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Structural and ferroelectric phase evolution in $[KNbO_3]_{1-x}[BaNi_{1/2}Nb_{1/2}O_{3-\delta}]_x$ (x = 0, 0.1)[1] CHRISTOPHER HAWLEY, Drexel University, LIYAN WU, University of Pennsylvania, GEOFFREY XIAO, Drexel University, ILYA GRINBERG, Bar Ilan University, ANDREW RAPPE, PETER DAVIES, University of Pennsylvania, JONATHAN SPANIER, Drexel University — The phase transition evolution for $[KNbO_3]_{1-x}[BaNi_{1/2}Nb_{1/2}O_{3-\delta}]_x$ (x=0, 0.1) is determined via complementary dielectric constant and Raman scattering measurements. Raman scattering by optical phonons over the range of 100-1000 cm^{-1} for -190°C $< T <$ 600°C reveals six discernible zone-center optical phonon modes. They are assigned to structural and ferroelectric phases in the solid solution $x = 0.1$ and compared with those for end member $x = 0$ and with the results of temperature-dependent dielectric permittivity. Rigorous peak fitting analyses of spectra collected from the solid solution and end member indicate structural and ferroelectric phase transition temperatures that are quite close to those for the $KNbO_3$ end member. Remarkably, despite the inclusion of 5 atomic % of ferroelectrically inactive Ni cations, the structural transition temperatures remain essentially unchanged. This is confirmed using density functional theory calculations to predict the polarization for $x = 0$ and 0.1 establishing that the ferroelectric-paraelectric T_c are comparable.

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