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High pressure X-ray study of the lattice dimerization in the S=1/2 chain quantum magnet TiOCl. COSTEL R. ROTUNDU, SIMES, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA, JIAJIA WEN, WEI HE, Department of Applied Physics, Stanford University, Stanford, CA 94305, USA, YEJUN FENG, YONGSEONG CHOI, DANIEL HASKEL, The Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA, YOUNG S. LEE, Department of Applied Physics, Stanford University, Stanford, CA 94305, USA and SIMES, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — TiOCl, composed of S=1/2 chains of Ti ions, is a good realization of a spin-Peierls system. Considerable effort has been put into doping the material with the goal of achieving metallization. Interestingly, high pressure resistivity shows a dramatic decrease of its insulating behavior, which may coincide with the emergence of charge density wave order. Therefore, high pressure of the structure with x-rays are important in further exploring the phase diagram. Upon cooling under normal pressure conditions, TiOCl exhibits a transition to an incommensurate nearly dimerized state at Tc2 = 92 K and to a commensurate dimerized state at Tc1 = 66 K. Here we map its complex temperature vs. pressure phase diagram with x-rays on a single crystal in a high pressure diamond anvil down to 6 K in temperature and to pressures up to approximately 14.5 GPa.

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