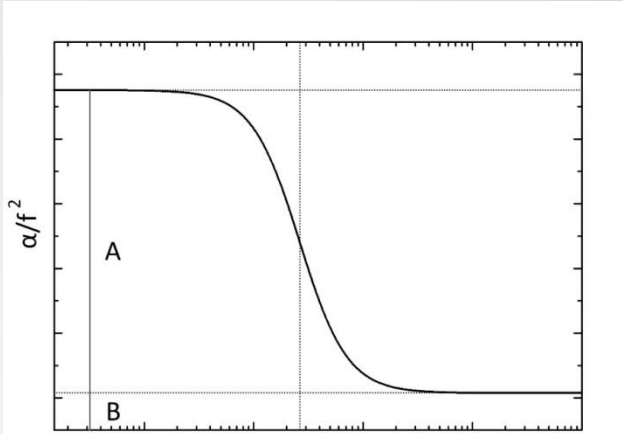
Typical ultrasonic relaxation spectra



Sound absorption vs frequency

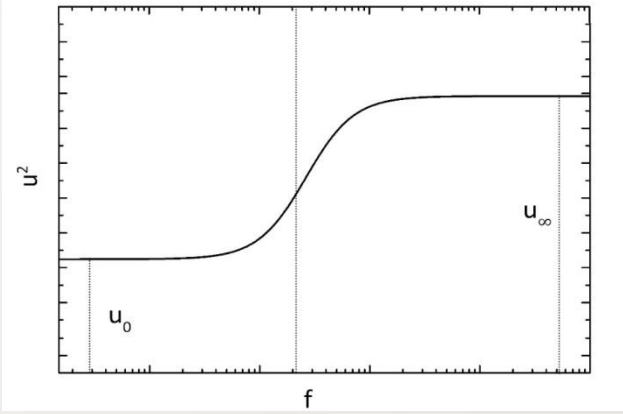
$$\frac{\alpha}{f^2} = \frac{A}{1 + \left({}^{f}/_{f_r}\right)^2} + B$$

Debye relaxation



Ultrasonic velocity vs frequency

$$\Delta u = \left(\mu^{ch}\right)_{max} u_0 u_\infty \frac{\left({}^{f}/_{f_r}\right)^2}{1 + \left({}^{f}/_{f_r}\right)^2}$$



Characteristic relaxation time:

$\tau_r = 1/(2\pi f_r)$

Time scales:

Vibrational spectroscopies: 10^{-12} - 10^{-14} s (ps region)

Acoustic spectroscopies: ns – ms

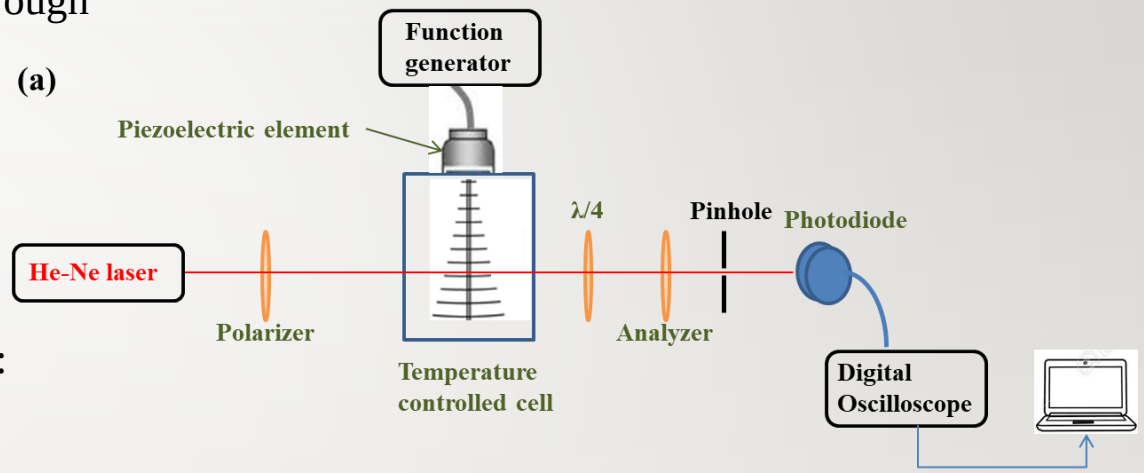
(Combination of Vibrational & Acoustic spectroscopies: wide frequency range from KHz - THz)

Acoustic spectroscopy – Ultrasonically-induced birefringence

Ultrasonic wave: forced orientation of molecules
laser: measurement of the orientation/disorientation process

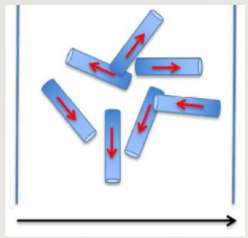
The **laser intensity change** is related to the induced **optical retardation δ(t)** through the equation:

$$I = I_0 sin^2\left(\frac{\delta}{2}\right)$$



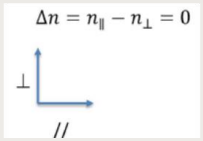
The **induced birefringence *Δn*** is associated to the **optical retardation** through:

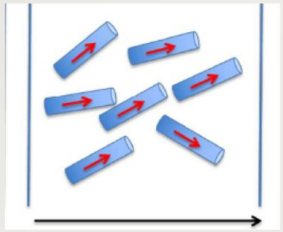
$$\Delta n = \frac{\delta\lambda}{2\pi d}$$



Field off **(isotropic medium)**

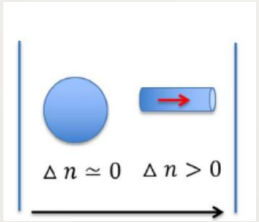
$\Delta n = n_{\parallel} - n_{\perp} = 0$





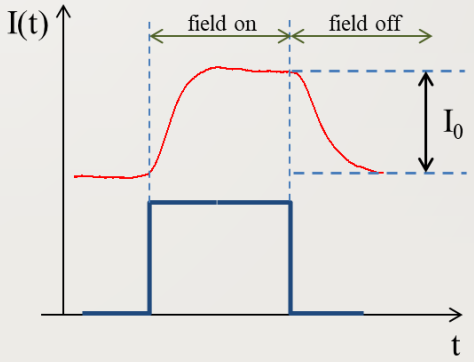
Field on **(anisotropic medium)**

$\Delta n = n_{\parallel} - n_{\perp} \neq 0$



Field on

(b)



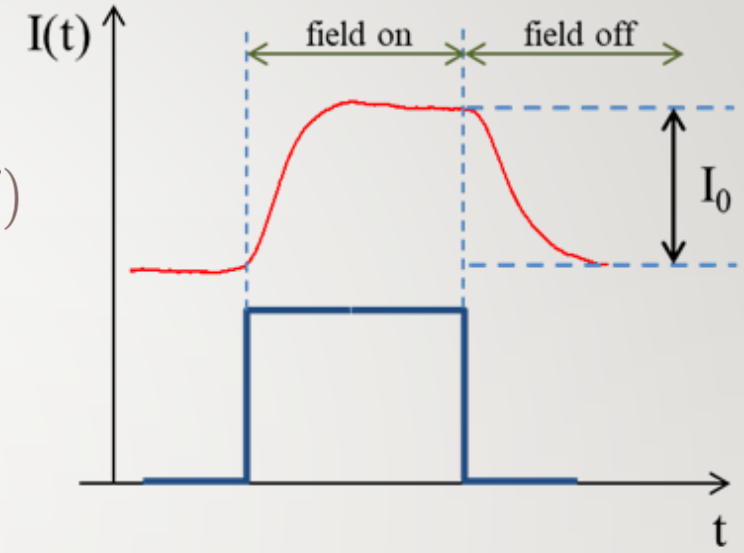
Ultrasonically-induced birefringence

During the acoustic **field-on** regime, The rise of the birefringence is given by a ***stretched exponential*** function:

forced orientation process: $\Delta n(t) = \Delta n_{max}\left(1 - e^{-(t/\tau)^{\beta}}\right)$

while after **sudden termination of the field**, the birefringence decay is:

Spontaneous rotational diffusion (disorientation relaxation): $\Delta n(t) = \Delta n_{max} e^{-(t/\tau)^{\beta}}$



Δn_{max}**:** corresponds to the **steady state birefringence (static birefringence)** when the acoustic field is on

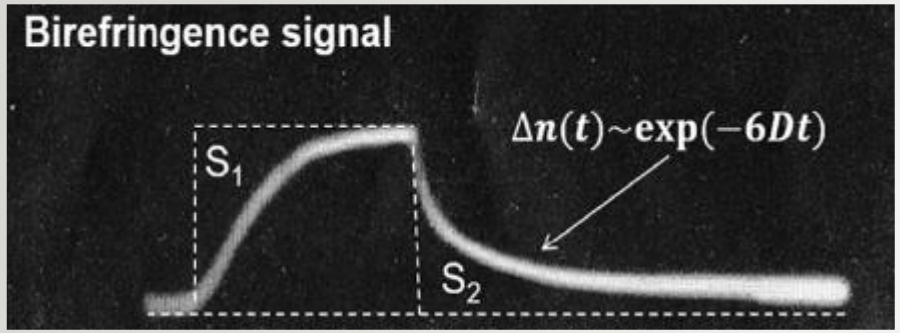
τ_{rise}, τ_{decay}**:** are the two different characteristic relaxation times for the rise and decay of the birefringence signal

β**:** is assigned to the width of the relaxation time distribution

β**=1:** simple exponential function **(Debye relaxation)**

The smaller the value of β, the larger is the distribution of the relaxation times.

