

ARTICLE

**Pressure-induced chemical decomposition of copper orthovanadate ( $\alpha$ -Cu<sub>3</sub>V<sub>2</sub>O<sub>8</sub>) - Supplementary Information**

Received 00th January 20xx,  
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

Daniel Díaz-Anichtchenko<sup>a</sup>, Robin Turnbull<sup>a,\*</sup>, Enrico Bandiello<sup>a</sup>, Simone Anzellini<sup>b</sup>, Srungarpu Nagabhusan Achary<sup>c</sup> and Daniel Errandonea<sup>a</sup>

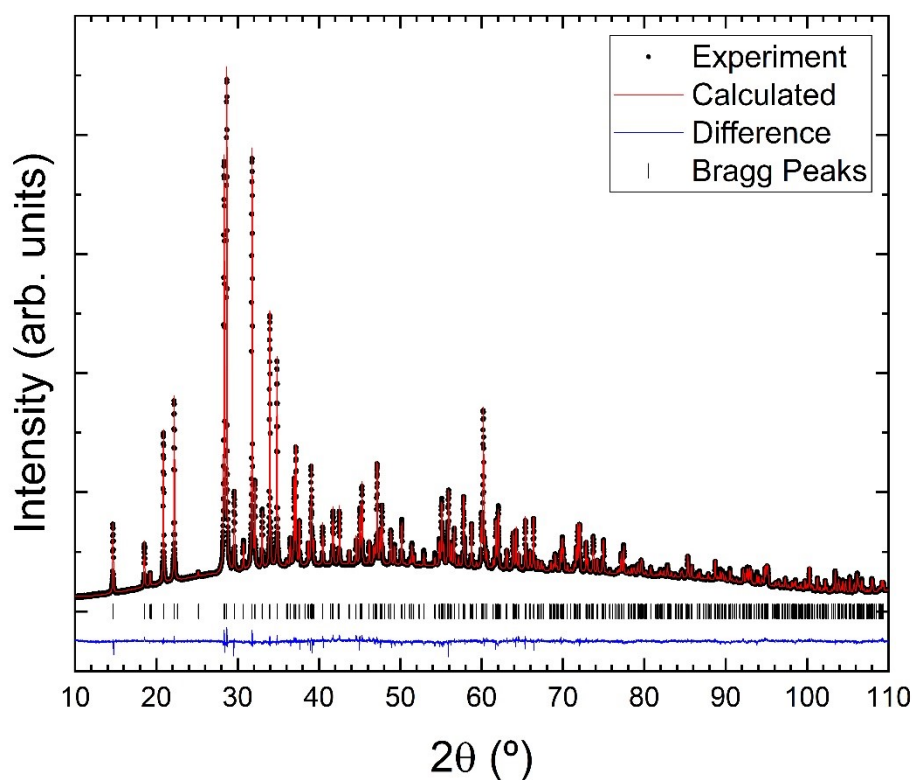
<sup>a</sup> A Departament de Física Aplicada-ICMUV, Universitat de València, Dr. Moliner 50, 46100 Burjassot, Spain \*Corresponding author: robin.turnbull@uv.es

<sup>b</sup> Diamond Light Source Ltd., Diamond House, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, UK

