HIGH RESOLUTION $^{15}$N NMR OF ANTIFERROELECTRIC PHASE TRANSITION IN A SINGLE CRYSTAL OF AMMONIUM DIHYDROGEN ARSENATE, NH$_4$H$_2$AsO$_4$

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We report high-resolution $^{15}$N NMR measurements of the paraelectric to antiferroelectric phase transition ($T_N$=216K) of the model hydrogen-bonded antiferroelectric NH$_4$H$_2$AsO$_4$ (ADA). We specifically examined whether the NH$_4^+$ ions undergo a displacive or an order-disorder behavior at the phase transition. The high-resolution NMR measurements on $^{15}$N-enriched single crystals were made initially on a Bruker Avance 600 NMR spectrometer at the NHMFL, and detailed measurements were made with a Varian UNITY INOVA 500 MHz wide-bore system. Variable temperature experiments with $^1$H-$^{15}$N cross polarization and proton decoupling using a spinning rate of 5 kHz have been carried out. The temperature dependence of the isotropic chemical shift, $\delta_{iso}$ (Figure 1), and of the spin-lattice relaxation time, $T_1$ (Figure 2), shows clear anomalies at the phase transition. These results are interpreted as evidence for the coexistence of an order-disorder and displacive behavior at the NH$_4^+$ site [1, 2].

**Fig. 1.** Temperature dependence of $\delta_{iso}$ of $^{15}$N in ADA. The arrow indicates the antiferroelectric transition temperature, $T_N$. A gradual change and then a clear jump mark the phase transition.

**Fig. 2.** Temperature dependence of $T_1$ for $^{15}$N in ADA at a resonance frequency of 50.7 MHz ($B_0$=11.4 T).

**References**
