Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

High-pressure structural investigation of the spin-Peierls compound TiOCl. A. PRODI, Massachusetts Institute of Technology, J. HU, NSLS, Brookhaven National Laboratory, E. ABEL, Massachusetts Institute of Technology, F.C. CHOU, National Taiwan University, Y.S. LEE, Massachusetts Institute of Technology — TiOCl is a S=1/2 layered Mott insulator which displays a spin-Peierls state at low-temperatures involving the dimerization of the Ti ions. Although carrier localization is expected to be weak, it has proven difficult to dope charges in the system through partial chemical substitution. To explore if TiOCl could instead host a bandwidth-driven insulator-to-metal transition under external pressure, we investigated the crystal structure at pressures up to 17 GPa by means of powder and single crystal synchrotron x-ray diffraction in diamond anvil cells.

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Date submitted: 20 Nov 2006 Electronic form version 1.4