Pressure-induced β→γ phase transition in copper(II) pyrovanadate ($Cu_2V_2O_7$) by single-crystal X-ray diffraction and absorption spectroscopy

Robin Turnbull[1,*], Javier Gonzáles-Platas[2], Fernando Rodríguez[3], Akun Liang[1], Catalin Popescu[4], Zhangzhen He[5], David Santamaría-Pérez[1], Alfonso Muñoz[6], Daniel Errandonea[1]

[1] *Departamento de Física Aplicada - Instituto de Ciencia de Materiales, MALTA Consolider Team, Universidad de Valencia, Edificio de Investigación, C/Dr. Moliner 50, Burjassot, 46100 Valencia, Spain.*

[2] *Departamento de Física - Instituto Universitario de Estudios Avanzados en Física Atómica, Molecular y Fotónica (IUDEA), MALTA Consolider Team, Universidad de La Laguna, Avenida Astrofísico Fco. Sánchez s/n, La Laguna, Tenerife E-38204, Spain.*

[3] *MALTA Consolider Team, Departamento de Ciencias de la Tierra y Física de la Materia Condensada, Facultad de Ciencias, Universidad de Cantabria, 39005 Santander, Spain.*

[4] *CELLS-ALBA Synchrotron Light Facility, 08290 Cerdanyola del Vallès, Barcelona, Spain.*

[5] *State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China*

[6] *Departamento de Física, Instituto de Materiales y Nanotecnología, MALTA Consolider Team, Universidad de La Laguna, La Laguna, E-38204 Tenerife, Spain.*

*e-mail: robin.turnbull@uv.es

We report an experimental high-pressure single-crystal synchrotron X-ray diffraction study of $Cu_2V_2O_7$ under compression to 4 GPa at ambient temperature. The results unambiguously reveal a previously unknown first-order pressure-induced phase transition from monoclinic β-$Cu_2V_2O_7$ to triclinic γ-$Cu_2V_2O_7$ at low pressures (< 0.40 GPa). The presentation will discuss the two structures and how they are related. The phase transition is associated with a volume collapse of approximately 7%, an increase in oxygen coordination (from 5 → 6) of half of the Cu^{2+} coordination complexes, and a reorientation of 1-dimensional chains composed of edge sharing CuO_6 units. The phase transition is also characterised by an indirect → indirect electronic bandgap decrease of approximately 0.2 eV as measured by absorption spectroscopy (1.93 → 1.75 eV) and calculated via density functional calculations (1.93 → 1.76 eV). The bandgap of γ-$Cu_2V_2O_7$, the pressure-induced structural evolution and isothermal compressibility tensor are reported here for the first time. β-$Cu_2V_2O_7$ is found to have by far the lowest bulk modulus (B_0 = 19(2) GPa) of any previously studied vanadate material.

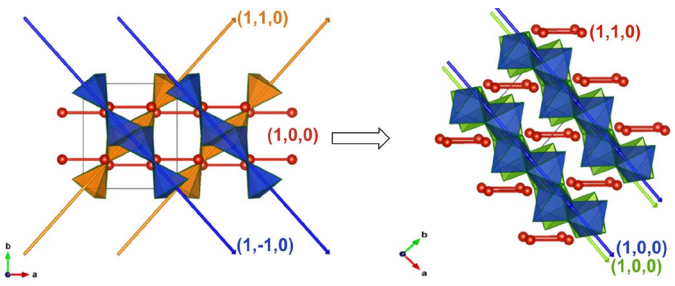


Figure 1: Crystal structures of β- and γ-$Cu_2V_2O_7$.