Ultrasonically-induced birefringence –Dipole moments



- ✓ **Stationary value (plateau) – Static birefringence Δn_{max}: size, shape**
- ✓ **Relaxation process – Dynamic birefringence $\Delta n(t)$: size, shape, charge distribution, permanent dipoles/induced dipoles**

S_1: area under the build-up curve
S_2: below the relaxation curve
Dotted square: the applied acoustic pulse

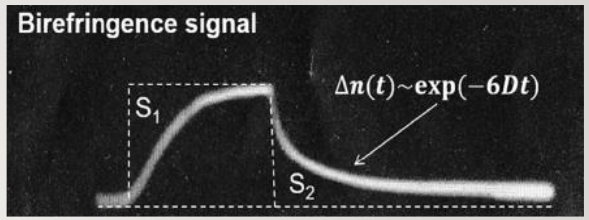
$$R = \frac{1 - \frac{S_1}{S_2}}{2\frac{S_1}{S_2} - 8} \propto \frac{permanent\ dipole\ moments}{induced\ dipole\ moments}$$

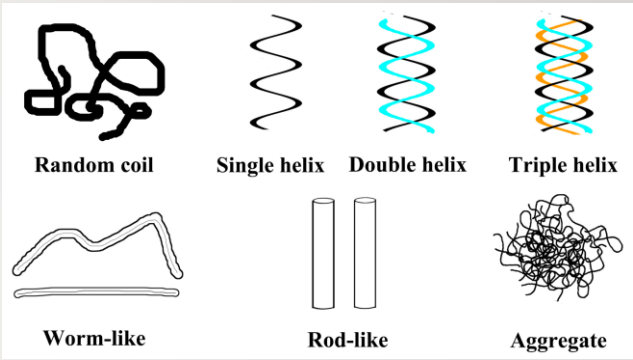
- S_1=S_2 then R=0: Permanent dipole moments=0 (pure induced dipoles)
  or permanent dipole moments >> induced dipole moments
- S_1=4S_2 then $R \rightarrow \infty$: Permanent dipole dominates the orientation mechanism

Ultrasonically-induced birefringence – Particle size and shape determination

The **relaxation time τ_{decay}** is directly related to the average **rotational diffusion coefficient, D_r**:

$$\Delta n(t) = \Delta n_{max} e^{-(t/\tau)^{\beta}} \longrightarrow D_r = \frac{\beta}{6\tau_{decay}\,\Gamma\left(\frac{1}{\beta}\right)}$$





✓ In general, the rotational diffusion constant of **right circular cylinders** is given by:

$$D_r = \frac{3kT}{\eta_0 \pi L^3}(\ln\,(L/d) - \gamma_r)$$

η_0: solvent viscosity
kT: thermal energy
L: rod length
d: rod diameter
γ_r : is a frictional factor

For **long cylinders**: $$\gamma_r = 0.877 - 7\left(\frac{1}{\ln\,(2L/d)} - 0.28\right)^2$$

For **long cylinders with spherical ends**: $$\gamma_r = 0.447 + 8.26[\ln\,(1 + (L/d))]^{-1} - \sum_{j=1}^{6} a_j (L/d)^{-j/4}$$

✓ The rotational diffusion constant for a **worm-like coil** about its minor axis is:

$$D_r = \frac{kT\lambda}{\eta_0 L^2}[0.506(2\lambda L)^{1/2} - 0.636\,\ln\,(b\lambda) - 1.548 + 0.64(b/a)]$$

✓ The rotational diffusion constant of the **weakly bending rod**, assuming that $\lambda L/2 \ll 1$ is:

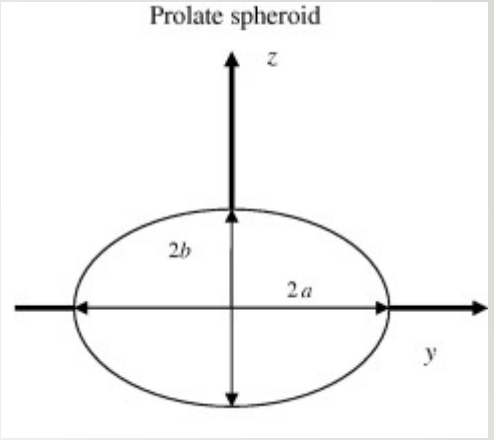
$$D_r = \frac{kT}{\eta_0 \pi L^3}[3\,\ln\,(L/b) - 7.0 + 4(b/a) + \lambda L(2.25\,\ln(L/b) - 6.66 + 2(b/a))]$$

Ultrasonically-induced birefringence – Particle size and shape determination

✓ For **prolate particles**:

$$D_r = \frac{\beta}{6\tau_{decay}\,\Gamma\left(\frac{1}{\beta}\right)}$$

$$\tau = \frac{\eta V^*}{kT}$$ Debye-Einstein equation (dilute solution)



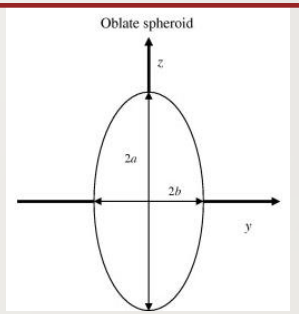
Hydrodynamic volume: $V^* = \frac{8\pi a^3}{9}\left(\frac{1-p^4}{(2-p^2)G(p)-1}\right)$

$$G(p) = \frac{1}{\sqrt{1-p^2}}\,ln\left[\frac{1+\sqrt{1-p^2}}{p}\right]$$

$$p = \frac{b}{a} = \frac{minor\ axis}{major\ axis} : axial\ ratio$$

✓ For **oblate particles**:

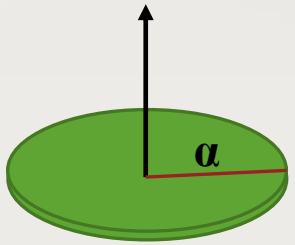
$$D_r = \frac{3kT}{16\pi\eta a^3}\left(\frac{(2-p^2)(1-p^2)^{\frac{1}{3}}\arctan\left(\sqrt{p^2-1}\right)-1}{1-p^4}\right)$$



✓ For **infinitely thin disks**:

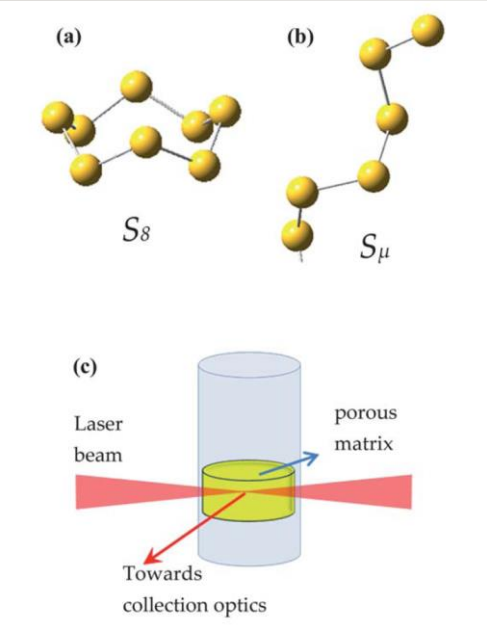
$$\tau = \frac{16\pi\eta\alpha^3}{9kT}$$

(under "stick" boundary conditions)
α: mean particle radii



Representative applications of Vibrational spectroscopy

Confinement & Thermo-aggregation phenomena in bulk and under confinement – The case of Sulfur



$$S_8 \rightleftarrows S_8^*$$

$$S_8 + (S_8^*)_{n-1} \rightleftarrows (S_8^*)_n$$

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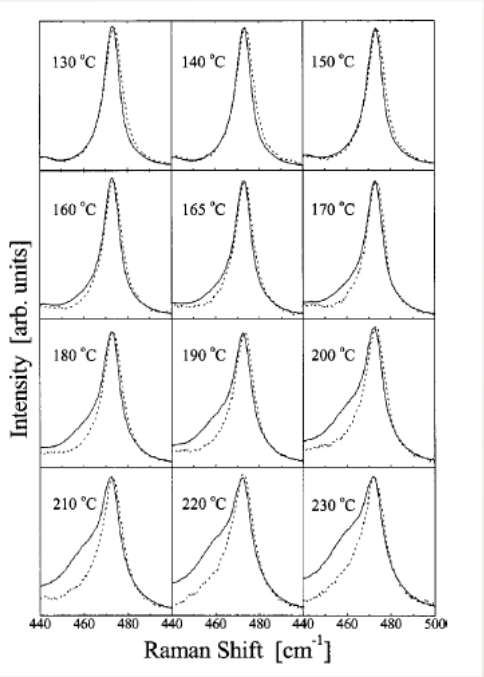
"Rounding" of the sulfur living polymerization transition under spatial confinement



