Spin Interactions in Ammonia and Method to Cross-check the Polarization

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Contents :

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2. NMR line shape structure in irradiated ammonia (NH_3).
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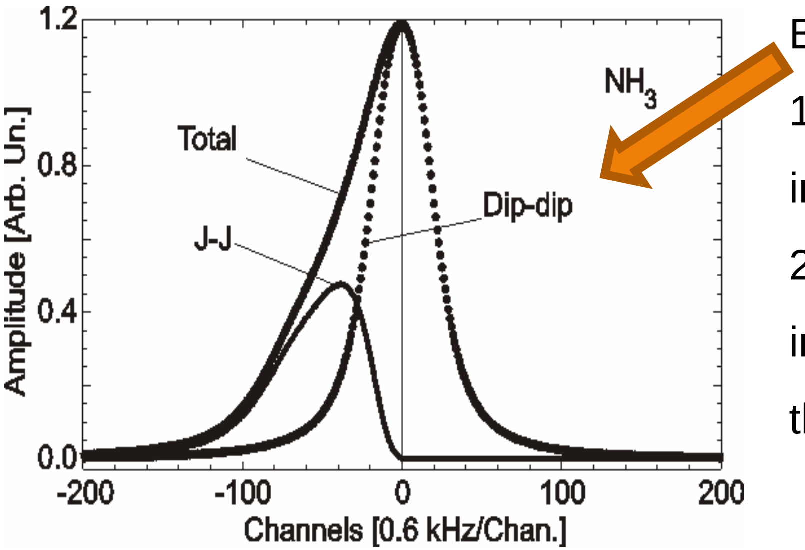
4. The correlation method for cross-checking the local polarizations in the long COMPASS target.
5. Conclusion.

We propose the ionising radiation as an universal way for the study of spin-spin interactions in solid dielectrics. Irradiated ammonia (NH3) [W. Meyer, et all., NIM A 215 (1983) 65] is a good example illustrating this method.



RUN-2007, COMPASS data, CERN, GENEVA.
Field 2.5 T, T=0.1 K, P = +93 %.

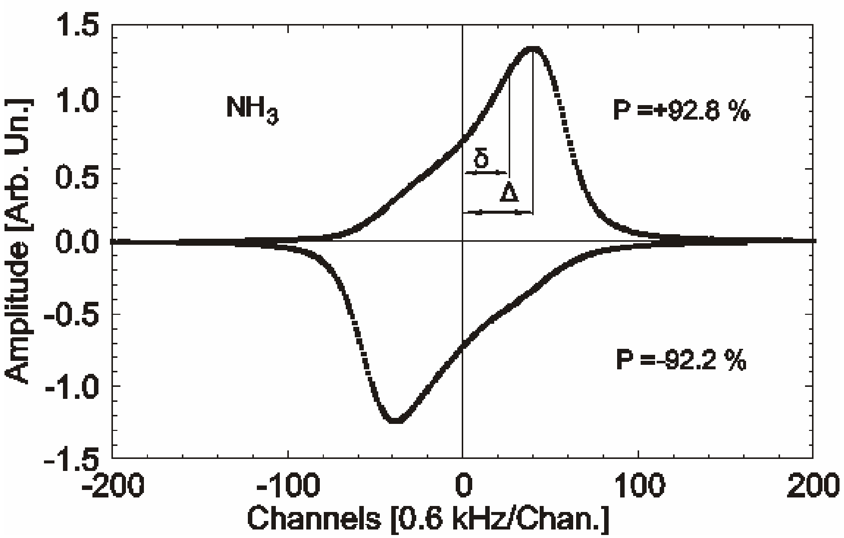
By our model – NH3 line shape consists of :

1.The symmetrical part due to the dipole-dipole interactions between the protons and

2.The asymmetrical part due to the indirect interactions between N and 3xH nuclear spins through F-electron spins.

At first we introduce the two consequences from this model.

Since the spectrum of DNP polarized protons incorporates also a mixture of nitrogen spectrum, their coupling effect can be detected directly on proton Larmor frequency!



