

**NUCLEAR MAGNETIC RESONANCE****Random Field and Cluster Dynamics in the Deuteron Glass D-RADP-50**

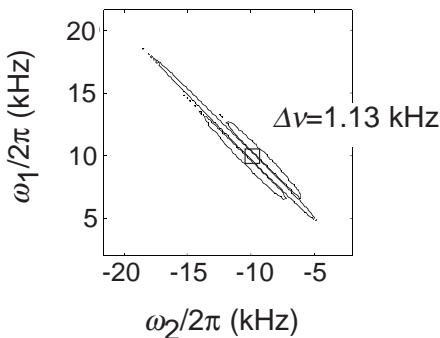
Th. König and R. Kind

The glass phase state in D-RADP-50 is characterized by short range ordered antiferroelectric clusters of nanometric size. While the hydrogen bonds within the clusters are strongly biased, they are less biased in the disordered inter-cluster regions. This leads to a strongly heterogeneous dynamics in these systems. For the investigation of the dynamical behavior one needs a microscopic method having the proper frequency window. While the frequency window of 1D-NMR extends from  $10^{12}$  to about  $10^3$  Hz, 2D-NMR methods cover a region between  $10^4$  and 1 Hz or even lower depending on the spin-lattice relaxation time  $T_1$ .

The following mechanisms in D-RADP-50 can lead to  $^{87}\text{Rb}$ -NMR-frequency fluctuations and thus to off-diagonal intensities in a 2D-NMR-exchange experiment: Intra-bond and inter-bond deuteron jumps, random-field or local polarization fluctuations, and spin diffusion.

$^{87}\text{Rb}$  2D-exchange difference NMR measurements in D-RADP-50 performed with a mixing time of  $t_{mix1} = 50$  ms revealed a cross-peak intensity at room temperature which was first assigned to spin diffusion. [1] The 2D difference spectrum drawn in Fig. 1 shows the diagonal-peak and the two cross-peaks. The characteristic time constant of this mechanism was found to be 8.3 ms. This is much too long for intra-bond hopping and much too short for spin diffusion.

Additional measurements are needed to rule out one of the two remaining possibilities.



$^{87}\text{Rb}$  2D-NMR exchange difference spectrum plotted as a contour plot of D-RADP-50 at room temperature. The square connecting the diagonal with the side lobes has a side length of  $\Delta\nu = 1.13$  kHz.

Reference: Th. König, Diss. ETH No. 12027 (1997).

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### Quadrupolar Glasses Containing $\text{HF}_2^-$ as Reorientable Units

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$\text{Rb}(\text{HF}_2)_{1-x}\text{Cl}_x$  is a model system for studying the properties of quadrupolar glasses. The aim of the measurements is to investigate the type of ordering of the reorientable  $\text{HF}_2^-$  molecules as a function of Cl content and temperature.

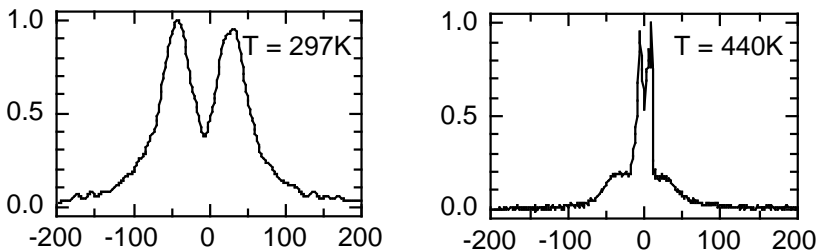
We expect that for low temperatures, the mixed crystal will be in a glass state, i.e. the  $\text{HF}_2^-$  molecules exhibit a short range correlated freeze out.

We have measured  $^1\text{H}$  and  $^{19}\text{F}$  NMR spectra in various powder samples ( $x = 0.05$  and  $0.1$ ) of  $\text{Rb}(\text{HF}_2)_{1-x}\text{Cl}_x$  as a function of temperature. The observed line shape transition at 430 K indicates the transition of the reorientable  $\text{HF}_2^-$  units from the slow motion regime to the fast motion regime (Fig.1). It coincides with the phase transition from a tetragonal to a cubic structure.

