$^{81}$Br and $^{127}$I NQR of Rare Earth Trihalogenides $\text{REX}_3$, $X = \text{Br, I}$*

T. A. Babushkina, A. A. Boguslavsky, and A. G. Dudareva
Institute of Biophysics, Ministry of Health, Moscow, USSR

Z. Naturforsch. 41 a, 190–191 (1986); revised version received November 5, 1985

The $^{81}$Br NQR spectra of $\text{REBr}_3$, $\text{RE} = \text{Dy, Ho, Yb, Sm}$, and the $^{127}$I NQR spectra of $\text{REI}_3$, $\text{RE} = \text{Dy, Ho, Sm}$, are reported. Additionally $^{127}$I NQR data of $\text{RbHoI}_3$, $\text{KSmI}_3$, and $\text{RbSmI}_3$ are given. The line shape of the $^{127}$I NQR of $\text{HoI}_3$ was studied in external magnetic fields up to 300 Gauss.

**Introduction**

Trihalogenides of rare earth elements show some differences in their crystal lattices. The chlorides and bromides of the light rare earth elements LaCl$_3$...GdCl$_3$; LaBr$_3$...PrBr$_3$, are isomorphous to UC$_3$ [1]. The trichlorides of the heavy rare earth elements are isomorphous to AIC$_3$ and the corresponding tribromides crystallize with the FeCl$_3$ type structure [2, 3]. Several tribromides REBr$_3$ (RE = Nd, Eu, Sm, Tb) and the iodides REI$_3$ (RE = La, Ce, Pr, Nd) are isomorphous to PuBr$_3$, whereas the majority of the REI$_3$ shows the BiI$_3$ type structure [4, 5].

NQR is quite a sensitive method with respect to details in the structure of the electrons surrounding the resonating nuclei, and changes in the crystal structure can easily be detected.

**Results and Discussion**

We have studied several tribromides and triiodides of rare earth elements, and a few compounds formed by rare earth triiodides and alkali iodides. In Table 1 the $^{81}$Br and $^{127}$I NQR frequencies are listed for $T = 77$ K (in a few cases for 290 K, too).

Since the compounds DyBr$_3$, HoBr$_3$, and YbBr$_3$, are isomorphous to FeCl$_3$ (C$_3$h−R 3, $Z = 6$), a single line $^{81}$Br NQR spectrum is expected and the experimental results are in accordance with this expecta-
Table 1. NQR frequencies of $^{81}$Br and $^{127}$I, quadrupole coupling constants, $e^2 \Phi_{zz} Q h^{-1}$ ($^{127}$I), and asymmetry parameters $\eta$ ($^{127}$I), in some trihalogenides of the rare earth elements. $v(81{Br})$ at $T = 11$ K.

<table>
<thead>
<tr>
<th>Substance</th>
<th>$v(81{Br})$/MHz</th>
<th>$v(127{I})$/MHz, $\Delta m = 1/2 - 3/2$</th>
<th>$v(127{I})$/MHz, $\Delta m = 3/2 - 5/2$</th>
<th>$e^2 \Phi_{zz} Q h^{-1}$/MHz</th>
<th>$\eta$ (%)</th>
<th>$T$/K</th>
</tr>
</thead>
<tbody>
<tr>
<td>DyBr$_3$</td>
<td>30.36</td>
<td>83.33</td>
<td>276.7</td>
<td>9.5</td>
<td>77</td>
<td></td>
</tr>
<tr>
<td>HoBr$_3$</td>
<td>31.194</td>
<td>82.80</td>
<td>278.3</td>
<td>13.5</td>
<td>290</td>
<td></td>
</tr>
<tr>
<td>YbBr$_3$</td>
<td>34.224</td>
<td>85.84</td>
<td>280.7</td>
<td>10.0</td>
<td>77</td>
<td></td>
</tr>
<tr>
<td>SmBr$_3$</td>
<td>24.985</td>
<td>72.76</td>
<td>242.5</td>
<td>9.0</td>
<td>300</td>
<td></td>
</tr>
<tr>
<td>Rbl•HoI</td>
<td>38.19</td>
<td>74.30</td>
<td>248.2</td>
<td>15.0</td>
<td>77</td>
<td></td>
</tr>
<tr>
<td>KI•SmI$_3$</td>
<td>41.09</td>
<td>80.64</td>
<td>270.3</td>
<td>12.5</td>
<td>77</td>
<td></td>
</tr>
<tr>
<td>3Rbl•2SmI$_3$</td>
<td>34.01</td>
<td>63.29</td>
<td>214.4</td>
<td>24.0</td>
<td>77</td>
<td></td>
</tr>
</tbody>
</table>

is rather small ($\approx 10\%$). This points out that there is a small deviation of the iodine positions from the ideal Bi$_3$ type structure in which the point symmetry of the iodine would be $3 (\eta = 0)$.

For SmI$_3$ the $^{127}$I NQR frequency ($1/2 \rightarrow 3/2$) was found to increase very little with decreasing temperature ($\sim 0.012$ kHz/degree). In the range $110 \leq T/K \leq 120$ the intensity of the line becomes very weak and at $T = 77$ K no $^{127}$I NQR signal was detected in the range $50 \leq v$/MHz $\leq 150$.

HoI$_3$ shows a very strong transition $3/2 \rightarrow 5/2$ and the signal to noise ratio is 100 on the oscilloscope. The $^{127}$I Zeeman spectrum on polycrystalline material was studied at $77$ K in a field $B_0 = 3 \cdot 10^{-2}$ T ($B_0 \parallel B_{HF}$). It was found that the shape of the band is very similar to that found for Sb in Sb$_2$O$_3$ and Re in NaReO$_4$ [7], but different from the shape expected in case of negligible dipole-dipole interactions. This effect can be observed by comparing the $^{35}$Cl Zeeman NQR powder spectrum of NaClO$_3$ and KClO$_3$, where in the latter compound dipolar interactions are very small.

The $^{127}$I NQR Zeeman powder spectrum (3/2 $\rightarrow$ 5/2) of SmI$_3$ is shown in Figure 1. It seems to be of interest to elaborate the theory of NQR line shape by incorporating dipole-dipole interactions.