Structural phase transition and charge-ordering effect in η-Na<sub>1.286</sub>V<sub>2</sub>O<sub>5</sub>, Fabienne Duc<sup>\*</sup> and Patrice Millet, Centre d'Elaboration de Matériaux et d'Etudes Structurales, UPR CNRS 8011, 29 rue Jeanne Marvig, BP 94347, 31055 Toulouse Cedex 04, France. E-mail: fduc@cemes.fr

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Charge ordering in mixed-valence transition metal oxides is a subject of great interest in solid state physics, very likely related to many electronic and magnetic properties that these compounds display. Within the transition metal oxides systems, vanadates offer an enormous playground of compounds where different valence states can coexist, and which may eventually give rise to quantum spin antiferromagnetic orderings. Recently, the detailed study of the V4+- rich zone of the sodium-vanadium-oxygen phase diagram has led to the structural characterization of the vanadium oxide bronze η-Na<sub>1.286</sub>V<sub>2</sub>O<sub>5</sub> [1-2] (also denoted by the stoichiometric formula Na<sub>9</sub>V<sub>14</sub>O<sub>35</sub>). The structure of the latter (space group P2/c) is built up of layers consisting of VO<sub>5</sub> square pyramids sharing edges and corners with their apical oxygens pointing up and down alternately to form double strings in the [100] direction. These double strings are isolated in the [001] direction via VO<sub>4</sub> tetrahedra and have a stair-like shape with a step every ten VO<sub>5</sub> square pyramids. This compound has been reported to exhibit [2] a spin-gap behaviour, although its magnetic susceptibility curve could not be fitted by theoretical equations for spin-gap systems. It is presently considered as a new type of low-dimensional system.

This contribution will give an overview of recent results [3] obtained by low temperature x-ray diffraction on the  $\eta$ -Na<sub>1.286</sub>V<sub>2</sub>O<sub>5</sub> phase. The x-ray data clearly reveal the existence, around 100 K, of a structural second-order phase transition, stabilizing a superstructure associated with charge ordering.

<sup>[1]</sup> Millet, P., Henry, J.-Y. & Galy, J. (1999). Acta Cryst. C55, 276-279.

<sup>[2]</sup> Isobe, M., Ueda, Y., Oka, Y. & Yao, T. (1999). J. Solid State Chem. 145, 361-365.

<sup>[3]</sup> Duc, F., Millet, P., Ravy, S., Thiollet, A., Chabre, F., Ghorayeb, A. M., Mila, F. & Stepanov, A. (2004). *Phys. Rev.* B **69**, in print.