

# **$^{81}\text{Br}$ NQR and $^1\text{H}$ NMR of Ethylammonium Tetrabromomercurate (II)**

## **$(\text{C}_2\text{H}_5\text{NH}_3)_2\text{HgBr}_4$ : Phase Transition and Molecular Motion**

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Crystals of  $(\text{C}_2\text{H}_5\text{NH}_3)_2\text{HgBr}_4$  were investigated by means of  $^{81}\text{Br}$  NQR,  $T_1$  of  $^1\text{H}$  NMR, and DTA measurements. The crystals undergo phase transitions at  $T_{c1} = 342$  K and  $T_{c2} = 96$  K. In phase III ( $T < T_{c2}$ ) sixteen  $^{81}\text{Br}$  NQR lines, and in both phase II ( $T_{c2} < T < T_{c1}$ ) and phase I ( $T_{c1} < T$ ) four lines were observed. The DTA peak positions at the  $T_{c1}$  transition depend strongly on the thermal history. In the cooling runs from the melt the crystals exhibited a strange thermal behavior. The  $\log T_1$  vs.  $T^{-1}$  curves of  $^1\text{H}$  NMR (42.5 MHz), measured in  $(\text{C}_2\text{H}_5\text{ND}_3)_2\text{HgBr}_4$  as well as  $(\text{C}_2\text{H}_5\text{NH}_3)_2\text{HgBr}_4$ , were characterized by V-shaped curves with a single minimum. They are explained by postulating  $C_3$  reorientational motions of  $\text{CH}_3$ - and  $\text{NH}_3$ -groups with the experimentally same correlation time and activation energy  $E_a$ . In Phase II, the  $E_a$  values were estimated as  $13.9 \text{ kJmol}^{-1}$  and  $14.2 \text{ kJmol}^{-1}$  for  $(\text{C}_2\text{H}_5\text{NH}_3)_2\text{HgBr}_4$  and  $(\text{C}_2\text{H}_5\text{ND}_3)_2\text{HgBr}_4$ , respectively. The  $^2\text{H}$  NMR spectra suggest that reorientation of the whole cations about the molecular axis is excited at high temperatures

*Key words:*  $(\text{C}_2\text{H}_5\text{NH}_3)_2\text{HgBr}_4$ ; Phase Transition; Molecular Motion; NQR; NMR.