THERMAL VIBRATIONS AND STATIC DISPLACEMENTS OF ATOMS IN HEXABORIDES $N^{11}B_6$ AND $^{154}Sm^{11}B_6$

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Crystal structures of $Nd^{11}B_6$ and intermediate-valence $^{154}Sm^{11}B_6$ have been studied by high-resolution powder neutron diffraction in the temperature range 20–300 K with the aim to compare structural parameters of atoms and their variation with temperature in both hexaborides in search of difference which might be related to the intermediate-valence state of Sm ion. It was found that thermal vibrations of intermediate-valence state of Sm ion and of the integer valence Nd ion can be satisfactory described by the Einstein model with characteristic temperature 120 K within the whole temperature range. A peculiar temperature dependences of the anisotropic temperature factors of the boron atoms were observed in

both compounds. It was shown that both in $Nd^{11}B_6$ and $^{154}Sm^{11}B_6$ the unusual temperature dependences of the mean-square displacements of the boron atoms can be satisfactory described by the Debye model only upon the assumption of static displacements of boron atoms.