NQR MEASUREMENTS OF $UPtGa_5$*

Harukazu Kato, Hironori Sakai, Shinsaku Kambe
Russell E. Walstedt

Advanced Science Research Center, Japan Atomic Energy Research Institute
Tokai, Ibaraki 319-1195, Japan

Yoshihumi Tokiwa and Yoshichika Ōnuki

Graduate School of Science, Osaka University
Toyonaka, Osaka 560-0043, Japan

(Received July 10, 2002)

Ga NQR measurements have been carried out for $5f$-antiferromagnet, $UPtGa_5$.The zero-applied-field NQR spectrum in the antiferromagnetic state can be explained as the resonance lines of a Ga nuclei, which is affected by the Zeeman interaction with the internal field from the uranium magnetic moments, as well as the quadrupole interaction. The hyperfine coupling constant in the antiferromagnetic state is evaluated.

PACS numbers: 76.60.–k, 75.50.Ee

In recent years, unconventional superconductivity has been found in $HoCoGa_5$-type compounds such as $CeT'In_5$ (T' = Co, Rh, Ir) [1–3]. In this context, magnetic properties of the same type of uranium compounds attract much interest. $UPtGa_5$ belongs to a large family of $UTGa_5$ compounds (T = ion group) and crystallizes in the $HoCoGa_5$-type structure [4]. There are two crystallographically inequivalent Ga sites, namely, Ga(1) at (1/2, 1/2, 0) and Ga(2) at (1/2, 0, u) with $u \sim 0.292$ [5]. $UPtGa_5$ is a $5f$-itinerant antiferromagnet with Néel temperature $T_N = 26$ K and an electronic specific coefficient $\gamma = 57$ mJ/mol K^2 [6]. We have previously reported the NMR measurements in the paramagnetic region, and have clarified the hyperfine parameters of Ga and Pt in $UPtGa_5$ [7]. However, in the previous NMR measurements with the external field applied, we could not find any resonance signals below T_N. In this paper, ^{69,71}Ga NQR measurements with zero

* Presented at the International Conference on Strongly Correlated Electron Systems, (SCES 02), Cracow, Poland, July 10–13, 2002.

applied field are reported. We have observed the Ga resonance lines both in the paramagnetic and antiferromagnetic states; the resonance frequencies in the antiferromagnetic state enable us to estimate the transferred field at Ga(2), which come from the uranium magnetic moments. The hyperfine coupling constant in the antiferromagnetic state is evaluated.

In general, a nucleus with the spin moment $I > 1/2$ in a noncubic environments is affected by quadrupole interactions, as well as Zeeman interactions under magnetic fields. The Hamiltonian can be written as,

$$H = -\gamma\hbar(H_0 + H_{\rm int})I_{z'} + \frac{h\nu_Q}{2}\left\{3I_z^2 - I^2 + \eta(I_x^2 - I_y^2)\right\}. \qquad (1)$$

Here, z' is the magnetic field direction. The axes x, y, z are the principal axes of the electrical field gradient (EFG) tensor V_{ij}, so that $|V_{zz}| > |V_{yy}| > |V_{xx}|$; γ is the gyromagnetic ratio; H_0 is the external magnetic field, and $H_{\rm int}$ is the internal field at the nuclear site; ν_Q is defined as $3e^2qQ/2I(2I-1)h$, where eq is the nuclear quadruple moment, and $eQ \equiv V_{zz}$. The asymmetry parameter η denotes $(V_{xx} - V_{yy})/V_{zz}$.

The eigenvalues of the Hamiltonian express the energy of the nuclear level. When the quadrupoler parameters (ν_Q, η) and the magnitude and the direction of the magnetic field (H_0, $H_{\rm int}$, θ, ϕ) are given, the resonance frequency ν in a NMR measurement can be deduced by solving the matrix elements numerically. It should be noted that six resonance lines are expected for each isotope of Ga (^{69,71}Ga; $I = 3/2$); transitions between any two of four levels are permitted because of the non-diagonal components come from the quadrupole interaction.

A polycrystalline sample of $UPtGa_5$ synthesized by arc-melting method [5] was used. All the measurements were performed by a conventional pulsed NQR spectrometer under zero applied field ($H_0 = 0$). In the paramagnetic region, a NQR line of Ga is expected to appear at the frequency $|\nu_Q|(1 + \eta/3)^{1/2}$ since $H_{\rm int} = 0$. In fact, we succeeded to observe resonance lines of ^{69}Ga(2), ^{71}Ga(2) and ^{69}Ga(1) at 27.53 MHz, 17.35 MHz, and 14.5 MHz, respectively. The observed resonance frequencies are consistent with the previous reported value of ν_Q and η [7]. Although the NQR line of ^{71}Ga(1) is expected to appear at about 9.1 MHz, we could not observe this resonance, probably because of its weak intensity.

The zero-applied-field NQR spectrum in the antiferromagnetic state is shown in Fig. 1. Since the ν_Q and η values have been evaluated [7], it is possible to discuss the internal field from the observed resonance peak position. That is, we calcurate the resonance frequcencies with $H_{\rm int}$ an explicit parameter at first, and then compare them with the observed frequencies. Here, let us focus on Ga(2). According to the neutron diffraction study [5], the magnetic structure of $UPtGa_5$ reserves a C_{2z} symmetry at the Ga(2) site.

