HIGH RESOLUTION ^{15}N AND ^{75}As NMR OF ANTIFERROELECTRIC PHASE TRANSITION IN A SINGLE CRYSTAL OF AMMONIUM DIHYDROGEN ARSENATE, $NH_4H_2AsO_4$

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High Resolution NMR has been used for investigating the paraelectric-antiferroelectric transition in $NH_4H_2AsO_4$ (ADA) at T_N~216K. Initial ^{15}N spectra were obtained on a Bruker DMX600 NMR spectrometer at 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 with spinning speed of 5 kHz have been carried out. Figure 1 shows the spectra around the phase transition. The isotropic chemical shift exhibits an approximately linear temperature dependence within 2K of T_N, and then changes discontinuously, followed by another almost linear dependence which is shown in figure 2(a) and 2(b). The sharp anomaly around T_N implies that the NH^{4+} ions undergo a displacive transition at T_N, whereas the protons in the O-H…O bonds undergo an order-disorder transition. The ^{15}N data thus support a mixed order-disorder-displacive mechanism for this transition. High-resolution ^{75}As NMR studies have also been carried out at room temperature using a Bruker NMR spectrometer operating at 830MHz at the NHMFL, shown in Figure 3. Sample spinning was at 35 kHz. Quadrupole coupling constant was found to be 9.2 MHz from spectral simulation, shown in figure 4. This result provides a new avenue for studying antiferroelectric transitions.

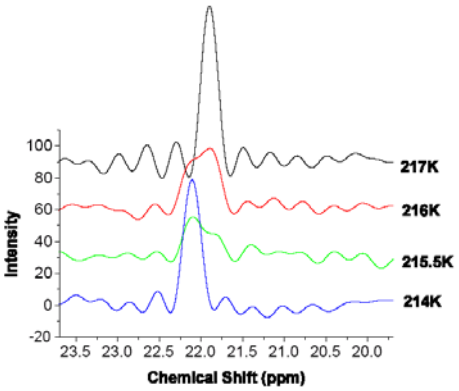

Figure 1

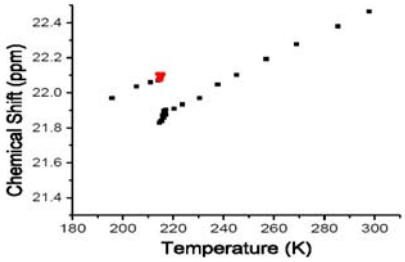

Figure 2a

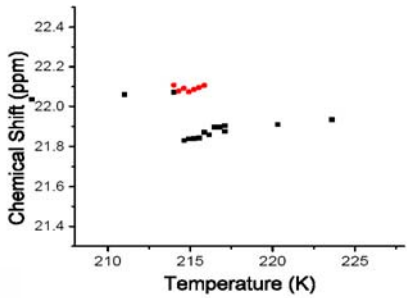

Figure 2b

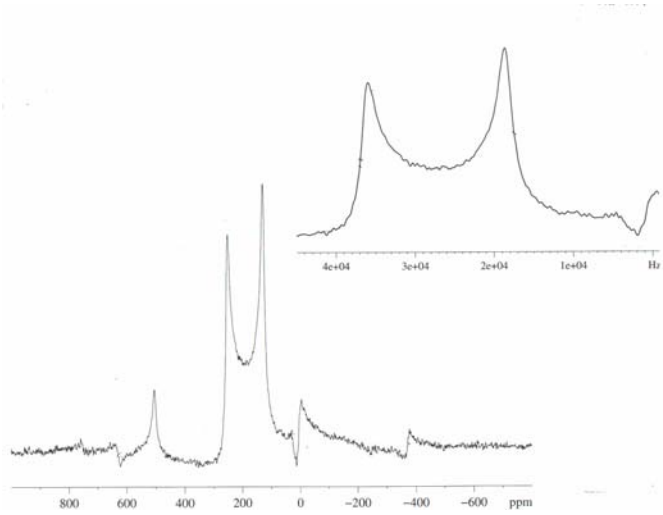

Figure 3

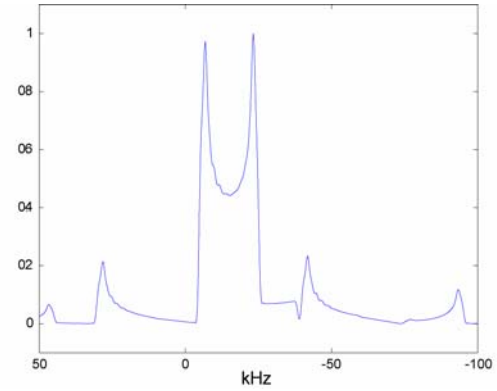

Figure 4