Structures of Perovskite-related layered $A_nB_nO_{3n+2}$

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Perovskite-related oxidic compounds $A_nB_nO_{3n+2}$ (where A = Ca, La or Sr and B = Ti or Nb) with n = 4, 4.5, 5, 6, and 7 have been the subject of much research, because of their one-dimensional metallic behavior which has been attributed to Peierls transition and charge-density wave [1,2]. Their structures are derived from the ABO_3 perovskite-type structure with additional layers of oxygen separating the slabs of BO_6 octahedra which are parallel to the (110) planes. The width of the slab is determined by the oxygen content and is given directly by the parameter n. In this study, single crystals of several of these compounds were prepared by floating-zone melting [1] and their crystal structures were determined at ambient conditions by single-crystal X-ray diffraction with synchrotron radiation using a CCD area detector. For some of these compounds superstructures were observed while some could be described by modulated structures. Particular attention is given to the distortions of the BO_6 octahedra and their variations across the width of the slabs, the different environments of the A cations, and the chemical ordering of these cations.

[1] Lichtenberg F., Herrnberger A., Wiedenmann K., Mannhart J., *Prog. Sol. State Chem.*, 2001, **29**, 1-70. [2] Kuntscher C. A., Schuppler S., Haas P., Gorshunov B., Dressel M., Grioni M., Lichtenberg F., Herrnberger A., Mayr F., Mannhart J., *Phys. Rev. Lett.*, 2002, **89** , 236403.

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