^{127}I NQR and Crystal Structure Studies of $[N(CH_3)_4]_2CdI_4$

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The temperature dependence of ^{127}I NQR and DSC as well as the crystal structure at room temperature of the title compound were determined. This compound shows a first-order phase transition of an order-disorder type at 245 K. Eight ^{127}I(ν_1: $m = \pm\frac{1}{2} \leftrightarrow \pm\frac{3}{2}$) NQR lines of 79.57, 81.86, 82.56, 83.36, 84.68, 87.72, 88.34, and 88.86 MHz, and corresponding eight ^{127}I(ν_2: $m = \pm\frac{3}{2} \leftrightarrow \pm\frac{5}{2}$) NQR lines were observed at liquid nitrogen temperature. Three ^{127}I(ν_1) NQR lines with an intensity ratio of 1:1:2 in the order of decreasing frequency were observed just above the transition point and two NQR lines except for the middle-frequency line disappeared around room temperature. This temperature behavior of NQR lines is very similar to that observed in $[N(CH_3)_4]_2HgI_4$. Another first-order phase transition takes place at 527 K. The structure of the room-temperature phase was redetermined: orthorhombic, Pnma, Z = 4, a = 1342.8(3), b = 975.7(2), c = 1696.5(3) pm. The NQR result of three lines with an intensity ratio of 1:1:2 is in agreement with this structure. The thermal displacement parameters of atoms in both cations and anions are large.

Key words: NQR; DSC; Crystal Structure; Phase Transition.