Nuclear Quadrupole Coupling of Nitrogen in ICN and N_2O*

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We have extended our measurements on $IC^{12}N^{14}$ to include the fourth rotational line ($J=3\rightarrow 4$) in the 1.18-cm region and have resolved the hyperfine structure caused by the nitrogen nucleus which is essentially superimposed upon that of the iodine nucleus. In our earlier observations which were made on the fifth rotational transition occurring in the millimeter region, only the hyperfine structure resulting from the I nucleus was resolved. A study of the nitrogen quadrupole coupling in $N^{14}N^{14}O$ has also been made.

Townes and his co-workers[2] in their study of BrCN and ClCN have observed quadrupole coupling for two nuclei in the same molecule. The theory of these rather complex spectra has been developed by Bardeen and Townes.[3] We have used this theory in our interpretation of the spectrum of ICN and N_2O.

Figure 1 shows some components of the $J=3\rightarrow 4$ transition of ICN at lower pressures, where the structure caused by nitrogen nucleus is evident. Since the N interaction is small compared to that of the I, the first-order theory developed by Bardeen and Townes[3] provides an adequate interpretation of the spectrum. From the measurements on these lines the nuclear quadrupole coupling of the nitrogen is determined as −3.80 mc, which is close to −3.66 mc, the value[2] obtained for ClCN, but significantly smaller than −4.67 mc, the value[4] for CH_3CN. It is of interest that the N coupling in N_2O[5] and in CH_3NC[4] is considerably smaller. The measurements on the $J=3\rightarrow 4$ transition yield a value of -2540 ± 25 mc for the nuclear quadrupole coupling of the iodine if the formula for the quadrupole coupling of a single nucleus as stated by Bardeen and Townes[3] is employed. This value is in satisfactory agreement with the value previously determined for the $J=4\rightarrow 5$ rotational transition, if the latter is multiplied by a factor of 5/4 to convert it to the same units.[4,6]

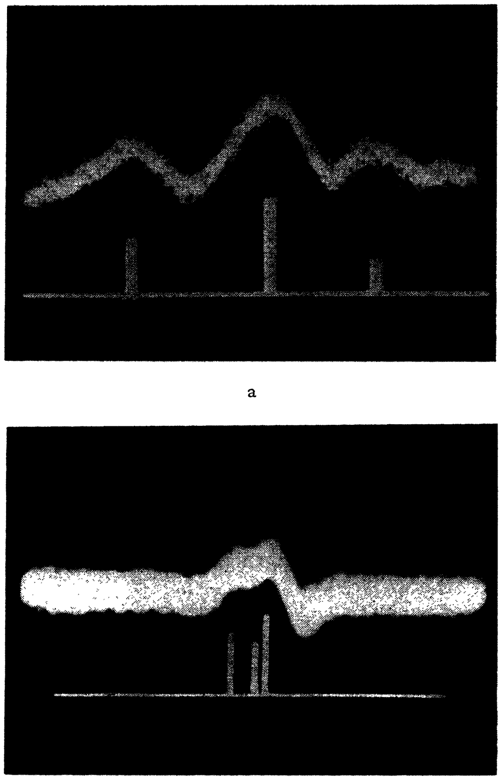

Fig. 1. Theoretical and observed nitrogen splitting of the $J=3\rightarrow 4$ rotational transition of ICN. a—$F_1=\frac{1}{2}\rightarrow\frac{3}{2}$ transition. Separation of outside peaks is 1290 *kc*/s. b—$F_1=\frac{11}{2}\rightarrow\frac{13}{2}$ transition. Separation of outside peaks is 74 *kc*/s.

