Abstract Submitted for the MAR05 Meeting of The American Physical Society

Hydrogen-Bond Nature in Isolated Hydrogen-Bonded Material h-MeHPLN and h-BrHPLN Studied by Neutron and X-ray Diffraction RYOJI KIYANAGI, Tohoku University, AKIKO KOJIMA, Chiba University, HI-ROYUKI KIMURA, MASASHI WATANABE, YUKIO N, Tohoku University, TO-MOYUKI MOCHIDA, Toho University, TADASHI SUGAWARA, The University of Tokyo — MeHPLN and BrHPLN are hydrogen-bonded dielectric materials. Though their crystal structures are essentially the same, their phase transition schemes are significantly different. MeHPLN undergoes a phase transition at 41 K, while h-BrHPLN does not show any phase transitions. When the hydrogen atom in the hydrogen-bond of BrHPLN is replaced with a deuterium atom (d-BrHPLN), successive phase transitions occur. In this study neutron and X-ray diffraction experiments were performed on h-MeHPLN and h-BrHPLN to elucidate the difference about the phase transition from the structural aspect. From the experimentally obtained electron and nuclear distributions, a local disordered electronic dipole moment was found in the hydrogen bond region at room temperature. The phase transition of h-MeHPLN was found to occur with the ordering of the moment. Meanwhile, the moment in h-BrHPLN remains disordered until very low temperature, suggesting a tunneling motion of the hydrogen atom.

> Ryoji Kiyanagi Tohoku University

Date submitted: 04 Dec 2004 Electronic form version 1.4