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High Resolution NMR ^{15}N and ^{31}P NMR Of Antiferroelectric Phase Transition in Ammonium Dihydrogen Arsenate and Ammonium Dihydrogen Phosphate OZGE GUNAYDIN-SEN, RANDALL ACHEY, RIQIANG FU, NARESH DALAL, Florida State University and National High Magnetic Field Laboratory — Natural abundance ^{15}N CPMAS NMR has been used to investigate the paraelectric-antiferroelectric phase transition of $NH_4H_2AsO_4$ (ADA) ($T_N \sim 216$K) and of $NH_4H_2PO_4$ (ADP) (148K), with a focus on the role of the NH_4^+ ion. Isotropic chemical shift of ^{15}N for ADA exhibits an almost linear temperature dependence to within $T_N \pm 1$K, and then changes discontinuously, followed by another almost linear dependence. The spectra of the paraelectric and antiferroelectric phases coexist around the T_N. The sharp anomaly around T_N implies that the NH_4^+ ions undergo a displacive transition, whereas the protons in the O$-$H$\cdots$O bonds undergo an order-disorder transition. The ^{15}N data thus support a mixed order-disorder-displacive mechanism for this transition. The ^{15}N data on ADP exhibit somewhat different behavior. ^{31}P CPMAS measurements will also be presented and discussed in terms of the above model.

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