

## Microsymposium

**MS17.O04**

### *Pressure-induced normal-incommensurate-commensurate phase transitions in $\text{TiPO}_4$*

M. Bykov<sup>1</sup>, E. Bykova<sup>1,2</sup>, L. Dubrovinsky<sup>2</sup>, M. Hanfland<sup>3</sup>, H. Liermann<sup>4</sup>, R. Kremer<sup>5</sup>, S. van Smaalen<sup>1</sup>

<sup>1</sup>University of Bayreuth, Laboratory of Crystallography, Bayreuth, Germany, <sup>2</sup>University of Bayreuth, Bavarian Research Institute of Experimental Geochemistry and Geophysics, Bayreuth, Germany, <sup>3</sup>ESRF, Grenoble, France, <sup>4</sup>Photon Sciences, FS-PE, DESY, Hamburg, Germany, <sup>5</sup>Max Planck Institute for Solid State Research, Stuttgart, Germany

The complex interplay between spin, charge, orbital, and lattice degrees of freedom has made low-dimensional quantum spin magnets with strong antiferromagnetic (AF) spin-exchange coupling prime candidates for studying unusual magnetic phenomena. A progressive spin-lattice dimerization in one-dimensional AF Heisenberg chains, which occurs below a critical temperature and induces a singlet ground state with a magnetic gap, is commonly referred to as spin-Peierls (SP) transition. Recently, the compounds  $\text{TiOX}$  ( $X = \text{Cl}, \text{Br}$ ) and  $\text{TiPO}_4$  have been intensively investigated due to their unconventional behavior [1,2]. Unlike standard SP systems,  $\text{TiOX}$  and  $\text{TiPO}_4$  undergo a sequence of normal-incommensurate-commensurate phase transitions on cooling at remarkably high transition temperatures. The transition temperatures are related to the direct exchange interactions between Ti ions, which increases strongly with decreasing the distance between the Ti ions, and therefore is very sensitive to the applied hydrostatic pressure. We have performed pressure-dependent single-crystal X-ray diffraction of  $\text{TiPO}_4$  using synchrotron radiation.  $\text{TiPO}_4$  undergoes a pressure-induced phase transition towards an incommensurate phase already below 10 GPa. This transformation is followed by the lock-in phase transition to the dimerized SP phase. Both structures are analogous to those at low temperatures, but reveal significantly larger modulation amplitudes. In this contribution we will present the detailed discussion of the high-pressure structures of  $\text{TiPO}_4$  and their behavior on compression. Furthermore, similarities and differences of high-pressure phase diagrams of  $\text{TiOCl}$  and  $\text{TiPO}_4$  and discrepancies between predicted and observed structures will be considered.

[1] A. Seidel, C. Marianetti et al., *Phys. Rev. B*, 2003, 67, 020405(R), [2] J.M. Law, C. Hoch, et al., *Phys. Rev. B*, 2011, 83, 180414(R)

**Keywords:** High-pressure, x-ray diffraction, Aperiodic crystals