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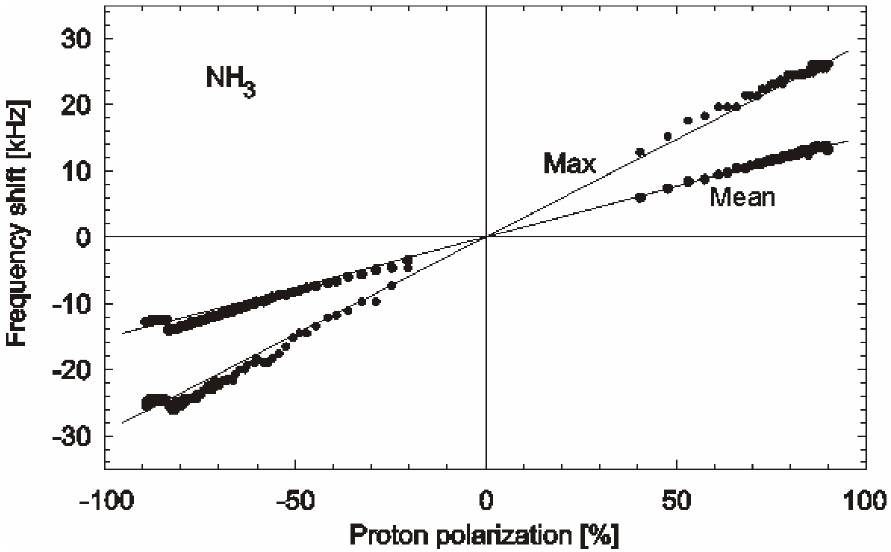
If ♎ **is** the mean centre position:

$$♎ = \frac{\sum N_j \cdot A_j}{\sum A_j} ,$$

where $\mathbf{N_j}$ is the channel number and $\mathbf{A_j}$ is the j-spectrum amplitude.

Than due to the 🖓-♎-different shifts, the proton spectrum is spread during polarization.

This plot show the 👎-(Max) and ♎ (mean) shifts over proton polarization.



RUN-2007, COMPASS data, CERN, GENEVA.
Field 2.5 T, T=0.1 K

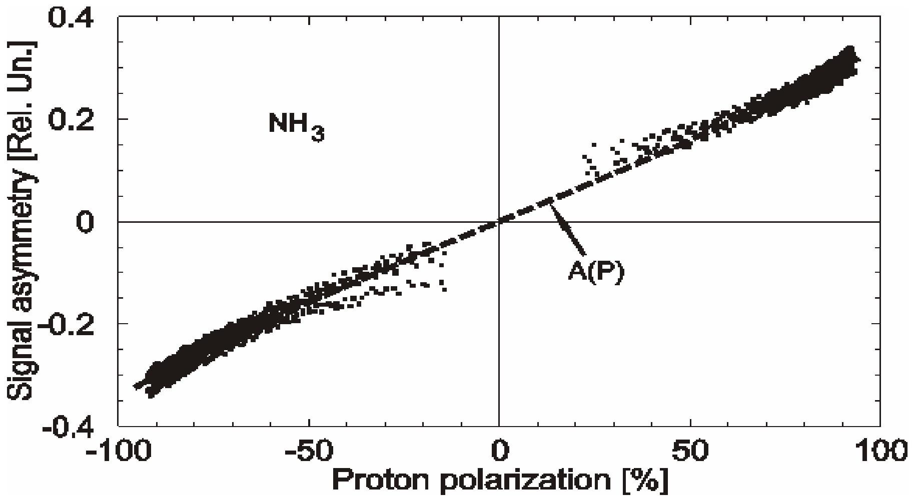
The first proposal :

Using selective RF-saturation one can decouple spins to study their mutual spin interactions.

This is a very power tool for quantitative searching of complicated spin interactions for example in bio-media!

The asymmetrical part of proton signal repeats the asymmetry of the nitrogen spectrum.

Remarks: N-spins have a huge quadruple moment



RUN-2007, COMPASS data, CERN, GENEVA.
Field 2.5 T, T=0.1 K .

Our data do not contradict with proposed model of spin-spin interactions and we consider its application also for the polarized target technique.

The method to cross-check polarization in the different NMR-probes

The long COMPASS target uses ten NMR probes for accurate spatial measurements of polarization. The best accuracy for the nuclear polarization is provided by the so-called integral method (TE-method).

