

## Poster-2-12

**Structural studies on new, layered K–Cu–Te oxides**Felix Eder,<sup>1</sup> Matthias Weil,<sup>2</sup> Ronald Miletich,<sup>3</sup> and Harishchandra Singh<sup>4</sup><sup>1</sup> University of Geneva, Department of Quantum Matter Physics, Laboratory for Quantum Material Discovery<sup>2</sup> Technical University of Vienna, Institute for Chemical Technologies and Analytics, Division of Structural Chemistry<sup>3</sup> University of Vienna, Department of Mineralogy and Crystallography<sup>4</sup> University of Oulo, Faculty of Science, Nano and Molecular Systems Research Unit

The family of layered alkali (*A*) transition metal (*M*) oxidotellurates(VI) with a composition of  $A_2M_2TeO_6$  can exhibit promising electrochemical properties (e.g.  $Li_2Ni_2TeO_6$  [1]) as well as frustrated 2D antiferromagnetism (e.g.  $Na_2Co_2TeO_6$  [2] and  $Na_2Ni_2TeO_6$  [3]) due to the honeycomb sublattice of the transition metal atoms.

The new phase  $K_2Cu_2TeO_6$  was synthesized using the hydroflux method [4]. Its crystal structure consists of  $[CuTe_2O_6]$  layers separated by  $K^+$  cations. The honeycomb sublattice of the Cu atoms is distorted due to the pronounced Jahn–Teller effect of Cu(II).

The structural evolution of  $K_2Cu_2TeO_6$  at increased temperatures and pressures was investigated by high-temperature synchrotron powder diffraction and high-pressure Raman spectroscopy. During the latter, hints of a second-order phase transition at pressures of 5–7 GPa were observed.

$K_2Cu_2TeO_6$  is prone to incorporate water molecules besides the  $K^+$  cations between the layers; this process can be tracked by the shifting of reflections to smaller angles in X-ray powder diffraction measurements. Furthermore, there exist two stoichiometric hydrates (mono-, and tetrahydrate) of  $K_2Cu_2TeO_6$ , which can be obtained under hydroflux conditions as well.

[1] Grundish, N. S. et al. (2019). Chem. Mater. 31(22), 9379-9388.

[2] Bera, A. K. et al. (2017). Phys. Rev. B 95, 094424.

[3] Kurbakov, A. I. et al (2020). J. Alloys Compd. 820, 153354.

[4] Bugaris, D. E. et al. (2013). Inorg. Chem. 52(7), 3836-3844.