Powder Zeeman NQR Study on the Absorption Forms for Nuclear Spin 5/2*

O. Ege, S. Nishijima, E. Kimura, H. Akiyama, S. Hamai, H. Negita

Department of Physics, Faculty of Education, Miyazaki University, Gakuen-kibanadai, Miyazaki 889-21, Japan
a Department of Chemistry, College of Education, Akita University, Tegata Gakuen-machi 1-1, Akita 010, Japan
b Computer Center, Hiroshima University of Economics, Gion, Asaminami, Hiroshima 731-01, Japan


For nuclei which have a nuclear spin of 5/2 and exhibit a small asymmetry parameter of the electric field gradient ($\eta$) at the nuclear site, line shapes of the Powder Zeeman NQR (PZNQR) spectra based on the transition between the energy levels $m_l = \pm 1/2$ and $\pm 3/2$ (the lower frequency line) were studied by means of computer simulations and experiments. (i) When an $\eta$ value is very small (type 1; $\eta = 0$), the line shape exhibits two shoulders like the style of the American football player. (ii) While an $\eta$ value is small (type 2; $0 < \eta < \text{around 0.01}$) but not zero, the line shape has two small peaks which are symmetrically located on the shoulders, as in the case of the small $\eta$ type of spin 3/2. (iii) When an $\eta$ value is not small (type 3; around 0.01 < $\eta$), the line shape has two symmetrical dips in stead of the peaks, which are also similar to the case of not small $\eta$ type of spin 3/2. As the $\eta$ value increases from around 0.01, the two dips grow and reach the maximum at the $\eta$ value of 0.349, and then become smaller and obscure in the range of $\eta$ larger than 0.349.

The observations of PZNQR spectra were performed for several compounds including the $^{127}$I and/or $^{121}$Sb nuclei to estimate the $\eta$ values, and gave the results as follows: very small for $^{127}$I (207.683 and 209.133 MHz, at 77 K) in SnI$_4$; very small for $^{127}$I (176.496 and 177.438 MHz, at 77 K) in Gal$_3$; small for $^{127}$I (265.102 MHz, at 77 K) in CH$_3$I; 0.33 for $^{127}$I (247.69 MHz, at 77 K) in C$_2$H$_5$I; 0.27 for $^{121}$Sb (58.23 MHz, at 290 K) in SbCl$_3$. The estimated $\eta$ values were compared to those obtained from the frequencies of two NQR lines for spin 5/2. They were in good agreement with each other for the small region of $\eta$, though somewhat large disagreements were seen in the cases of not small $\eta$ values.

Key words: NQR; Nuclear Quadrupole Resonance; Zeeman effect; Powder Zeeman NQR; Spin 5/2.

Reprint requests to Dr. O. Ege; Fax: +81-985-58-2892.