Static and Dynamic Structures of $InBr_x$ (x = 1.4, 1.5, 1.75, and 2) Studied by ^{81}Br NQR and ^{115}In NMR

Koji Yamada, Hiroshi Mohara, Tomotaka Kubo, Takashi Imanaka, Kazue Iwaki, Hiroshi Ohki, and Tsutomu Okuda

Graduate School of Science, Hiroshima University,
Kagamiyama 1-3, 739-8526 Higashi-Hiroshima, Japan

Reprint requests to Dr. K. Y.; E-mail: kyamada@sci.hiroshima-u.ac.jp

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Structure and bonding properties of $InBr_x$ (In_5Br_7, In_2Br_3, In_4Br_7 and $InBr_2$) were studied by ^{81}Br and ^{115}In NQR, and ^{115}In NMR. The ethane-like $[Br_3In^{II}\text{-}In^{II}Br_3]^{2-}$ anion was confirmed in In_5Br_7 or In_2Br_3 by ^{81}Br NQR and the anion was characterized by the high quadrupole coupling constant at the ^{115}In site ($e^2Qq/h \approx 350$ MHz). On the other hand, In_4Br_7 showed successive phase transitions and was characterized as $[In^{I}]_5[In^{III}Br_4]_2[In^{III}Br_6]$ by means of ^{81}Br NQR and ^{115}In NMR below 370 K. A disordered structure at the cationic sublattice was supposed at Phase I above 370 K. NMR signals assigned to the In^{I} could not be detected for the powdered sample, however, all quadrupole coupling constants (e^2Qq/h) and chemical shifts (σ_{iso}) could be determined using a single crystal. The In^{I} sites show relatively large e^2Qq/h and also show larger distribution of the chemical shift suggesting a diversity of the In^{I} coordination similar to the isoelectronic main group elements such as Sn^{II} or Sb^{III}.

Key words: ^{115}In NMR; Single Crystal; Quadrupole Coupling Constant; Phase Transition.