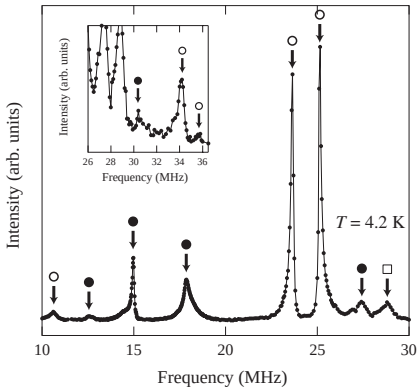

Fig. 1. Zero-applied-field NQR spectrum in the ordered state. The open and closed circles indicate the resonance lines come from ^{69}Ga(2) and ^{71}Ga(2), respectively. Peaks indexed by open square come from Ga(1).

From consideration of symmetry [8], it is found that the induced field by the magnetic moments cannot break the C_{2z} symmetry at Ga(2). Therefore, $H_{\rm int}$ at the Ga(2) site should be parallel to the [001] direction of the crystal, which coincides with the EFG x-axis of Ga(2) [7]. Under this constraint of the internal field direction, the adjustable parameter is only $H_{\rm int}$. The good agreement between the calcurated and observed frequencies is shown with regard to Ga(2). Here, $H_{\rm int} = 5.9$ kOe is given at 4.2 K.

Unfortunately, we could not find all of the Ga(1) lines due to their weak signal intensities; most of the resonance lines of Ga(1) are suspected to be hidden by the strong resonance peaks of Ga(2). There appear fewer signals of Ga(1), so that they could not be analyzed in a similar way to the Ga(2) lines. Hence, $H_{\rm int}$ for Ga(1) could not be evaluated in this measurements.

The temperature dependence of $H_{\rm int}$ is shown in Fig. 2. For comparison, we also plotted a square root $\sqrt{I_{\rm mag}}$ of the magnetic Bragg peak intensity in the previous neutron diffraction study [5]. It is noted that $\sqrt{I_{\rm mag}}$ is proportional to the amplitude of the ordered moments. As shown in Fig. 2, $H_{\rm int}$ and $\sqrt{I_{\rm mag}}$ show a similar temperature dependence. This clearly indicates that $H_{\rm int}$ is the transferred hyperfine field come from the magnetic moments at the uranium site; the relation of $H_{\rm int} = A_{\rm hf}^{\rm AF} \times \langle m \rangle$ is realized. Here, $\langle m \rangle$ is the magnitude of the ordered moments, and $A_{\rm hf}^{\rm AF}$ denotes the hyperfine coupling constant in the antiferromagnetic state. Since $\langle m \rangle$ is estimated to be 0.24 $\mu_{\rm B}$ at the lowest temperature [5], we can evaluate $A_{\rm hf}^{\rm AF}$ of Ga(2) to be $\pm$ 24.6 kOe/$\mu_{\rm B}$. The magnitude of $A_{\rm hf}^{\rm AF}$ is rather larger than that of the hyperfine coupling constant $A_{\rm hf}^{\rm para}$ in the paramagenetic state, which has been estimated to be a few kOe/$\mu_{\rm B}$ [7]. At present, we have no defi-

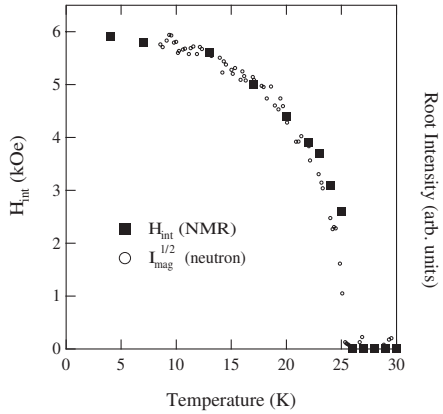

Fig. 2. Temperature dependence of $H_{\rm int}$. For comparison, the square root $\sqrt{I_{\rm mag}}$ of the magnetic Bragg peak intensity are shown.

nite explanation for the change of the hyperfine coupling constant. Further discussions are mentioned in the forthcoming reports.

In summary, we have carried out the zero-applied-field NQR measurements for $UPtGa_5$. From the spectrum in the antiferromagnetic state, we succeeded in evaluating the magnitude of the internal field at Ga(2). The hyperfine coupling constant in the antiferromagnetic state is evaluated.

REFERENCES

[1] H. Hegger, C. Petrovic, E.G. Moshopoulou, M.F. Hundley, J.L. Sarrao, Z. Fisk, J.D. Thompson, *Phys. Rev. Lett.* **84**, 4986 (2000).

[2] C. Petrovic, R. Movshovich, M. Jaime, P.G. Pagliuso, M.F. Hundley, J.L. Sarrao, Z. Fisk, J.D. Thompson, *Europhys. Lett.* **53**, 354 (2001).

[3] C. Petrovic, P.G. Pagliuso, M.F. Hundley, R. Movshovich, J.L. Sarrao, J.D. Thompson, Z. Fisk, P. Monthoux, *J. Phys.: Condens Matter* **13**, L337 (2001).

[4] Yu.N. Grin, P. Rogl, K. Hiebl, *J. Less. Common. Met.* **121**, 497 (1986).

[5] Y. Tokiwa, Y. Haga, N. Metoki, Y. Ishii, Y. Ōnuki, *J. Phys. Soc. Jpn.* **71**, 725 (2002).

[6] Y. Tokiwa, S. Ikeda, Y. Haga, T. Okubo, T. Iizuka, K. Sugiyama, A. Nakamura, Y. Ōnuki, *J. Phys. Soc. Jpn.* **71**, 845 (2002).

[7] H. Kato, H. Sakai, Y. Tokiwa, S. Kambe, R.E. Walstedt, Y. Ōnuki,*J. Phys. Chem. Sol.*, **63**, 1197 (2002).

[8] S. Demuynck, L. Sandratskii, S. Cottenier, J. Meersschaut, M. Rots, *J. Phys.: Condens Matter* **12**, 4629 (2000).