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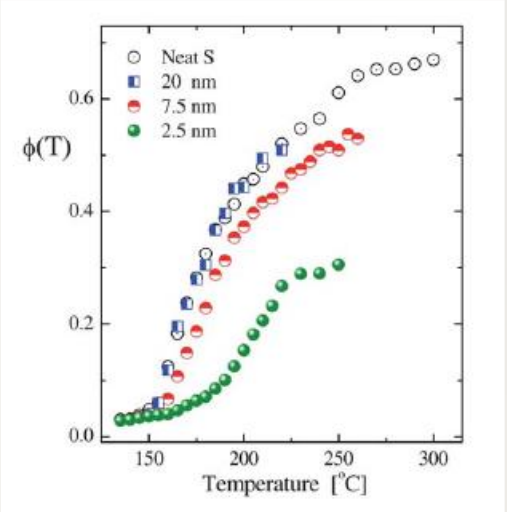
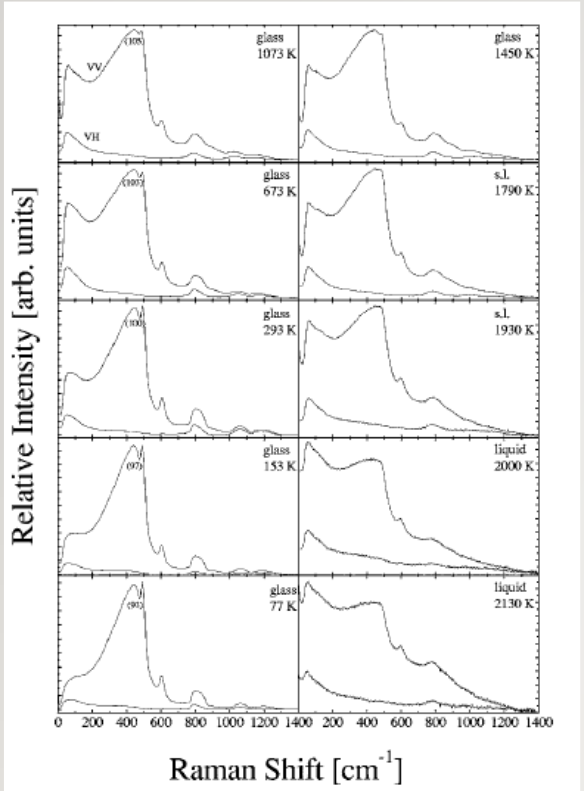
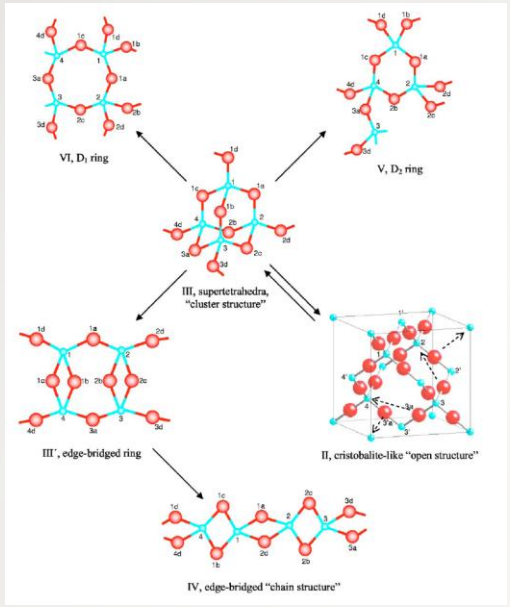
www.rsc.org/softmatter
PAPER

Confinement effects on liquid–liquid transitions: pore size dependence of sulfur's living polymerization



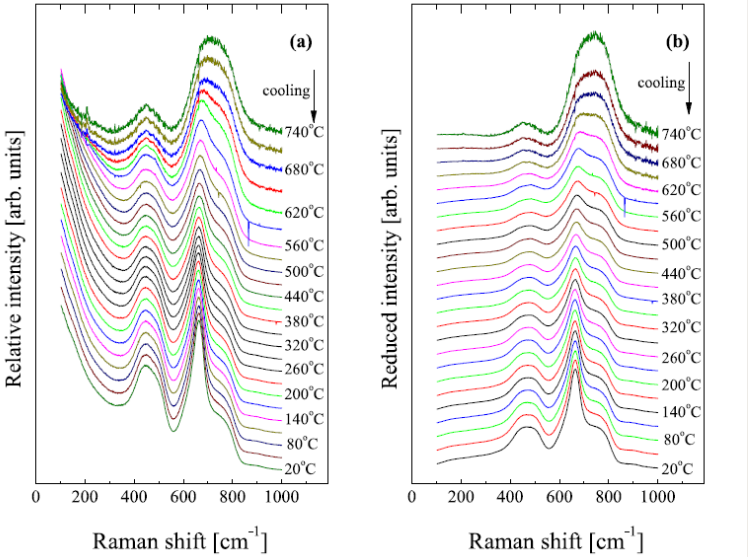
Temperature-induced structural changes (High-melting point oxides)





THE JOURNAL OF CHEMICAL PHYSICS **124**, 014504 (2006)

Temperature- induced structural changes in glassy, supercooled, and molten silica from 77 to 2150 K

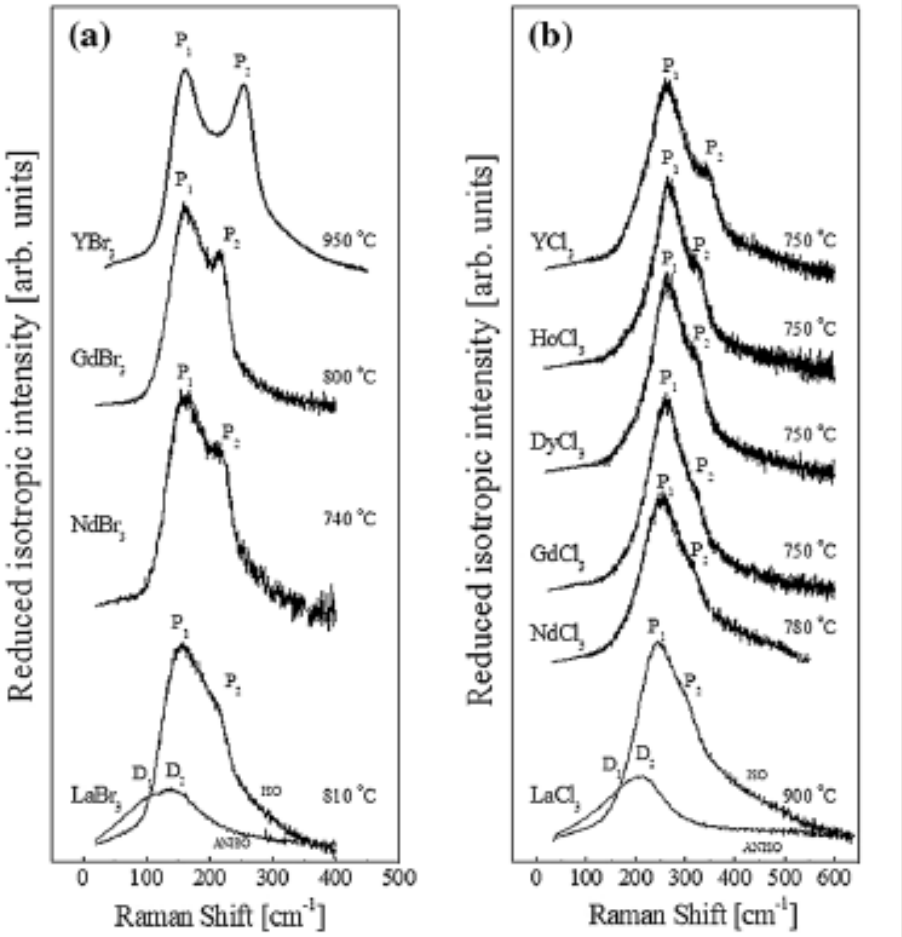


THE JOURNAL OF CHEMICAL PHYSICS **142**, 154503 (2015)

CrossMark click for updates

Glass-forming ability of TeO_2 and temperature induced changes on the structure of the glassy, supercooled, and molten states

2D Raman correlation spectroscopy



Chem. Pap. (2017) 71:1529–1539
DOI 10.1007/s11696-017-0147-2

CrossMark

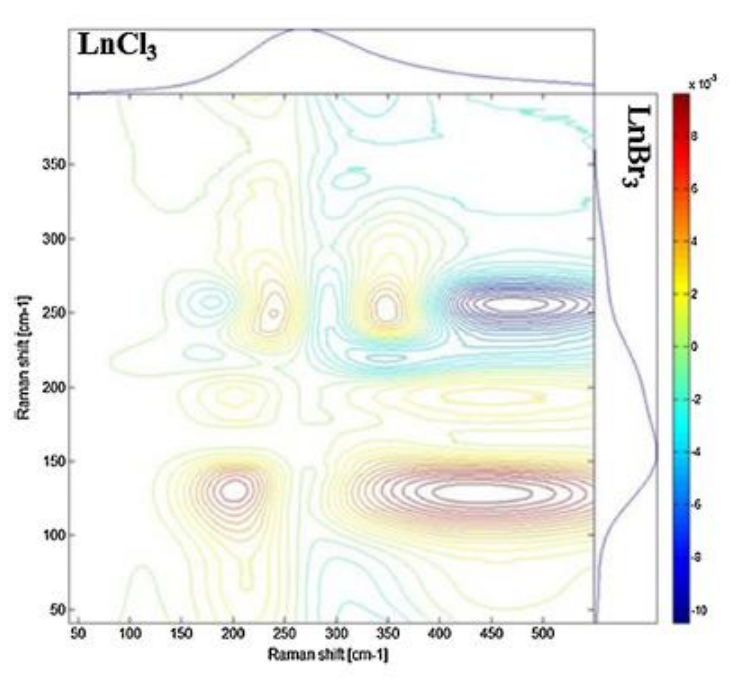
ORIGINAL PAPER

Correlating changes in structure and dynamical properties in LnX_3 (Ln = Y, Ho, Dy, Gd, Nd, La and X = Cl, Br) ionic melts

$$X(\nu_1, \nu_2) = \Phi(\nu_1, \nu_2) + i \cdot \Psi(\nu_1, \nu_2)$$

Synchronous and asynchronous spectral changes

Assignment of spectral changes to specific species



Vibrational dynamics & dephasing from "steady-state" experiments: Liquids under confinement