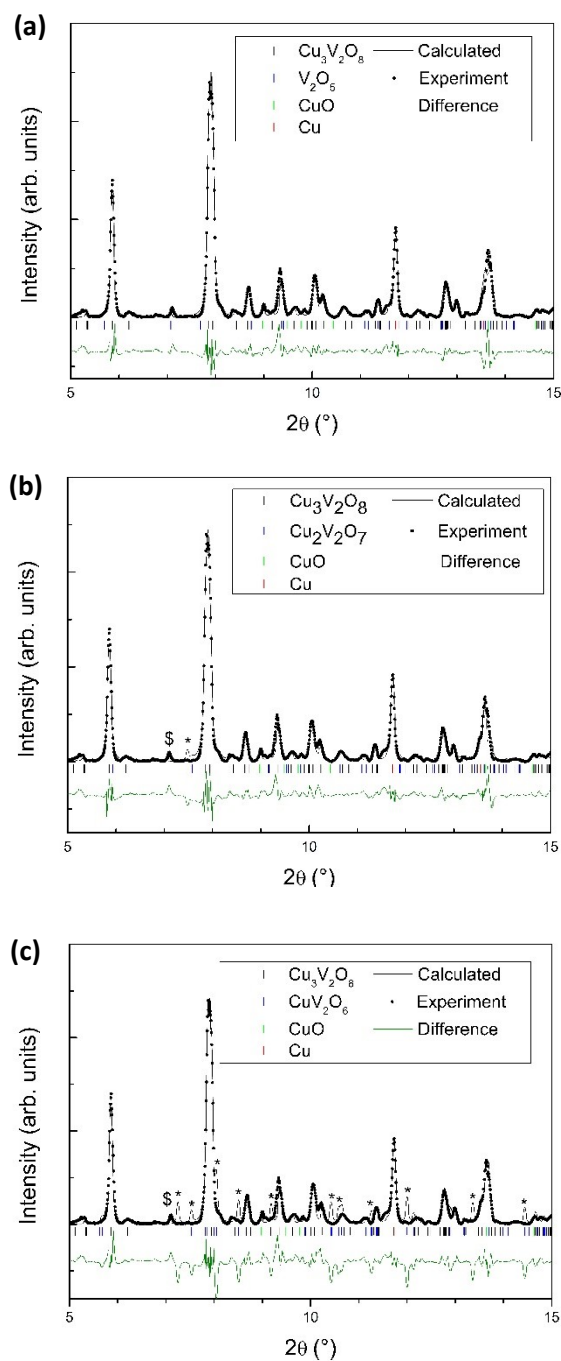
<sup>c</sup> Chemistry Division, Bhabha Atomic Research Centre, Mumbai 400085, India

Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/x0xx00000x

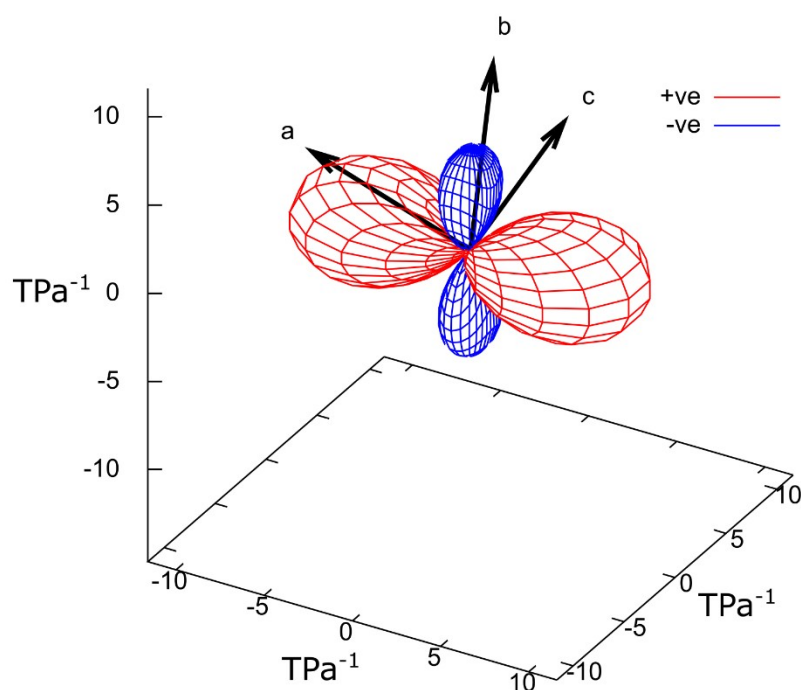
## Supplementary Information



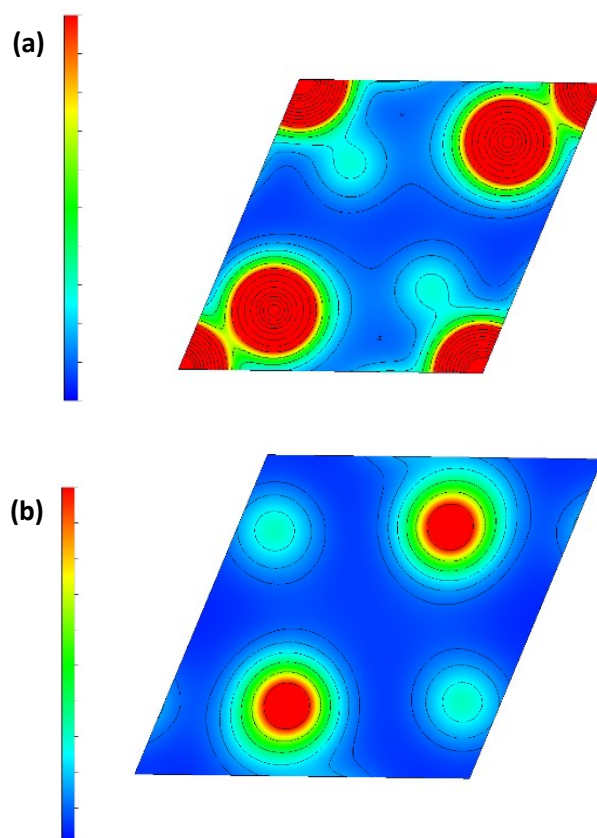
**Supplementary Figure 1 | Integrated powder XRD pattern of  $\alpha$ - $\text{Cu}_3\text{V}_2\text{O}_8$  acquired at ambient conditions.** The experimental data are shown in black. The calculated Rietveld profile is shown in red. The difference between the experimental data and the Rietveld profile is shown in blue. Tick marks indicate the positions of the Bragg reflections. The determined crystal parameters are shown in Table 1.



