## Abstract Submitted for the MAR09 Meeting of The American Physical Society

Effects of Magnetic Ordering on Phonon Spectra in Iron-based Superconductors: First Principle Calculation and Theoretical Analysis HIROKI NAKAMURA<sup>2</sup>, MASAHIKO MACHIDA<sup>3</sup>, CCSE, JAEA, ALFRED BARON<sup>4</sup>, Spring-8/RIKEN, TATSUO FUKUDA<sup>5</sup>, Spring-8/JAEA, SHINICH SHAMOTO<sup>6</sup>, MNRC JAEA — Recently, inelastic x-ray scattering measurements on single crystals of PrFeAsO<sub>y</sub> (y $\sim$ 0.2) have reported that phonons related with Fe-Fe and Fe-As bondings are significantly more softened than those obtained by the first principle calculations [1]. However, it is noted that any previous calculations do not include the magnetic degree of freedom. Therefore, we performed the phonon structure calculations by taking into account the magnetic structure in mother compounds. The magnetic calculations are in better agreement with the observed softening. We show the results and clarify the reason.

[1] T. Fukuda et al, J. Phys. Soc. Jpn. 77, 103715 (2008).

Masahiko Machida CCSE, Japan Atomic Energy Agency

Date submitted: 26 Nov 2008 Electronic form version 1.4

<sup>&</sup>lt;sup>1</sup>JSPS, Superclean MEXT Project

 $<sup>^{2}</sup>$ CREST JST & TRIP JST

 $<sup>^3</sup>$ CREST JST & TRIP JST

<sup>&</sup>lt;sup>4</sup>TRIP JST

<sup>&</sup>lt;sup>5</sup>TRIP JST

<sup>&</sup>lt;sup>6</sup>TRIP JST