JOURNAL OF CHEMICAL PHYSICS VOLUME 118, NUMBER 18 8 MAY 2003

Short-time dynamics of glass-forming liquids: Phenyl salicylate (salol) in bulk liquid, dilute solution, and confining geometries

the isotropic and anisotropic Raman

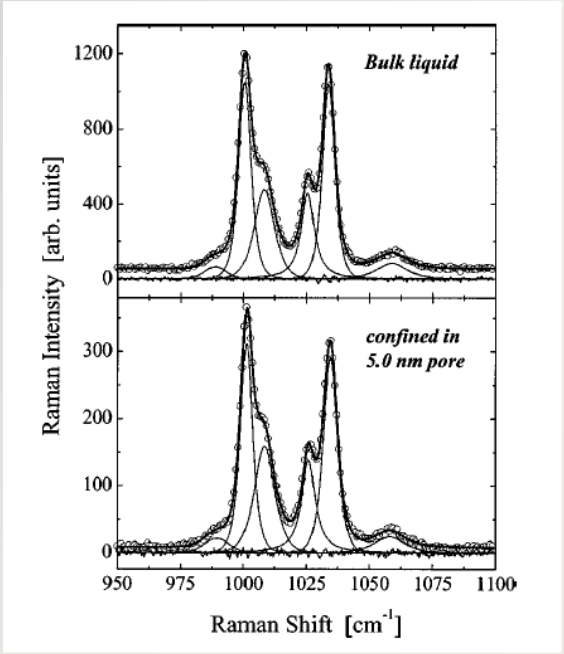
$$I_{iso}(\omega) = I_{VV}(\omega) - \frac{4}{3} I_{HV}(\omega) \quad \text{and} \quad I_{aniso}(\omega) = I_{HV}(\omega)$$

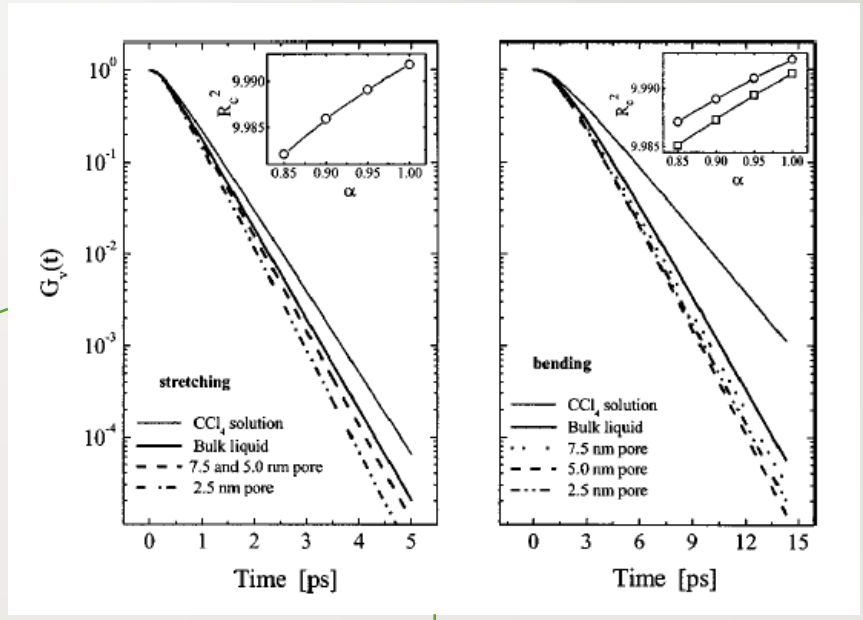
IFFT

Time-correlation functions of vibrational relaxation and reorientation:

$$G_V(t) = \int_{-\infty}^{+\infty} I_{iso}(\omega)\exp(i\omega t)dt$$

$$G_R(t) = \left(\int_{-\infty}^{+\infty} I_{aniso}(\omega)\exp(i\omega t)dt \right) / G_V(t)$$





Kubo model (simple liquids)

$$-\ln G_V(t)/M_2\tau_\omega^2 = \exp(-t/\tau_\omega) - 1 + t/\tau_\omega$$

τ_ω **time between collisions** in the medium and therefore allows for conclusions about **translational** and **collision dynamics**

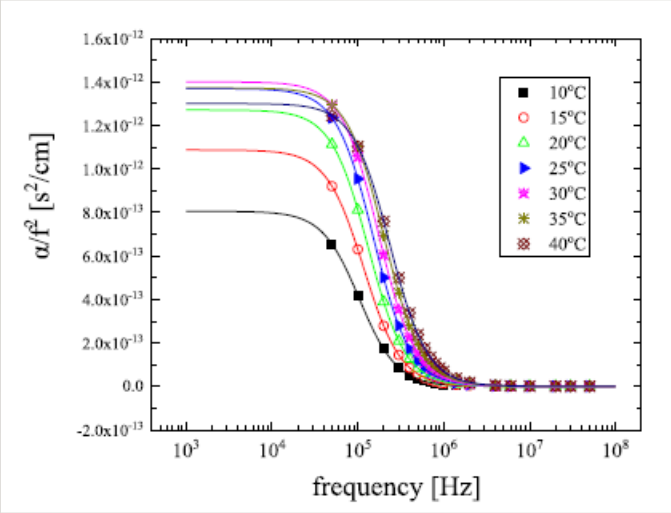
M_2**:** vibrational second moment. Sensitive to intermolecular forces. When M_2 increases repulsion forces prevail over attraction and vice-versa

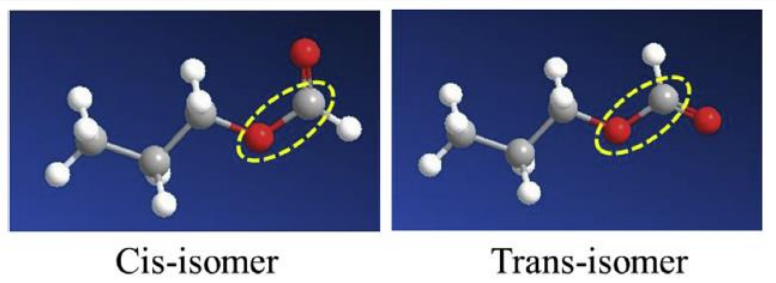
Rothschild model (complex liquids)

$$-\ln G_V(t)/M_2\tau_\omega^2 = \sum_{n=0}^{\infty} \frac{(-1)^n (t/\tau_\omega)^{2+n\alpha}}{n!(1+n\alpha)(2+n\alpha)}$$

Representative applications of Acoustic spectroscopies

Conformational changes of simple organic molecules





Propyl formate (neat liquid)

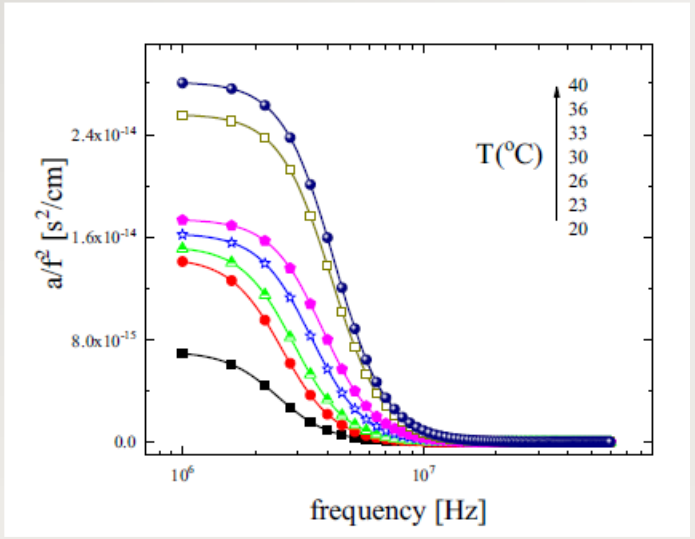
Journal of Molecular Structure 1212 (2020) 128146

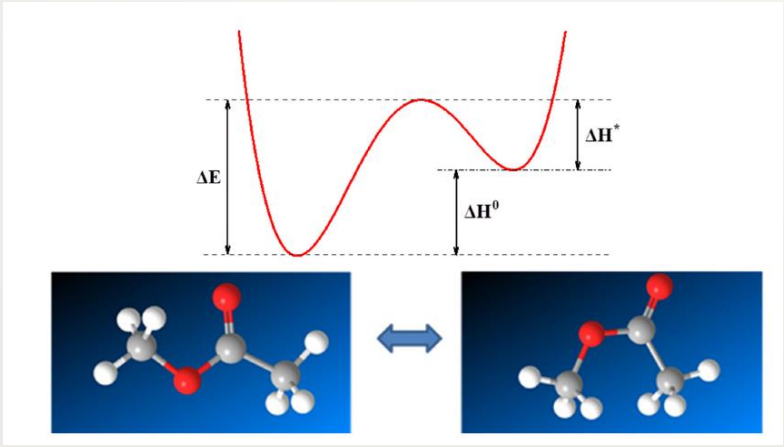
Contents lists available at ScienceDirect

Journal of Molecular Structure

journal homepage: http://www.elsevier.com/locate/molstruc

Exploring conformational change profile of n-propyl ester of formic acid by combining ultrasonic relaxation spectroscopy and molecular orbital calculations





Methyl acetate dissolved in EthOH

Journal of Molecular Liquids 302 (2020) 112519

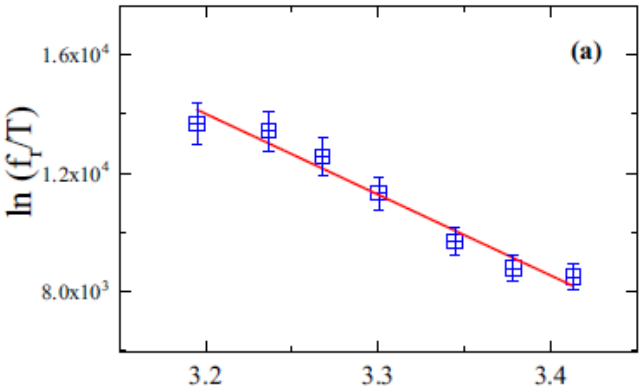
Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

