RELATIVE INTENSITIES OF NUCLEAR QUADRUPOLE RESONANCE LINES OF Sb^{121} *IN ANTIMONY TRICHLORIDE*

V. S. GRECHISHKIN and I. A. KYUNTSEL'

Perm State University

Submitted to JETP editor April 30, 1962

J. Exptl. Theoret. Phys. (U.S.S.R.) **43**, 1712-1713 (November, 1962)

The relative line intensities of antimony isotopes are studied in crystalline antimony trichloride. Transition probabilities are calculated. A forbidden transition has been detected in an indirect manner. The theoretical calculations are compared with the experimental data.

THE nuclear quadrupole resonance (NQR) of the isotope Sb^{121} in $SbCl_3$ was first observed by Dehmelt and Krüger.[1] Since the spin of the nucleus Sb^{121} is $^5/_2$, then in correspondence with the selection rules for the magnetic quantum number, $\Delta m = \pm 1$, two NQR lines can be observed, belonging to the transitions $\nu(\pm {}^1/_2 \rightarrow \pm {}^3/_2)$ and $\nu(\pm {}^3/_2 \rightarrow \pm {}^5/_2)$. The transition $\nu(\pm {}^1/_2 \rightarrow \pm {}^5/_2)$ is designated as a "forbidden" transition. It can be observed if the asymmetry parameter η is sufficiently large. In the work of Dehmelt and Krüger [1] this transition was not observed.

We have made some theoretical calculations of the probabilities of all three transitions in $SbCl_3$. The method of calculation differs little from that described earlier.[2,3] If we symbolize the levels by 1, 2, 3 in correspondence with the values of m $= \pm {}^1/_2, \pm {}^3/_2$, and $\pm {}^5/_2$, the wave functions ψ_1, ψ_2, and ψ_3 turn out to be mixed. Since each is doubly degenerate, then in general we have to calculate four probabilities for each transition for different orientations of the radiofrequency field. For Sb^{121} in $SbCl_3$ we have $eQq_{zz} = 376{,}902$ Mc, $\eta = 16\%$ (Q is the quadrupole moment of the nucleus, q_{zz} a tensor component of the gradient of the crystalline electric field).

The results of the calculation are presented in Table I. If the radio-frequency field is oriented in the X direction in a monocrystal, the intensity of the transition $\nu(\pm {}^1/_2 \rightarrow \pm {}^3/_2)$ is almost twice as great as in polycrystalline form. The transition intensity ratios in polycrystalline form are $W_{1,2}^2 : W_{2,3}^2 : W_{1,3}^2 = 1 : 0.59 : 0.0058$.

We observed the first transition ($\nu_{1,2}$) at 58,156 Mc at room temperature with a signal-to-noise ratio of about 70 (the spectrum was recorded with a synchronous detector). If the line was observed on an oscilloscope, this ratio was about 3. The second transition ($\nu_{2,3}$) was accordingly observed at 112,596 Mc at +18.6°C. In oscilloscope presentation the signal-to-noise ratio was 1.6. Thus, we get from experiment $W_{1,2}^2 : W_{2,3}^2 = 1 : 0.54$, which agrees well with the theoretical results. Since the intensity of the "forbidden" transition is 100 times weaker than the intensity of the transition $\nu_{2,3}$, a search of the spectrum in the region of 170 Mc (the spectrum was recorded on a pen recorder) was futile. In view of the fact that the NQR frequency varies with temperature we took the temperature dependence of the frequency of the $\nu_{1,2}$ transition. The results are presented in Table II.

Thus, the NQR signals were observed right up to the melting point (73°C). No kind of structural transition was detected in this crystal. On the basis

Table I

Orientation of radiofrequency field	Contribution from cross transitions			Contribution from direct transitions			Square of the total transition probability		
	$W_{1,2}^2$	$W_{2,3}^2$	$W_{1,3}^2$	$W_{1,2}^2$	$W_{2,3}^2$	$W_{1,3}^2$	$W_{1,2}^2$	$W_{2,3}^2$	$W_{1,3}^2$
$H_1 \parallel X$	4.44	2.2	0.02	0	0	0	4.44	2.2	0.02
$H_1 \parallel Y$	3.1	2.1	0.02	0	0	0	3.1	2.1	0.02
$H_1 \parallel Z$	0	0	0	0.09	0.0002	0.005	0.09	0.0002	0.005
Polycrystal	2.51	1.53	0.01	0.09	0.0002	0.005	2.6	1.53	0.015

Table II

Signal-to-noise ratio	t, °C	$\nu_{1,2}$, Mc/sec	Signal-to-noise ratio	t, °C	$\nu_{1,2}$, Mc/sec
3	27.3	58.1310	2	58.5	57,816
3	31,3	58,0968	1,8	64	57.7584
3	35.1	58.0536	1,8	67.8	57,7062
3	39.4	58.0014	1,7	69.6	57,686
3	45,5	57,9564	1,6	70.4	57,686
2,5	50,7	57,9096			

of the temperature dependence, the temperature coefficient of frequency was estimated, and this permitted the prediction of the frequency of the corresponding transitions at different temperatures.

Since the direct method of observation gave no information about the presence of the "forbidden" transition, an indirect method was employed to detect it. A powerful (~20 W) generator at a frequency close to 170 Mc was constructed. By applying a saturating field of frequency ≈170.5 Mc at room temperature, we observed a diminution in the intensity of the transition $\nu_{1,2}$ by a factor of 1.2. In this case, saturation of the "forbidden" transition occurred and the difference in population between the levels 1 and 2 was decreased.

In conclusion the authors express their sincere gratitude to N. E. Aĭnbinder for checking the numerical calculations and to M. A. Kitsenko for his assistance with some of the measurements.

[1] H. G. Dehmelt and H. Krüger, Z. Physik **130**, 385 (1951).

[2] G. M. Volkoff and G. Lamarche, Can. J. Phys. **32**, 493 (1954).

[3] V. S. Grechishkin and N. E. Aĭnbinder, FTT **3**, 2981 (1961), Soviet Phys. Solid State **3**, 2175 (1962).

Translated by L. M. Matarrese
297