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High pressure structural and vibrational studies of β- and α-In2Se3-like Ga2S3

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Tetradymite α-Bi2Te3 (space group (S.G.) R-3m, centrosymmetric) is well known to be found in a few group-V A2X3 compounds (A=As, Sb, Bi) at room conditions (RC). Under high temperature (HT), this R-3m can be obtained in the In2Se3, the β phase [1], which belongs to the group-III A2X3 compounds (A=Al, In, Ga). A few theoretical works have shown that this β- In2Se3-like structure is stable above the theoretical Tc calculated, following a tendency of Al2X3 > Ga2X3 > In2X3 [2], starting from the α-In2Se3-type structure (s.g. R3m, non-centrosymmetric), which is stable at RC. Such structure is dynamically stable for all this family at RC [2], unlike the β-In2Se3-like structure [3]. The seeking of centrosymmetric and non-centrosymmetric structures, together with the easiest way to switch between them, are being studied for ferroelectric, pyroelectric, and piezoelectric applications, among others.

Multiple high-pressure works on such A2X3 compounds, both from V and III groups have been released for years, where in situ high-pressure x-ray diffraction (HP-XRD) measurements have been deployed to characterize the phase transitions (PTs) observed and the related structural changes. In addition, other experimental techniques are employed, supported by DFT calculations, to fully understand these PTs. In this sense, α-In2Se3 undergoes a PT to β-In2Se3 at above 10-12 GPa, after transforming into β'-In2Se3 at 1 GPa [4]. Very recently, Ga2S3 transforms into this β-In2Se3-like structure was observed at about 16 GPa [7]. Evidence of such PT has been stressed in subsequent works [8, 9]. What is more unexpected, after this α'-β'PT on Ga2S3, two other polymorphs have been synthesized upon decreasing pressure, at 9.0 and 3.0 GPa, respectively [8]. However, further information about the nature of both polymorphs was not given.

In this work, we have confirmed this β'-Ga2S3 under HP via XRD and Raman measurements, joint theoretical simulations. Upon decreasing pressure, α-In2Se3-like structure matches quite well with the 1st polymorph observed at 9.0 GPa (φ-Ga2S3). Raman signatures and pressure dependence of structural parameters have allowed us to discern such β'- φ PT. The 2nd polymorph below 1.0 GPa has been identified with a disordered zincblende (γ-Ga2S3). To complement our results, we discuss the relation between the PTs of both Ga2X3 and AGa2X4 compounds.

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