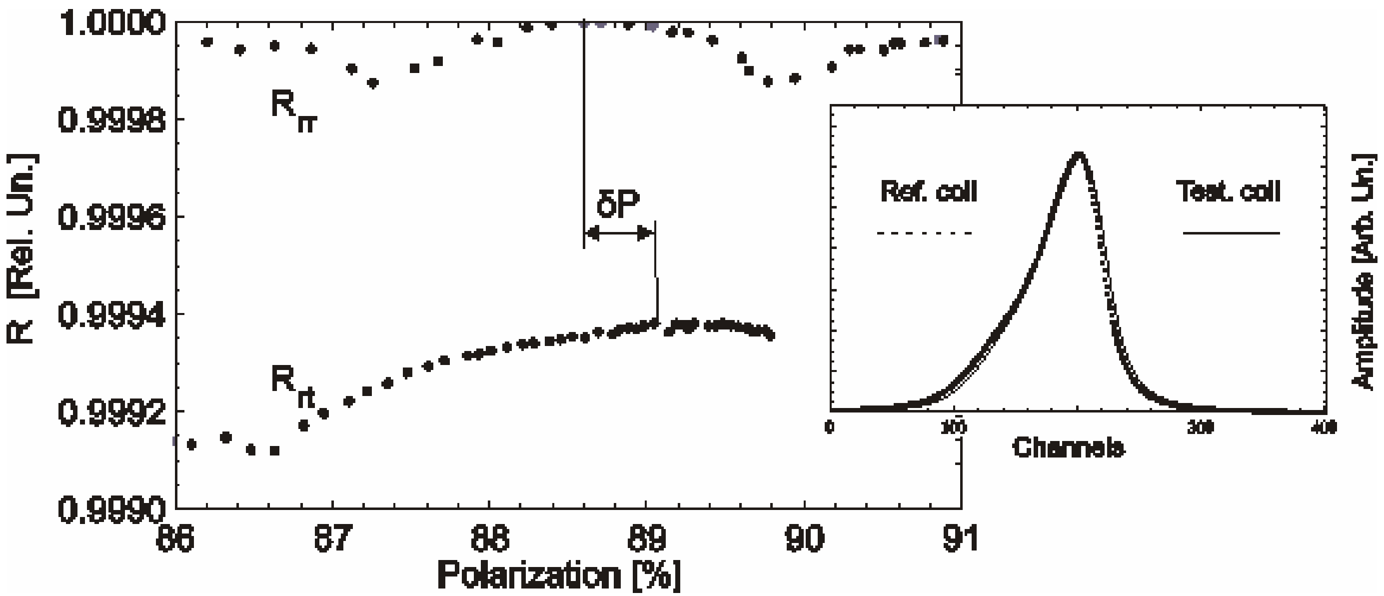
Here we compare the NMR line shape asymmetries from different probes using the correlation coefficient between a reference spectrum and all other spectrum.

$$R = \frac{\sum (A_j - A)(B_j - B)}{\sqrt{\sum (A_j - A)^2 (B_j - B)^2}} \qquad [-1 \le R \le 1]$$

Where: A_j **and** B_j are spectral amplitudes in (1, 2, 3, .Nj…1000) channels;

A and B are their mean values.

The variation of correlation coefficient during built-up target polarization

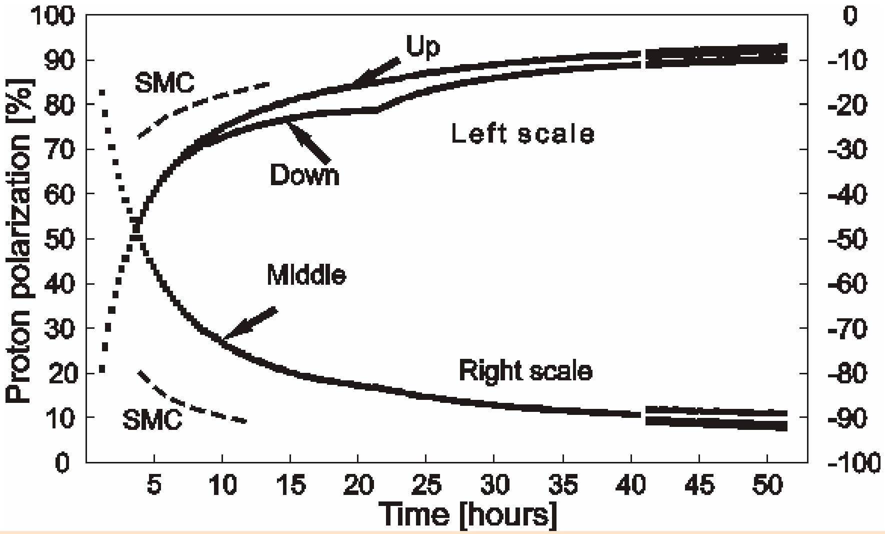


Rrr –correlation between the reference and non reference spectra for the same probe;

Rrt – the same reference spectrum but the different probe;

ΔP – the difference between TE-polarizations and the maximum correlation coefficient.

Using correlations between signals, one can slightly correct TE-constants within their error-bars and finally this help us to improve the accuracy of the relative polarizations in the cells.



Dashed built-up curves have been obtained with fresh doped ammonia.

Solid curves were obtained with the same material after 12 years stored in liquid N_2 with about half spin concentration of the fresh material.

The solid curves show the averaged built-up polarization in 2007 after the correction of TE-constant within their error-bars. This method enables self-consistent approximation between TE-polarizations and their maximum correlation coefficients.

Summary

1. **NMR line shape in NH_3 is formed by the proton dipole-dipole and indirect coupling between spin species in molecules.**
2. **It was shown that F-electrons couple the spins allowing a very effective method for the study of their spin-spin interactions by spin decoupling in "frozen mode" at superlow temperatures.**
3. **The method can be applied for the any solid dielectric including probably and bio-media.**
4. **NMR line shape asymmetry in NH_3 can be used for "cross-checking" polarizations taken by different Q-meter probes. This allows the a fine correction of TE-constant within their error-bars , providing the final accuracy of ±1.5 % for the proton polarizations.**