The powder samples have the drawback that they are chemically not very stable at temperatures above 400 K and set possibly HF free.

For  $x = 0.05$  proton spin-lattice relaxation time ( $T_1$ ) measurements between 265 and 374 K have been performed. A frequency-resolved experiment revealed that the central peak of the proton spectrum relaxes faster than the rest, which may be assigned to freely rotating  $\text{HF}_2^-$  ions.  $T_1$  is for 260 K in the order of 3 s, reaches its minimum of 0.6 s at room temperature and grows again above room temperatures to values of about 1 s. The  $^{19}\text{F}$  spin-lattice relaxation time at room temperature was found to be in the order of 10 s.

First  $^1\text{H}$  and  $^{19}\text{F}$  measurements on a single crystal, grown from a solution of 50%  $\text{RbCl}$  and 50%  $\text{RbHF}_2$ , have been performed between room temperature and 77 K. The spectra show that the quality of the crystals is probably not sufficient for our investigations.



$^{19}\text{F}$  spectra of  $\text{Rb}(\text{HF}_2)_{0.9}\text{Cl}_{0.1}$  at 297 K and 440 K, respectively.

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## Dynamics in Polymer Glasses

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An interesting feature in polymer glasses is the heterogeneity of the relaxation in these systems. The basic question concerns the probability distribution function of the single particle autocorrelation time which is believed to be characteristic for the correlation length of the local order. While  $T_1$ -measurements yield information about fast fluctuations, the 2D-NMR measurements cover the low frequency spectrum down to  $1/T_1$ .

In the framework of her diploma thesis Paola Cereghetti has performed extended deuterium 2D-NMR-exchange measurements on partially deuterated PMMA using four-pulse sequence methods. The aim was to observe the  $CD_3$  rotational jumps around the methyl group symmetry axis directly. The measurements were mainly performed at 40 K.

The experiments showed some off-diagonal intensity in the 2D-spectrum which, however, could not be assigned to the motion under investigation. Several improvements of the probe-head have brought a gain in signal intensity and a wider irradiation spectrum. Moreover, the phase corrections for a pure 2D-absorption spectrum were performed in a more sophisticated way. We could improve the signal detection substituting the formerly used four-pulse sequence by a five-pulse sequence. In this way the 2D-time domain signal was unambiguously collected and we obtained a well defined 2D-spectrum after Fourier transformation.

Further problems arose because of the long spin lattice relaxation time of the sample, particularly at 40 K, where it is in the order of 18 s. It turned out that to obtain an acceptable signal-to-noise ratio prohibitively long measuring times were needed. Exchange-difference measurements were also tried, but the limiting parameter was also here the measuring time.

From former  $T_1$ -measurements we know that the probability distribution of  $\tau_c$  has a width of more than 4 orders of magnitude at 40 K. Though part of this distribution falls into the observation window of the five pulse-experiment the corresponding off-diagonal intensity in the 2D-spectrum is probably too small to be detected unanimously.

At present we investigate an isotactic modification of the sample. We are interested whether the ester methyl dynamics is affected by the change in the polymer conformation from syndiotactic to isotactic. We started with spin alignment relaxation time measurements using a broad band pulse sequence in order to equally excite the whole  $^2H$ -spectrum.

## **Magnetic Field Dependence of the Vapor-Cell Zeeman Optical Trap**

T. Marty

Cold atoms are an interesting starting point for different fields of physics, such as precision microwave spectroscopy or collisional studies of ultracold atoms with each other. While the magneto-optical trap is widely used to produce samples of cold atoms, a three-dimensional description of the capture process is far too complicated to be solved analytically. Even for numeric computations the problem has to be considerably simplified. In this work the magnetic field dependence of the vapor-cell Zeeman optical trap has been investigated for cesium atoms. The measured dependence of the number of trapped atoms on laser detuning and magnetic field gradient is compared by contour plots with a theoretical one-dimensional model of the capture process that includes the spatially changing magnetic field.

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