

## **Influence of cation disorder on the mineral physics of ankerite**

**AZZURRA ZUCCHINI<sup>1,\*</sup>, TIZIANA BOFFA BALLARAN<sup>2</sup>, MAXIMILIANO FASTELLI<sup>1</sup>, DAVIDE COMBONI<sup>3,†</sup>,  
MICHAEL HANFLAND<sup>4</sup>, FRANCESCO FRONDINI<sup>1</sup>, AND PAOLA COMODI<sup>1</sup>**

<sup>1</sup>Department of Physics and Geology, University of Perugia, Piazza Università, 06100 Perugia, Italy

<sup>2</sup>Bayerisches Geoinstitut, University of Bayreuth, D-95440 Bayreuth, Germany

<sup>3</sup>Department of Earth Sciences “Ardito Desio”, University of Milan, Via Mangiagalli 34, 20133 Milano, Italy

<sup>4</sup>European Synchrotron Radiation Facility, 71 avenue des Martyrs, 38000 Grenoble, France

### **ABSTRACT**

The structural evolution and compressibility of ordered and disordered ankerite were investigated at pressures up to  $\sim 25$  GPa using synchrotron single-crystal X-ray diffraction in a diamond-anvil cell. Ordered ankerite (space group  $R\bar{3}$ ) undergoes a discontinuous phase transition between 12.15 and 13.45 GPa to a high-pressure structure called ankerite-II (space group  $P\bar{1}$ ) that has Ca in an eightfold coordination. Disordered ankerite ( $R\bar{3}c$  space group) does not undergo a phase transition in the investigated pressure range.

A Birch-Murnaghan equation of state was used to fit the volume compressibility. Ordered ankerite [ $K_{0V} = 95(1)$  GPa,  $K' = 3.8(3)$ ] appears slightly more compressible than disordered ankerite [ $K_{0V} = 99(1)$  GPa,  $K' = 2.7(1)$ ]. The phase transition in ordered ankerite has a change in volume of  $\sim 0.6\%$  and  $K_{13.45V} = 110(11)$  GPa,  $K' = 7(3)$  for ankerite-II. The possible significance of this different behavior of ordered and disordered ankerite is discussed.

**Keywords:** Ankerite, high pressure, synchrotron, single-crystal X-ray diffraction, compressibility