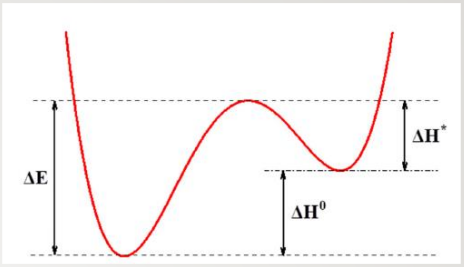
Conformational energy barriers in methyl acetate – Ethanol solutions: A temperature-dependent ultrasonic relaxation study and molecular orbital calculations

Thermodynamic analysis of Conformational changes

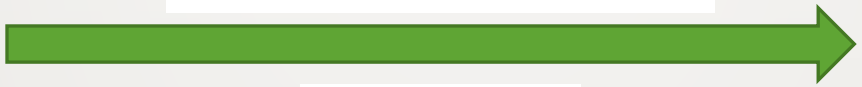


$$\frac{1}{2\pi f_r} = \frac{h}{k_B T} exp\left(\frac{\Delta H^* - T\Delta S^*}{RT}\right)$$

Activation enthalpy ΔH^*



$$\frac{T\mu_{max}}{u^2} = (constant) \times \exp\left(-\frac{\Delta H^0}{RT}\right)$$

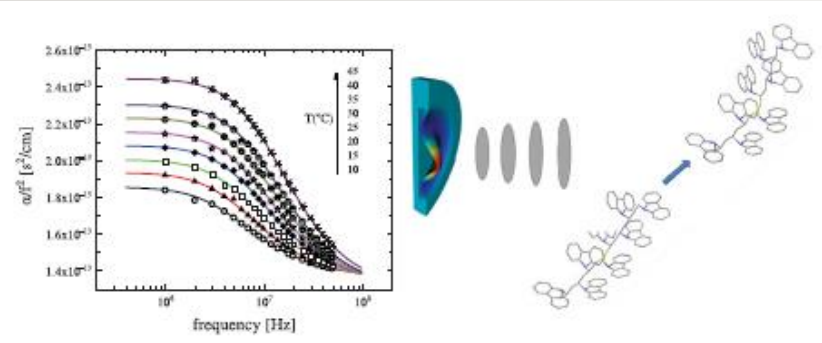


Enthalpy difference ΔH^0
between cis- and trans-isomers

$$\mu_{max} = \frac{1}{2} A u f_r$$

The experimentally estimated
energy barrier value was found equal to:
$\Delta E_{experimental} = \Delta H^* + \Delta H^0$

Fingerprints of segmental and normal mode motion of a polymer chain in ultrasonic absorption measurements



MOLECULAR PHYSICS e1802075
https://doi.org/10.1080/00268976.2020.1802075
Taylor & Francis
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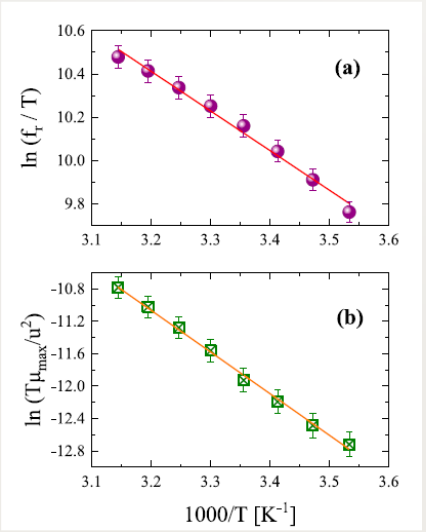
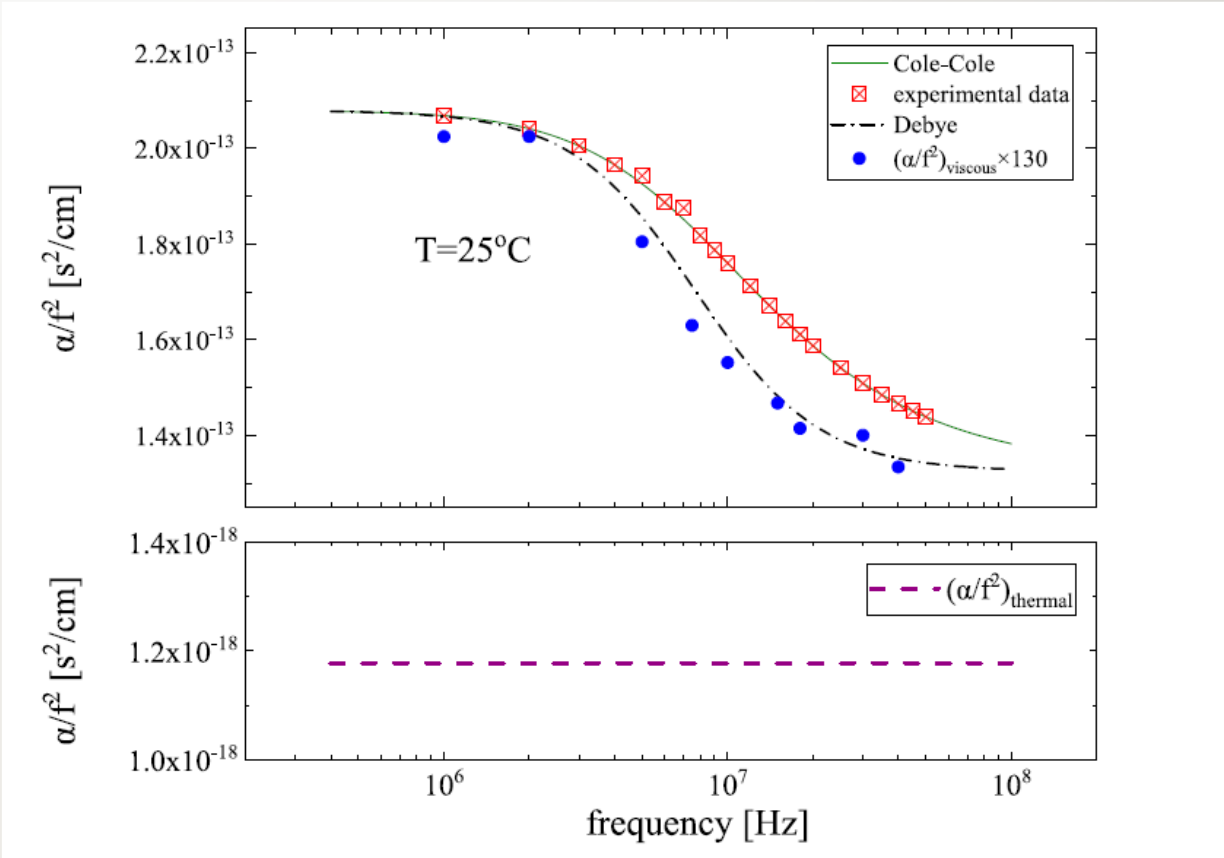
RESEARCH ARTICLE
Check for updates

Non-Debye segmental relaxation of poly-N-vinyl-carbazole in dilute solution

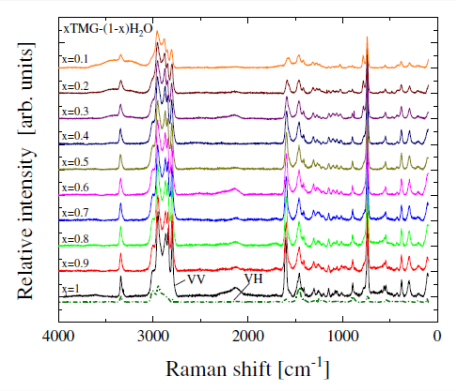
The data were best fitted using the real part of the Cole–Cole distribution function instead of Debye

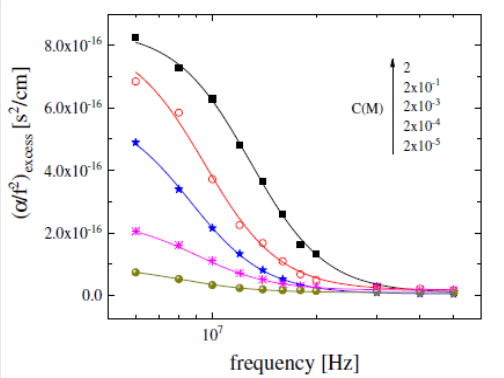
$$\frac{a}{f^2} = \frac{A\left\{1 + \left(\frac{f}{f_r}\right)^{\beta}\cos\left(\frac{\pi\beta}{2}\right)\right\}}{1 + 2\left(\frac{f}{f_r}\right)^{\beta}\cos\left(\frac{\pi\beta}{2}\right) + \left(\frac{f}{f_r}\right)^{2}} + B$$

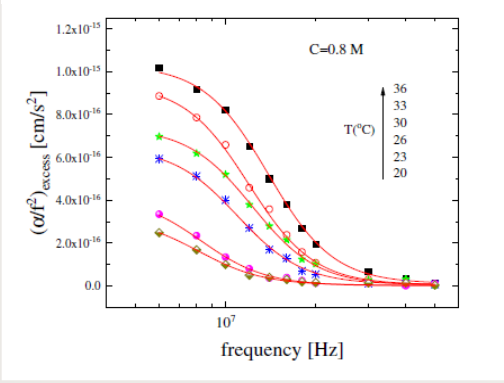




Proton-transfer reaction in amine solution: The case of 1,1,3,3, tetramethyl guanidine







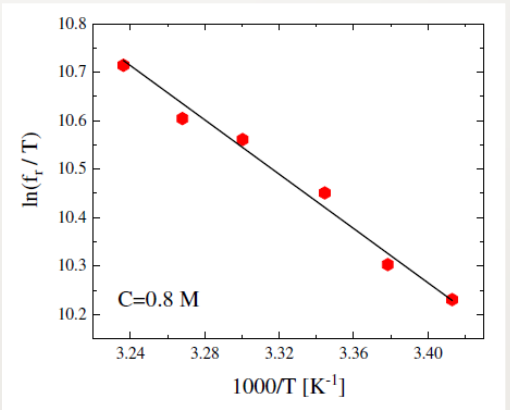
Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 229 (2020) 117958

