Pulsed terahertz study and spectral analysis of a simple solution: HCl in CCl₄

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Recent advances in generation of high intensity radiation in the far-infrared (FIR) spectral region¹ have suggested the possibility of performing a FIR spectral hole burning measurement to determine the homogeneous rotational dephasing time of a dipolar rotor in condensed media. Knowledge of the individual rotational line widths and shifts would be needed for such a study. This paper describes the first steps, in terms of both measured and calculated line shapes, in studying
sented QWD46
do the anisotropic potential time auto-
correlation function (APTAFl). Although on
average the solution is isotropic, the anisotropic
intermolecular potential is important be-
cause anisotropy in the orientational fluctua-
tions of the HCl molecules is determined by
the interaction between the HCl dipole and the
surrounding solvent molecules. These solute-
bath interactions are responsible for the rota-
tional line broadening and shifting observed in
the experimental data.

The APTAF may be determined by molecu-
lar dynamics simulation of the system and bath
and experimentally determined anisotropic
potential parameters from gas phase micro-
wave and radio frequency spectra, although
for the HCl/CCI4 gas a microscopic model in
and has been shown to approximate the time
scale of the decay and shape of the simulated
correlation function reasonably well.

The calculated fit normalized to the experimen-
tal data is shown in Fig. 2. A best fit was
obtained when the interaction strength pa-
rameter \( \lambda^2 = 165 \) and the APTAF decay time \( \tau = 0.10 \) (in reduced units where \( \lambda^2 \) and \( \tau \) have units of mass \( \text{cm}^2 \) and \( \text{ps} \) respectively). These results are qualita-
tively consistent with FT-IR spectra and simula-
tions of HCl in Ar and SF6. While CCI4 is
most similar in mass to SF6, the polarizability of
11.2 is almost twice the value of SF6 and seven
times the value of Ar. A larger solvent polarizability means that the dipolar
solute induces a proportionally larger dipole
moment on the neighboring solvent mole-
cules. Hence the dipole-induced dipole in-
teraction between HCl and CCI4 is stronger
than between HCl and SF6 and much stronger
than between HCl and Ar. This trend sug-
ests that the stronger the dipole-induced dipole
interaction in the solution, the greater the degree
of line broadening and shifting in the corre-
sponding absorption coefficient spectrum.
From these results we conclude that THz hole
burning studies should be carried out in low
polarizability (even atomic) solvents at low
temperature.

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QWE 2:30 pm–4:00 pm
Room 337

Atomic Interference
John E. Thomas, Duke University, President

QWE1 (Invited) 2:30 pm
Atom holography
Fujio Shimizu, University of Tokyo, Japan

We generated an ultracold Ne atomic beam
in the 1s3 (J = 0) metastable state by optical
pumping of the 1s5 atoms stored in a magneto-
opical trap. The atomic beam was then dif-
fracted by a computer-generated binary holo-
graphic mask. The atom interference interfer-
eogram can be obtained from the pro-
cessing of a single frame of the holographic
image. The atom diffraction pattern shows the
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