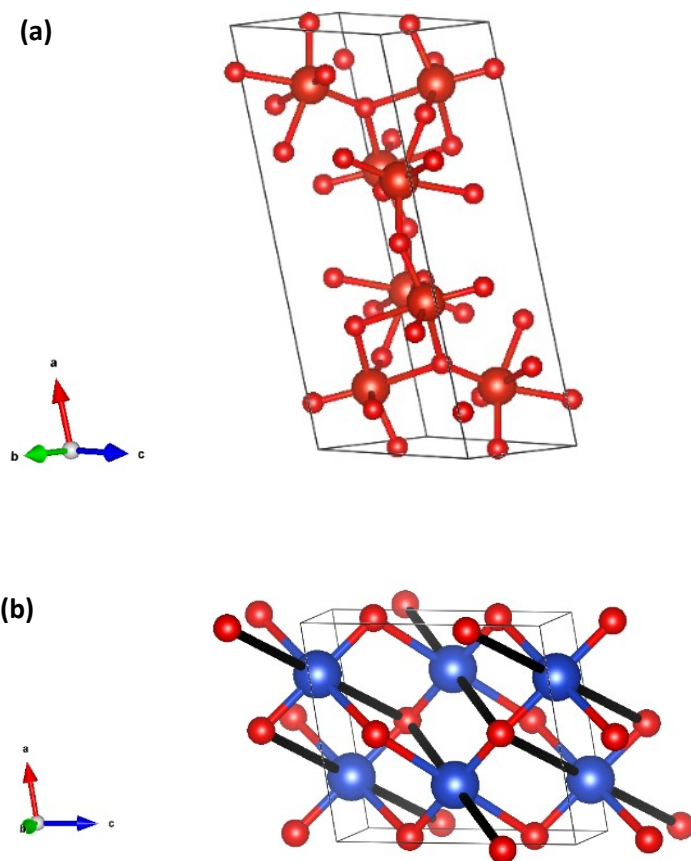
**Supplementary Figure 2 | Integrated XRD pattern acquired at 1.9 GPa (after the onset sample decomposition) fitted with different phase mixtures.** The phase mixtures consist of  $\alpha\text{-Cu}_3\text{V}_2\text{O}_8$  plus: (a)  $\text{CuO} + \text{V}_2\text{O}_5$ , (b)  $\text{CuO} + \text{Cu}_2\text{V}_2\text{O}_7$  and (c)  $2\text{CuO} + \text{CuV}_2\text{O}_6$ . Tick marks correspond to the calculated Bragg peak positions. Asterisks indicate calculated peaks which are not observed experimentally, and '\$' indicates experimental peaks which are not predicted from the selected phases.



**Supplementary Figure 3 | Compressibility indicatrix of  $\alpha\text{-Cu}_3\text{V}_2\text{O}_8$  at ambient pressure.** The directions  $a$ ,  $b$ , and  $c$  are, respectively, equal to the vectors  $e_{v1}$ ,  $e_{v2}$ , and  $e_{v3}$  shown in Table 2.



**Supplementary Figure 4 |** Electron localization in the  $a$ - $b$  plane of  $\alpha$ - $\text{Cu}_3\text{V}_2\text{O}_8$  showing (a) copper atoms, and (b) vanadium atoms.



**Supplementary Figure 5 | Crystal structures of (a) CuO and (b) V<sub>2</sub>O<sub>5</sub>.** Both belong to crystallographic space group C12/c1 (number 15).