Contents lists available at ScienceDirect

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

journal homepage: www.elsevier.com/locate/saa

Proton-transfer in 1,1,3,3 tetramethyl guanidine by means of ultrasonic relaxation and Raman spectroscopies and molecular orbital calculations



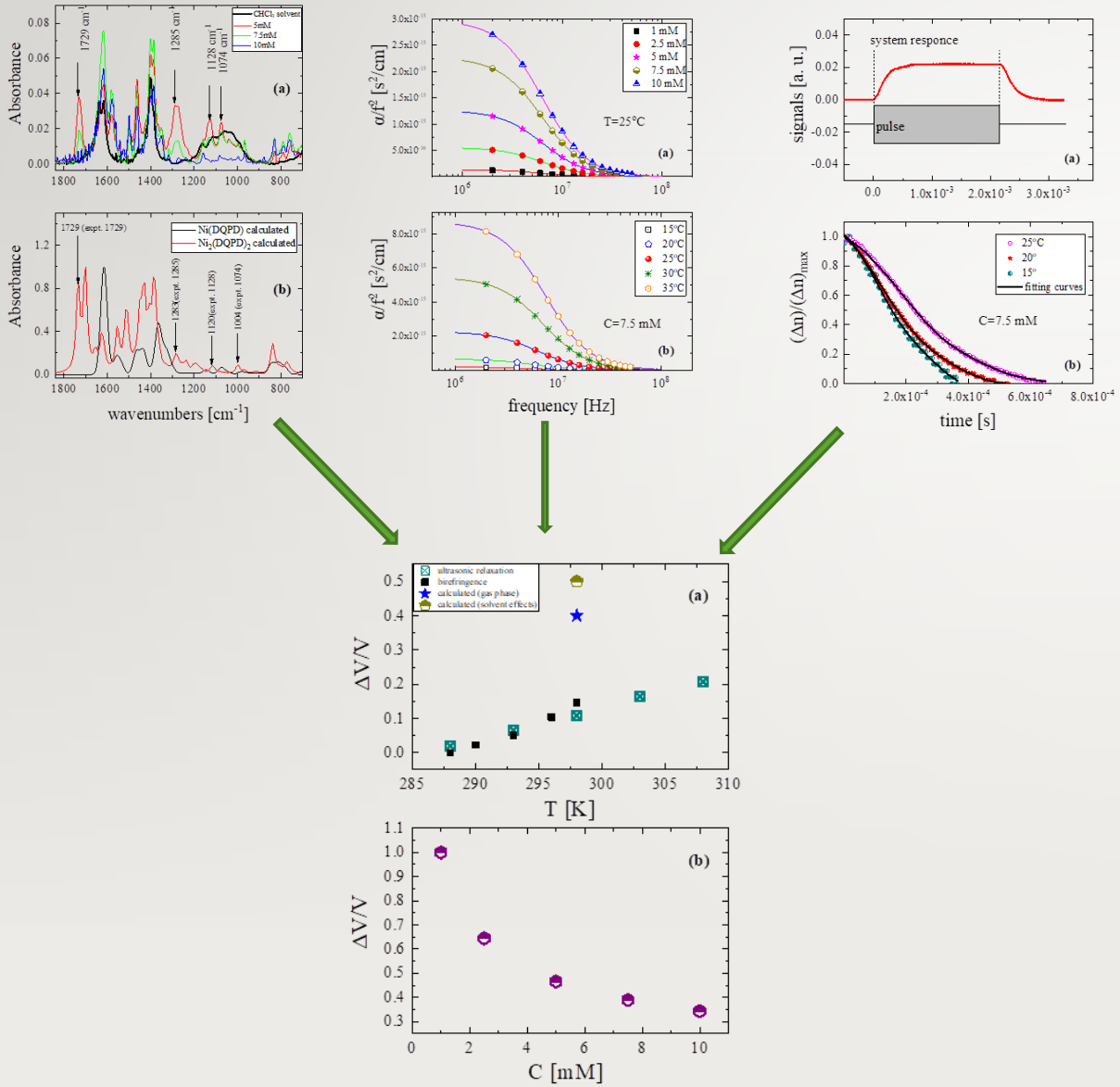
$$\frac{1}{2\pi f_r} = \frac{h}{k_B T} exp\left(\frac{\Delta H^* - T\Delta S^*}{RT}\right)$$

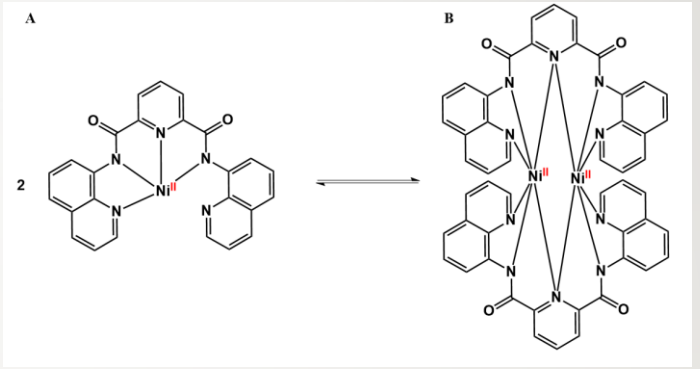
$$TMG + H_2O \rightleftharpoons TMGH^+ \cdots OH^- \rightleftharpoons TMGH^+ + OH^-$$

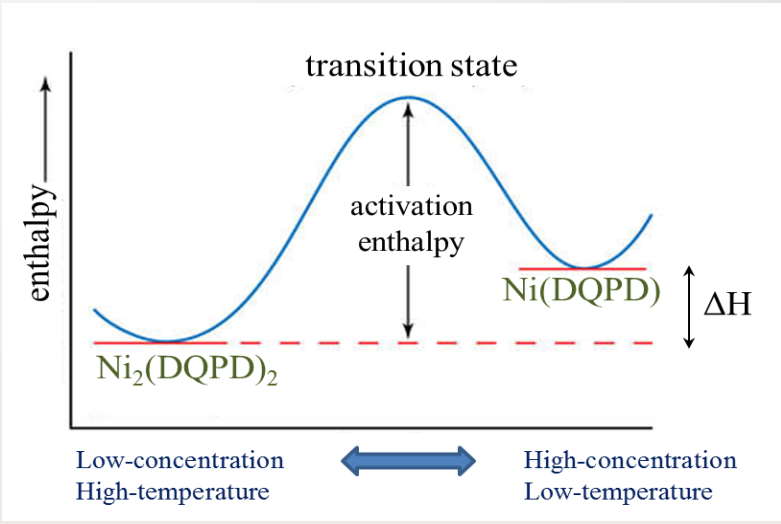
The activation enthalpy ΔH^* of proton-transfer is obtained from the slope of this graph and found equal to $\Delta H^* = 5.56 \pm 0.34$ kcal/mol

Probing the equilibrium between mono- and di-nuclear nickel(II)-diamidate {[NiII(DQPD)]x, x = 1,2} complexes in chloroform solutions by combining acoustic and vibrational spectroscopies and molecular orbital calculations

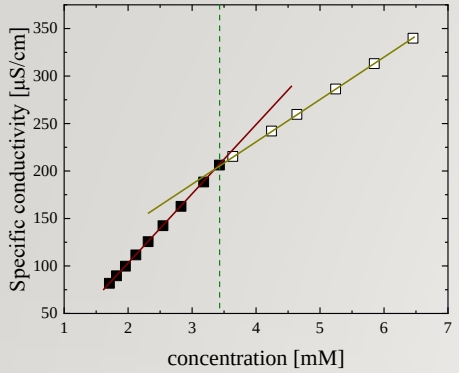
(In collaboration with Professor T. Kabanos)

