^{81}Br NQR and ^{1}H NMR of Guanidinium Hexabromoantimonate(V) $[C(NH_2)_3]SbBr_6$: Phase Transition and Molecular Motion

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Z. Naturforsch. **57 a,** 399–402 (2002); received January 18, 2002

Presented at the XVIth International Symposium on Nuclear Quadrupole Interactions, Hiroshima, Japan, September 9-14, 2001.

Guanidinium hexabromoantimonate(V) $[C(NH_2)_3]SbBr_6$ was prepared. It was black in color at room temperature and showed a tendency to turn yellow by loosing bromine in open air. Six ^{81}Br NQR lines were observed at 77 K. On heating, four of the six lines faded out around 200 K, while the remaining two lines could be observed up to room temperature. This temperature behavior suggests a preferential libration or reorientation around a pseudo C_4 axis of the octahedral $[SbBr_6]^-$ anion. DTA measurement revealed a small heat anomaly at T_{c1} = 273 K (on heating), showing a thermal hysteresis, and a sharp and large anomaly at T_{c2} = 314 K. The temperature dependence curve of ^{1}H NMR T_1 is characterized by a single minimum of 26 ms (32 MHz) near 280 K, which is assigned to the C_3 reorientation of the planar $[C(NH_2)_3]^+$ cations. Its activation energy (E_a) is 43.3 kJ/mol.

Key words: $[C(NH_2)_3]SbBr_6$; Phase Transition; Molecular Motion; ^{81}Br NQR; ^{1}H NMR T_1.