Abstract Submitted for the SHOCK19 Meeting of The American Physical Society

Shock Compression Response of Calcium Fluoride $(CaF_2)^1$ SETH ROOT, MICHAEL DESJARLAIS, PATRICIA KALITA, CHAD MCCOY, SCOTT ALEXANDER, Sandia National Laboratories — Fluorite, a textbook crystal structure named after CaF_2 , is observed in many materials such as Mg_2Si , and CeO_2 . Specifically, CaF_2 is a useful material for studying the fluorite structure because it is readily available as a single crystal. Under static compression, CaF_2 is known to have at least three solid phases: fluorite, cotunnite, and a Ni₂In phase. Along the Hugoniot CaF_2 undergoes a fluorite to cotunnite phase transition, however, at higher shock pressures it is unknown whether CaF_2 undergoes another solid phase transition or melts directly from the cotunnite phase. Historical work by Al'shuler et al [1]. showed that CaF_2 became highly incompressible above 100 GPa. In this work, we conducted planar shock compression experiments on CaF_2 using Sandia's Z-machine and a two-stage light gun up from 60 GPa to 900 GPa. Additionally, we conducted decaying shock experiments at the Omega Laser Facility to measure temperature along the Hugoniot. We use density functional theory (DFT) based quantum molecular dynamics (QMD) simulations to provide insight into the CaF_2 state along the Hugoniot. We also compare the experimentally measured temperatures to the DFT calculations. [1] L. V. Al'tshuler *et al.* Sov. Phys. Solid State 15, 969, (1973)

¹SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

> Seth Root Sandia National Laboratories

Date submitted: 28 Feb 2019

Electronic form version 1.4