

Phase Transitions and Crystal Structure of Dimethylammonium Tribromomercurate(II), $(\text{CH}_3)_2\text{NH}_2\text{HgBr}_3$, as Studied by ^{81}Br NQR and Single Crystal X-ray Diffraction*

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The temperature dependence of the ^{81}Br NQR frequencies of the title compound has revealed the presence of three phases (I, II and III, in the order of decreasing temperature): T_{c1} (II - I) = (318 ± 10) K and T_{c2} (III - II) = (202 ± 1) K. The transitions were confirmed by thermal analysis (DTA). Both of the II-I and I-II transitions exhibited strong hysteresis (*i. e.*, superheating and supercooling, respectively). The crystal data, determined by single crystal X-ray diffraction, are: monoclinic, space group P2/a, $a = 1384.8(3)$, $b = 934.7(4)$, $c = 1452.0(2)$ pm, $\beta = 104.10(1)^\circ$, $Z = 8$, $R = 0.076$. The crystal has two crystallographically independent cations $(\text{CH}_3)_2\text{NH}_2^+$ and an infinite chain of anions almost in the c -direction. The anion chain is considered to consist of a HgBr_2 molecule and two different HgBr_4^{2-} anions which are interconnected *via* weak intermolecular $\text{Hg}\cdots\text{Br}$ bonds. The splitting patterns of the ^{81}Br NQR spectra indicate that rearrangements of the Hg-Br bonds are slight at the III-II transition but serious at the II-I transition. Some of the ^{81}Br NQR lines show anomalous temperature coefficients, attributable probably to thermal motions of cations.

Key words: $(\text{CH}_3)_2\text{NH}_2\text{HgBr}_3$; X-Ray Analysis; NQR; Phase Transition; Crystal Structure.

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