



Contribution ID: 67

Type: ORAL CONTRIBUTION

14N NQR study of proton position and dynamics in some hydrogen bonded organic ferroelectrics

Thursday, 16 September 2010 11:50 (20 minutes)

nuclear quadrupole resonance

Are you a student, a delegate from developing countries or a participant with physical needs and would like to apply for a sponsored accommodation. Please answer with yes or no.

no

Please specify whether you would prefer an oral or poster contribution.

oral

Summary

Three hydrogen bonded organic systems: phenazine–chloranilic acid (1:1), 1,2-diazine–chloranilic acid (2 : 1) and 2,3,5,6-tetra(2'-pyridyl)pyrazine-chloranilic acid (1:2) have been recently studied by ^{14}N nuclear quadrupole resonance (NQR). Several ^1H - ^{14}N nuclear quadrupole double resonance techniques have been used to obtain the ^{14}N NQR spectra.

In phenazine-chloranilic acid (1:1) the ^{14}N NQR parameters suggest that donor orbital populations of the two nitrogen atoms in a phenazine molecule become nonequivalent in the ferroelectric phase below $T_c = 253\text{ K}$, while they are both equal in the paraelectric phase. In the deuterated compound besides the ferroelectric transition at $T_c = 286\text{ K}$, a neutral to ionic transition was found at $T = 188\text{ K}$ associated with the proton transfer from chloranilic acid to phenazine.

Protons involved in the H-bond system in 1,2-diazine–chloranilic acid (2 : 1) are assumed to be in jumping motion in the double-minimum potential corresponding to the two extreme electronic states of $\text{O}-\text{H}\cdots\text{N}$ and $\text{O}\cdots\text{H}-\text{N}^+$. The ^{14}N nuclear quadrupole coupling tensor is used to determine the population of the states. The NQR data suggest that not only the population but also the electron distribution of the extreme electronic states itself changes with temperature.

The complete ^{14}N nuclear quadrupole resonance spectrum has been measured in ferroelectric and paraelectric 2,3,5,6-tetra(2'-pyridyl)pyrazine-chloranilic acid (1:2). The quadrupole coupling tensors are assigned to various nitrogen positions in the crystal structure. Two types of asymmetric $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds are observed in the ferroelectric phase. A slow dynamics influencing the ^{14}N NQR spectrum and relaxation has been observed in the paraelectric phase. The analysis of the ^{14}N NQR spectra in the paraelectric phase shows that above T_c each hydrogen bond exchanges between the two types observed in the ferroelectric phase. The change of the type of hydrogen bond is associated with the transfer of protons within the bond.

Primary author: Prof. SELIGER, Janez (University of Ljubljana)

Co-authors: Prof. ASAJI, Tetsuo (Department of Chemistry, College of Humanities and Sciences, Nihon University, Tokyo, Japan); Mr ŽAGAR, Veselko ("Jozef Stefan" Institute, Ljubljana)

Presenter: Prof. SELIGER, Janez (University of Ljubljana)

Session Classification: Resonance Methods

Track Classification: Resonance Methods