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Pressure and Temperature Dependent Raman Spectroscopy of Chalcogenide Perovskites NELSON GROSS, SAMANTHE PERERA, XI-UCHENG WEI, State University of New York at Buffalo, YIYANG SUN, None, SHENGBAI ZHANG, Rensselaer Polytechnic Institute, HAO ZENG, B. A. WEIN-STEIN, State University of New York at Buffalo — Inorganic semiconductors known as chalcogenide perovskites including BaZrS₃ and its alloys, show potential for application in photovoltaics. The phonon frequencies of BaZrS₃ have been investigated using Raman spectroscopy as a function of temperature from 14 K to 295 K at 1 atm, as well as a function of pressure up to 8.9 GPa at 295 K and up to 6.8 GPa at 120 K. In the range measured, pressure shifts of Raman peaks show no mode softening, indicating a robust and stable material in the Pnma space group. Due to this stability, BaZrS₃ serves as an excellent prototype for alloys occupying the same phase but having different unit cell volume. This volume change provides a method for band-gap tuning with the goal of more efficient energy harvesting. Results of these studies will be discussed.

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