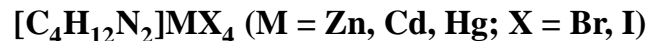


# NQR Study of Piperazinium Tetrahalogenometalates(II)



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The <sup>81</sup>Br and <sup>127</sup>I NQR ( $\nu_1: m = \pm 1/2 \leftrightarrow m = \pm 3/2$  transition) frequencies in the title compounds were measured as functions of temperature. Four NQR lines were observed for each bromide or iodide in the temperature range investigated. Piperazinium tetrabromocadmate(II) was obtained as a monohydrate (**1**) containing isolated  $\text{CdBr}_4^{2-}$  anions, piperazinium dications, and water molecules (monoclinic,  $\text{P2}_1/\text{c}$  at 293 K). The crystal structure of piperazinium tetraiodocadmate(II) (**2**) was found to consist of isolated  $\text{CdI}_4^{2-}$  anions and dications (orthorhombic,  $\text{P2}_12_12_1$  at 293 K). The structures of others seem to be similar to that of (**2**). The DSC measurement of (**1**) showed heat anomalies at ca. 363, 386 and 556 K, that of the anhydrous sample only at 556 K, which suggests that the former two heat anomalies are due to dehydration. All the other compounds exhibited also a phase transition around 550 K and decomposed above 600 K. Disappearance (or remarkable weakening in intensity) of the NQR lines was observed at 330 - 350 K in all compounds, indicating the pronounced excitation of librational motions of anions and/or cations. The NQR results indicate that the covalent character of M-X bond is in the order  $\text{Zn-X} < \text{Cd-X} \ll \text{Hg-X}$ .

*Key words:* NQR; DSC; Piperazinium Tetrahalogenometallate(II); Bond Character; Phase Transition.