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Magnetic ground state of PbVO₃ and origin of the large tetragonal distortion KENGO OKA, IKUYA YAMADA, MASAKI AZUMA, MIKIO TAKANO, YUICHI SHIMAKAWA, Inst. Chem. Res., Kyoto Univ., SOSHI TAKESHITA, KOHKI H. SATOH, AKIHIRO KODA, RYOSUKE KADONO, Inst. Mater. Str. Sci., KEK, HIROSHI KOJITANI, MASAKI AKAOGI, Gakushuin Univ. — Magnetic property of PbTiO₃-type perovskite PbVO₃ with a large tetragonal distortion $(c/a=1.23)^1$ was investigated. Long-range antiferromagnetic ordering with $T_N = 45$ K was found by a μ SR measurement. Magnetic susceptibility of multi domain crystal showed a broad maximum centered at 180 K indicated the 2-dimensional nature in magnetism. This is consistent with the d_{xy} orbital ordering predicted by the band calculation.² We propose a mechanism that the pyramidal coordination with a short vanadium-apical oxygen bond is stabilized to lift the orbital degeneracy in this d^1 system. Accordingly, PbMnO₃ (Mn⁴⁺, d^3) newly stabilized at 15 GPa has a pseudo cubic structure like PbCrO₃. This scenario explains the pressure induced tetragonal to cubic, insulator to metal transition¹ of PbVO₃ and similar large tetragonal distortion of BiCoO₃. [1]A. A. Belik, et al., Chem. Mater., 18 (2006) 798. [2]Y. Uratani, et al., Jpn. J. Appl. Phys., 44 (2005) 7130.

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