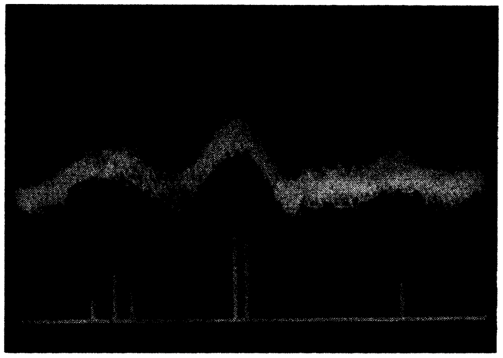

Fig. 2. Theoretical and observed nitrogen splitting of the $J=0\rightarrow 1$ transition of $N^{14}N^{14}O$. Separation of two outside peaks is 765 *kc*/s.

The $J=0\rightarrow 1$ rotational transition of N_2O has recently been studied by Coles, Elyash, and Gorman,[5] who obtained a quadrupole coupling for N^{14} in the central position as −0.27 mc and in the end position as −0.84 mc. The first value was determined from $N^{15}N^{14}O$. The latter was obtained from $N^{14}N^{14}O$ by neglecting the effects of the central N^{14}. In the calculated spectrum of $N^{14}N^{14}O$ shown in Fig. 2 we have taken into account the effects of both the central and end nitrogens. In these calculations we have used the value −0.27 mc for the central N^{14} mentioned above and have chosen the quadrupole coupling for the end N^{14} so as to give the best agreement with our own measurements. The value obtained in this way for the nuclear quadrupole coupling of N^{14} in the end position of N_2O is -1.03 ± 0.10 mc.

We wish to thank J. Bardeen and C. H. Townes for sending us a prepublication copy of their paper on the calculation of nuclear quadrupole effects.

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** Frederick Gardner Cottrell Fellow.

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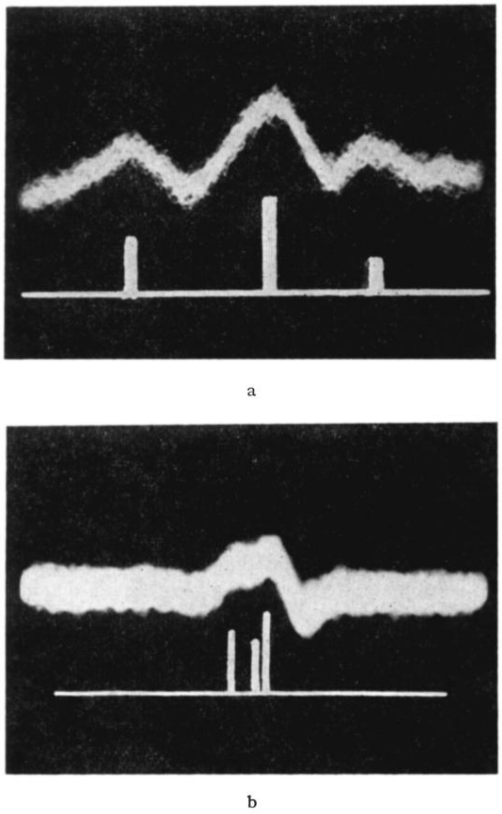

a

b

FIG. 1. Theoretical and observed nitrogen splitting of the $J=3\to4$ rotational transition of ICN. a—$F_1=\frac{1}{2}\to\frac{3}{2}$ transition. Separation of outside peaks is 1290 *kc*/s. b—$F_1=\frac{11}{2}\to\frac{13}{2}$ transition. Separation of outside peaks is 74 *kc*/s.

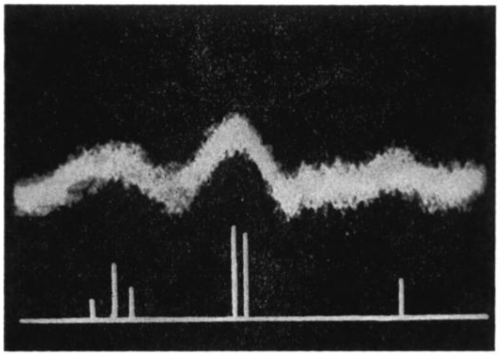

FIG. 2. Theoretical and observed nitrogen splitting of the $J=0\rightarrow1$ transition of $N^{14}N^{14}O$. Separation of two outside peaks is 765 *kc*/s.