CRYSTAL STRUCTURE, LOCAL SODIUM ENVIRONMENTS AND ION DYNAMICS IN Na_{0.8}Ni_{0.6}Sb_{0.4}O₂, A NEW MIXED ANTIMONATE

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At 298 K cation conducting mixed antimonate Na_{0.8}Ni_{0.6}Sb_{0.4}O₂ exhibits an O3-type structure, with sodium ions in a distorted octahedral coordination, space group R-3m, a = 3.0496(1)Å, c = 16.4060(4)Å. ²³Na NMR reveals two main types of sodium local environments, ascribed to the different distribution of sodium vacancies in the second coordination sphere, (NaO₆)Na₄□₂ and (NaO₆)Na₅□ (populations ratio 2:1 at 215-230 K). These data agree with the model of local order for x≈0.79 and disagree with the model of random vacancy distribution. The temperature increase results in the sites averaging and NMR lines narrowing. The activation energy for the motion of sodium cations within one site estimated from ²³Na NMR data is ca. 1.0 kJ/mol at 215-288 K, much lower than the activation energy of both sodium hopping between the sites in a crystallite (ca. 22 kJ/mol at 330-370 K) and long-range transfer in ceramic material (ca. 48 kJ/mol at 294-775 K).