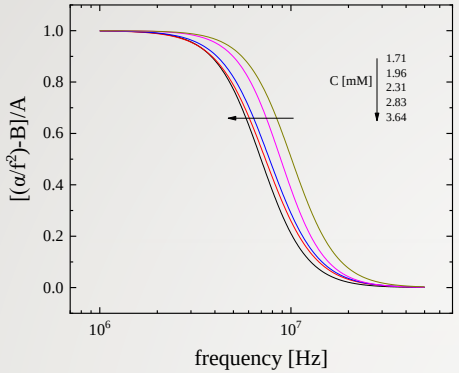


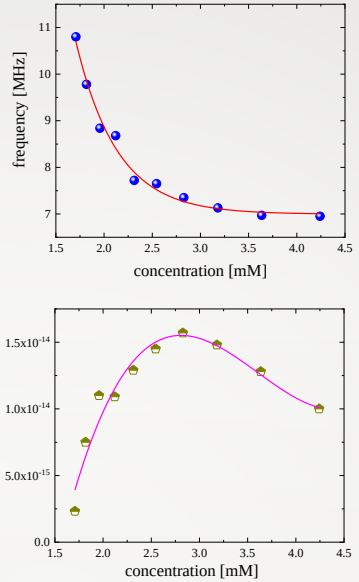




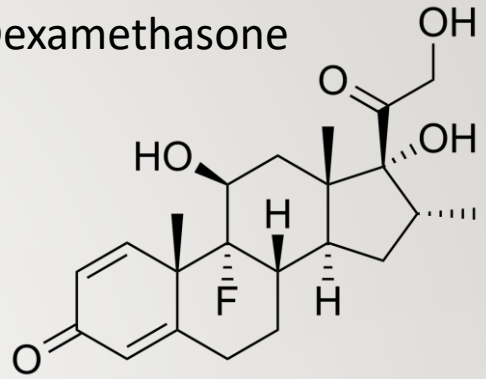
Molecular aggregation in Dexamethasone

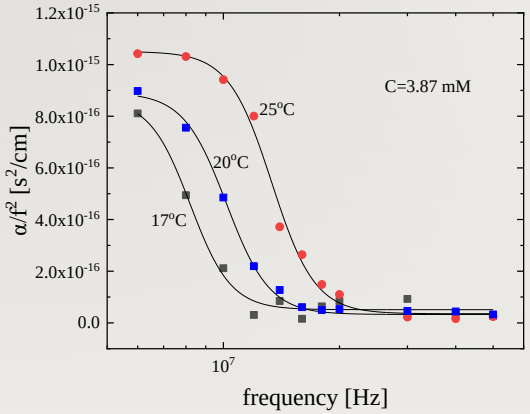


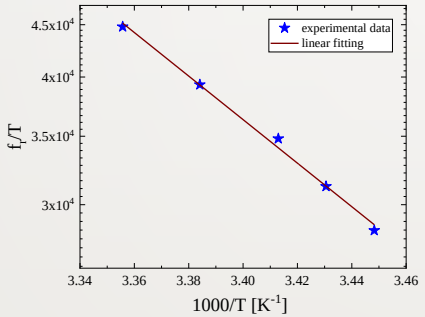


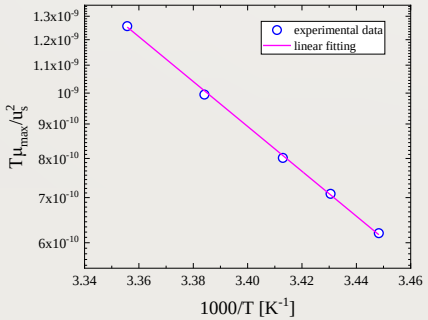


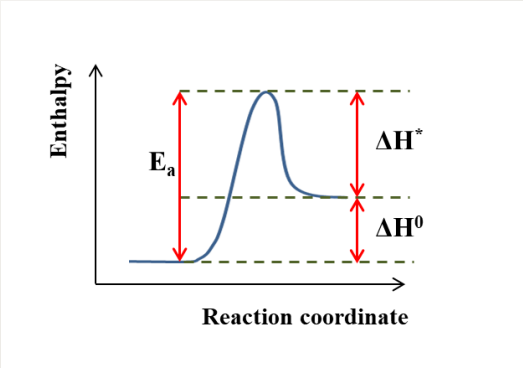
Dexamethasone



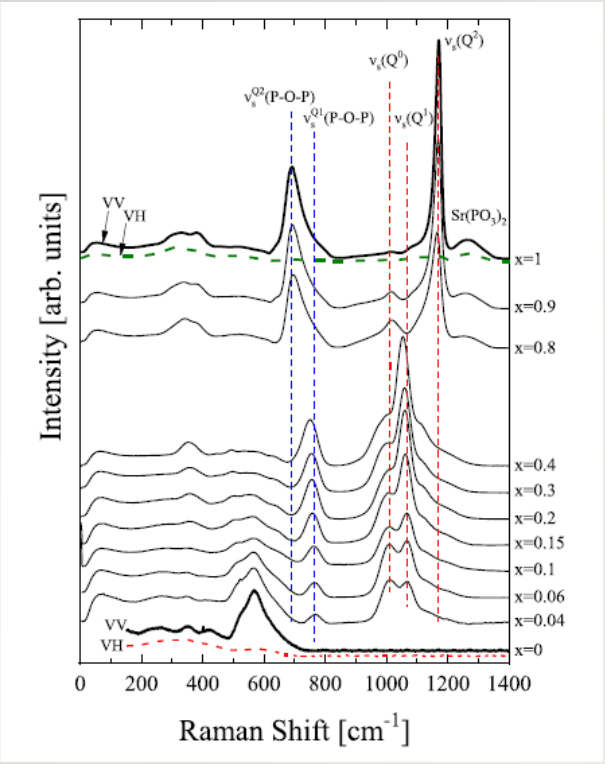


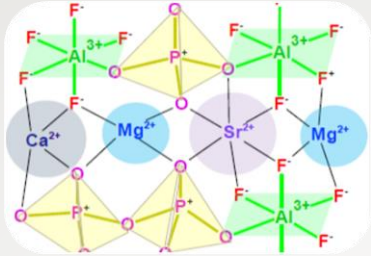


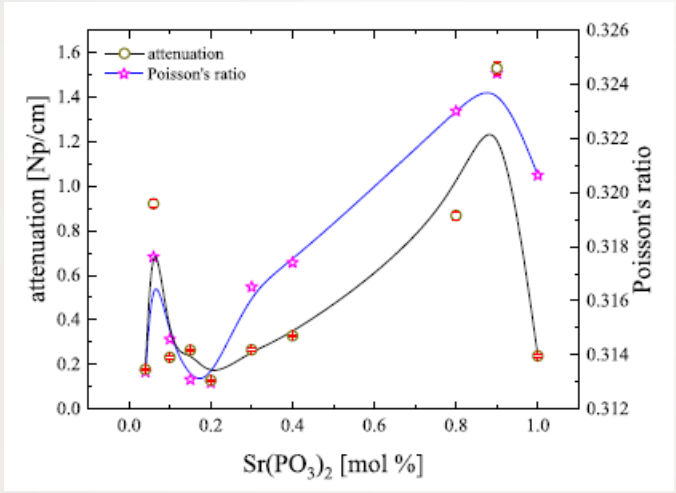


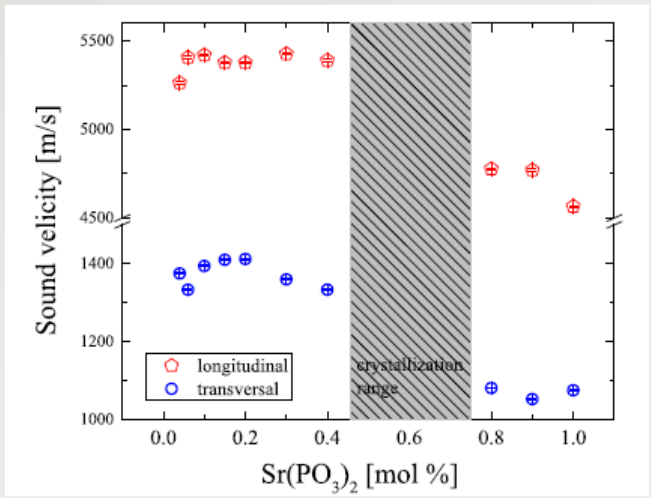


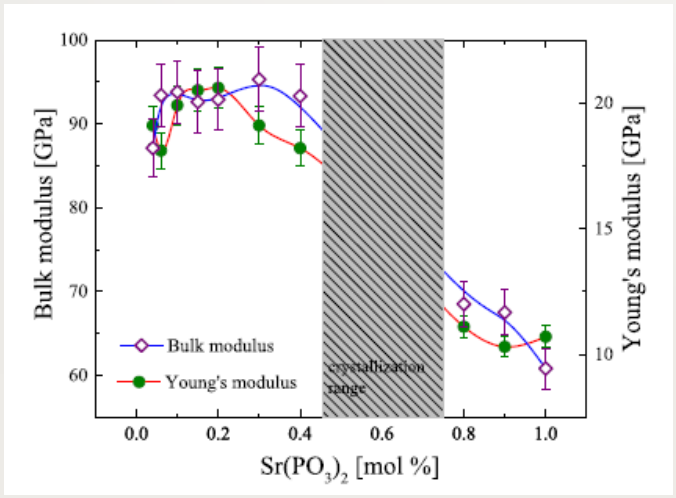
Elastic properties of a Fluorophosphate glass network: an ionic to covalent transition

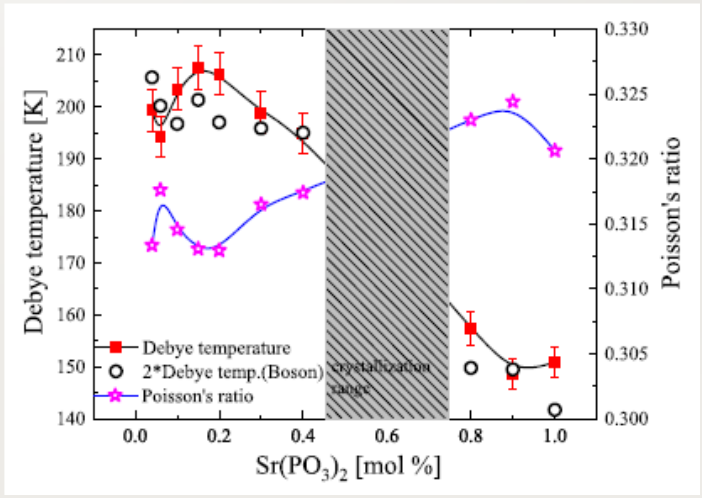












Journal of Physics and Chemistry of Solids 125 (2019) 43–50

Contents lists available at ScienceDirect

Journal of Physics and Chemistry of Solids

journal homepage: www.elsevier.com/locate/jpcs

Ionic to covalent glass network transition: Effects on elastic and vibrational properties according to ultrasonic echography and Raman spectroscopy

