Three-dimensionally aligned V trimers in various vanadates

T. Katsufuji ^{a, b}, M. Ikeda^a, J. Miyazaki^a, T. Kajita^a, K. Takubo^a, Y. Nagamine^c, S. Mori^c, K. Kato^d, and M. Takata^d

^aDepartment of Physics, Waseda University, Tokyo, Japan ^bPRESTO, JST, Saitama, Japan

Department of Material Science, Osaka Prefecture University, Sakai, Japan

^dRIKEN/SPring-8, Hyogo, Japan

We found that V^{3+} ($3d^2$) trimers are formed and three-dimensionally aligned as a phase transition in three different series of vanadates [AV₁₀O₁₅, A₂V₁₃O₂₂, and AV₁₃O₁₈ (A=Ba,Sr)], in which V ions occupy a part of the fcc lattice in the high-temperature phase. ¹ We also found that this V trimerization substantially affects the transport and magnetic properties of these compounds. From various measurements, e.g., resonance x-ray scattering, NMR, and optical measurement, we conclude that this V trimerization and the change of various properties can be attributed to the orbital ordering of V t_{2g} states with spin-singlet formation. The present result implies that such V trimers are local objects that are rather universally observed in a certain class of compounds ($3d^2$ ions on a fcc lattice), and can be regarded as "molecules of ions" in the crystal.

¹J. Miyazaki and T. Katsufuji *et al.*, Phys. Rev. Lett. **104**, 207201 (2010); T. Kajita and T. Katsufuji *et al.*, Phys. Rev. B **81**, 060405(R) (2010); M. Ikeda and T. Katsufuji *et al.*, Phys. Rev. B **82**, 104415 (2010); M. Ikeda and T. Katsufuji *et al.*, Phys. Rev. B **83**, 134417 (2011).