## MS.40.4

**Multiferroic CuWO₄ under pressure: Comparison of PXRD and SXRD studies**

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3$d$-transition metal tungstates are interesting due to their scintillating detection properties and their use for the search of rare events in particle physics. Cuproscheelite ($CuWO_4$) has been also proposed as a material for the production of positive electrodes of lithium rechargeable batteries. Furthermore, from the fundamental point of view, $CuWO_4$ has attracted attention as a multiferroic material with an intriguing magnetic phase diagram showing low dimension antiferromagnetism at 90 K; quite above the Neel temperature $T_N$ = 23 K. The Jahn-Teller (JT) effect around the $Cu^{2+}$ ions is responsible for this antiferromagnetic phase. Due to the JT distortion of the $CuO_6$ octahedra the symmetry of cuproscheelite is lowered from the monoclinic wolframite structure (SG. $P2/c$) to a triclinic distorted structure (SG. $P\bar{1}$). Based on our optical absorption [1] and Raman spectroscopy [2] studies at high pressure (HP), it has been found that $CuWO_4$ undergoes a structural phase transition at 10 GPa. Otherwise, *ab initio* calculations [2] predict a wolframite-like structure for the HP phase. On top of that, according to calculations, the phase transformation involves an antiferromagnetic to ferromagnetic transition and a quenching of the JT distortion. In order to study the compressibility, solve the HP structure, and understand the mechanism of the phase transition, we have performed powder x-ray diffraction (PXRD) under different quasi-hydrostatic conditions up to 20 GPa. Experiments were performed at Diamond and APS synchrotrons. We also carried out single crystal x-ray diffraction (SXRD) at pressures smaller (7 GPa) and higher (13.4 GPa) than the transition pressure. These experiments were performed at HASYLAB synchrotron, Hamburg. Results showed that the compound's compressibility is affected by the presence of non-hydrostatic stresses. Depending upon the pressure-transmitting medium the bulk modulus of the low-pressure phase ranges from 139 to 171 GPa. We also found that only under non-hydrostatic conditions a second phase transition takes place at 17 GPa. On the other hand, SXRD experiments allowed us to solve the structure of the HP phase of $CuWO_4$, which has a monoclinic-type structure with space group $P2/c$. Interestingly, the JT effect plays an important role in this phase transition and, in contrast to the theoretical predictions, it is reduced but not suppressed.

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## MS.40.5

**Phase transitions in carbon dioxide at high pressures and temperatures**

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We report on the electronic, structural, and thermodynamic properties of carbon dioxide phases up to 200 GPa and 10 000 K obtained from first-principles theory. The liquid region of the phase diagram is divided into several regimes – molecular and polymeric among others, based on a detailed analysis of local structure and molecular composition. The finite-temperature stability of several solid phases has been examined and the melting curve has been calculated up to 150 GPa. Liquid free energies were evaluated explicitly using a new and efficient method. The issue of carbon-oxygen demixing in the Earth's mantle will also be addressed.

**Keywords: pressure, transition, computation**

## MS.41.1

**Is a more predictable QTAIM possible?**

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The Quantum Theory of Atoms in Molecules (QTAIM) [1] has been extremely successful, providing an orbital invariant theory of chemical bonding based on an observable, the electron density, amenable to experimental determination. Two different operating modes coexist in the QTAIM. In the first, or local mode, chemical descriptors are correlated to the values of operator densities obtained a critical points. The second, or global mode, is based on basin averaged quantities. It is our opinion that the QTAIM has not reached the predictability of the standard Molecular Orbital (MO) paradigm due to the prevalence of the first mode over the second. A set of recent developments that expand both the scope and the predictive power of the QTAIM are considered here. We will first describe the Interacting Quantum Atoms (IQA) [2] approach, which provides an exact energetic decomposition within the QTAIM valid at general geometries. Then we will turn to how a statistical description of chemical bonds through the consideration of electron number distribution functions (EDF) [3] in real space may help recover many well-known concepts derived through MO pictures.

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## MS.41.2

**Halogen bonding from charge density analysis**

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Directional intermolecular interactions of diverse strengths [1],