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The Crystal Structure of Zn_3As_2 ¹ LYDIA S HARRIS, Brigham Young University - Idaho, STACEY J SMITH, BRANTON J CAMPBELL, JOHN S COLTON, Brigham Young University — In the course of trying to produce doped semiconductors, the Colton lab happened upon a sample of ZnO that had been doped with Zn_3As_2 . In the difficulty to reproduce such a sample, they became interested in studying Zn_3As_2 itself, as the literature disagrees on what the structure is. It is likely that Zn_3As_2 has a structure isomorphic to Cd_3As_2 due to their number of valence electrons. It is generally agreed upon that these isomorphic structures are a $2 \times 2 \times 4$ super structure of anti-fluorite with a 25% cation deficiency. In this work, two different purity samples of Zn_3As_2 are studied and compared to several candidate structures obtained from the literature and additional symmetry arguments. The method of studying the crystalline structure is X-ray diffraction (XRD). The structure was solved using single crystal (SC) XRD, and is presented in this work. The structure found using SC-XRD is also compared to powder XRD data.

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