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 212 (2019) 363–370

Contents lists available at ScienceDirect

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

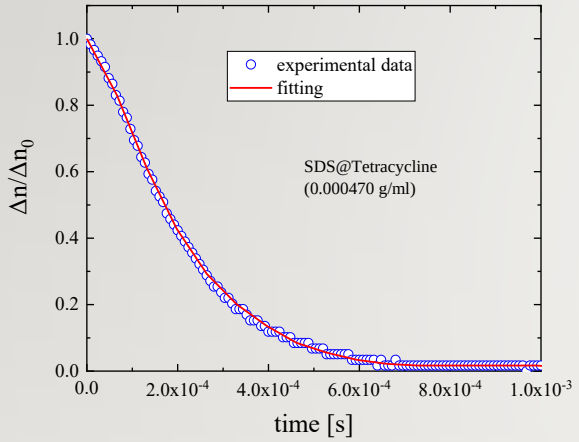
journal homepage: www.elsevier.com/locate/saa

Transverse phonons and intermediate-range order in Sr-Mg fluorophosphate glasses

Probing morphological alterations of simple and complex micelles by means of ultrasonically-induced transient birefringence experiments:

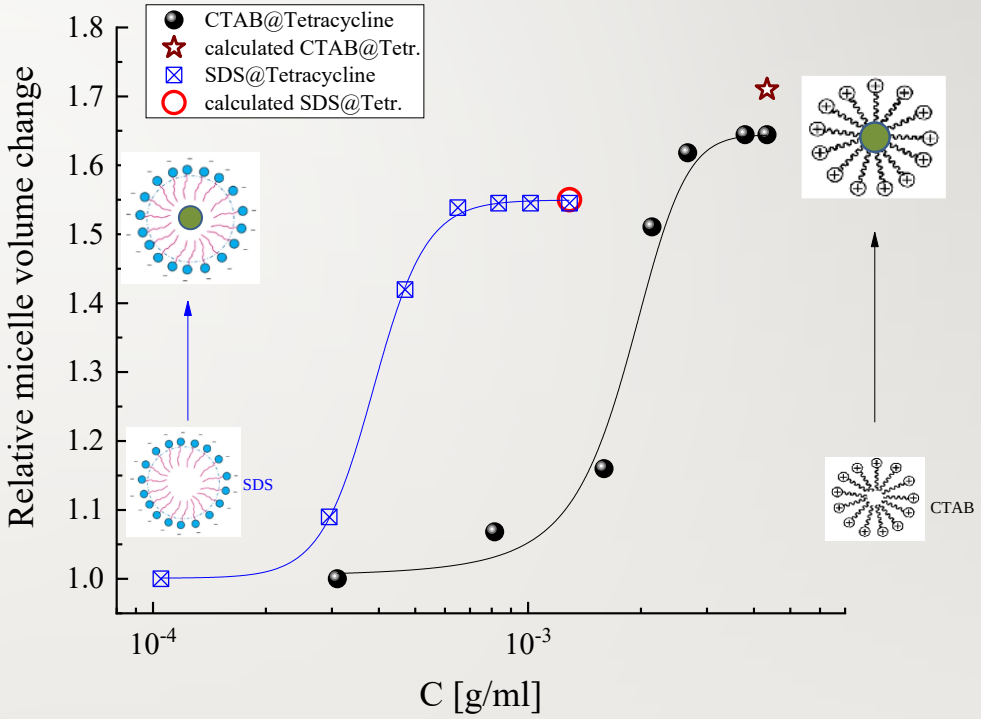
Tetracycline water soluble formulations with enhanced antimicrobial activity

(In collaboration with Professor S.K. Hadjikakou)



$$\tau = \frac{\eta V_h}{k_B T}$$

Fitting with a stretched exponential function



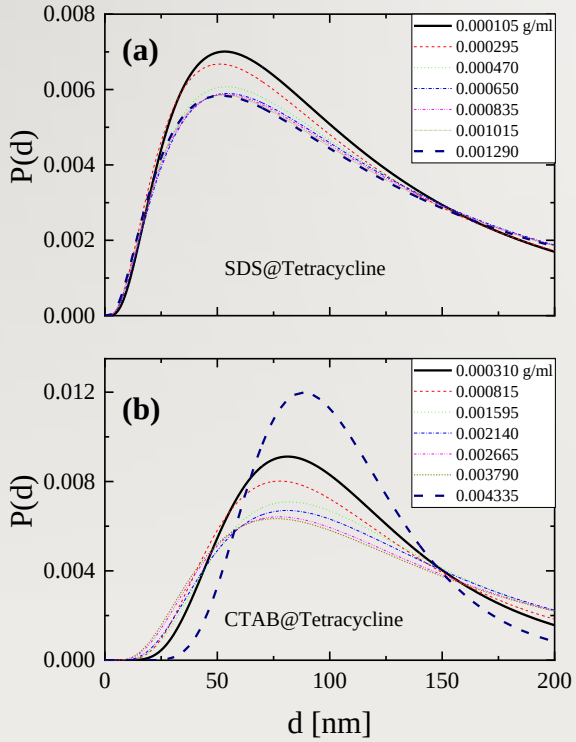
The ***size distribution*** is assumed to follow a log-normal behavior: $$P(d) = \frac{1}{d\sigma\sqrt{2\pi}} exp\left\{-\frac{[ln(d/d_m)]^2}{2\sigma^2}\right\}$$

d_m: the median
σ: the breadth of the size distribution

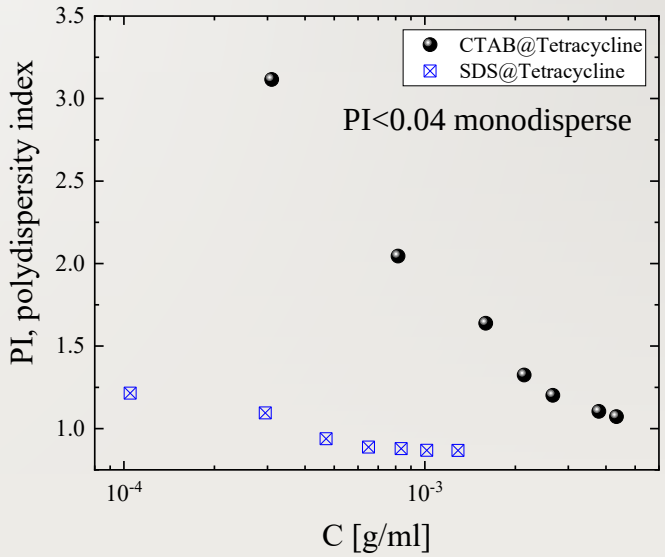
Both parameters can be estimated as the solution of the following system of equations:

$$\lim_{t\to 0}\left\{\frac{d}{dt}\left(ln\frac{\Delta n(t)}{\Delta n_0}\right)\right\} = -\frac{6d_m^3}{F_\Theta} exp(15\sigma^2/2)$$ the initial logarithmic derivative

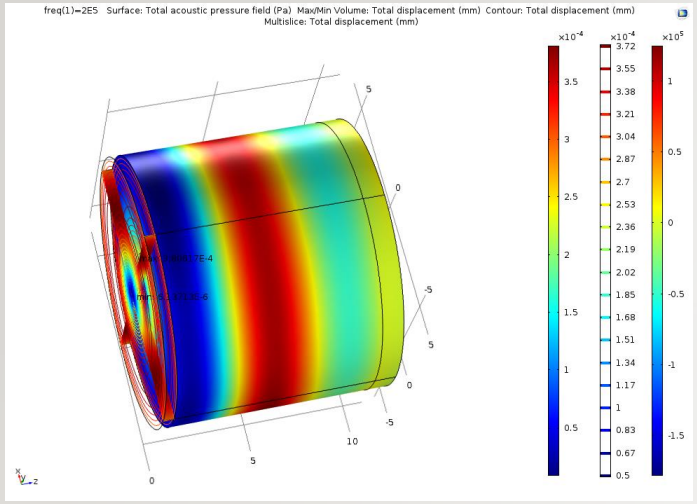
$$\int_0^\infty \frac{\Delta n(t)}{\Delta n_0} dt = \frac{exp(9\sigma^2)}{D_{WJ}}$$ the area under the birefringence trace



Polydispersity
PI = the square of the standard deviation divided by the mean particle diameter

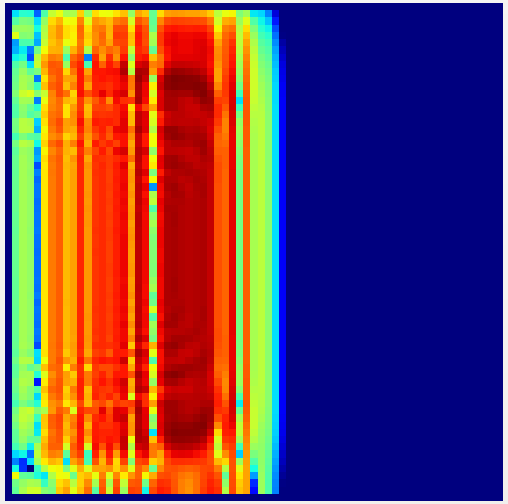


Representative simulation results in 3D, in 2D and using electrical circuits



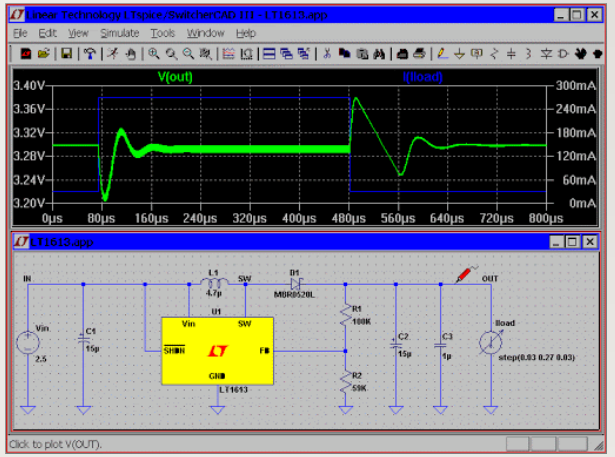
COMSOL

3D



FEM

2D



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Εργαστήριο Φυσικοχημείας

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