

Supporting Information

A simulation study on phase transition behavior of solid nitrogen at extreme conditions

Han Qin ^a, Sheng-Hai Zhu ^{b,*}, Zhen Jiao ^c, Fu-Sheng Liu ^d, Zheng-Tang Liu ^e, Qi-Jun

Liu ^{d,†}

^a School of Science, Key Laboratory of High Performance Scientific Computation,
Xihua University, Chengdu 610039, China

^b Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065,
China

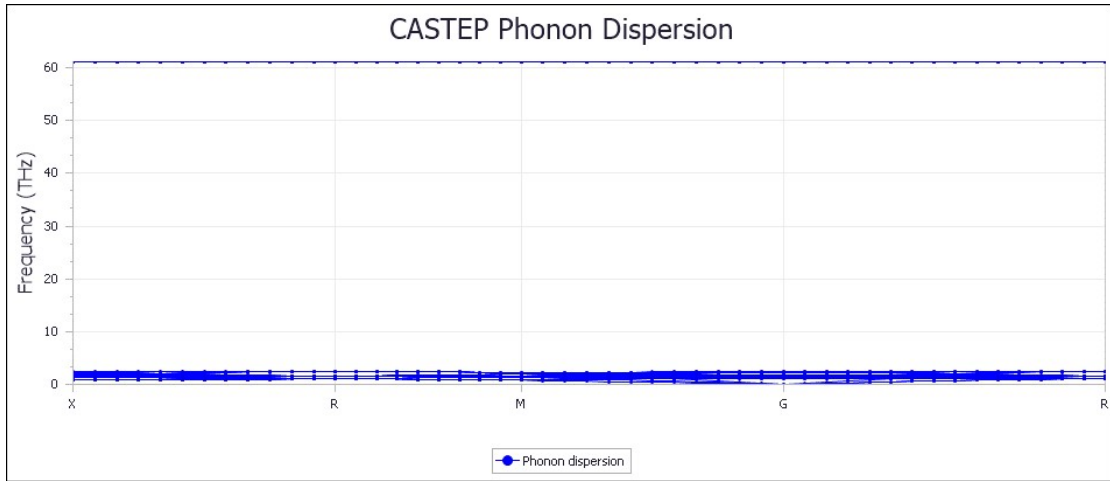
^c Physics of Interfaces and Nanomaterials, MESA Institute for Nanotechnology,
University of Twente, P.O. Box 217, 7500AE Enschede, The Netherlands

^d Bond and Band Engineering Group, School of Physical Science and Technology,
Southwest Jiaotong University, Chengdu 610031, China

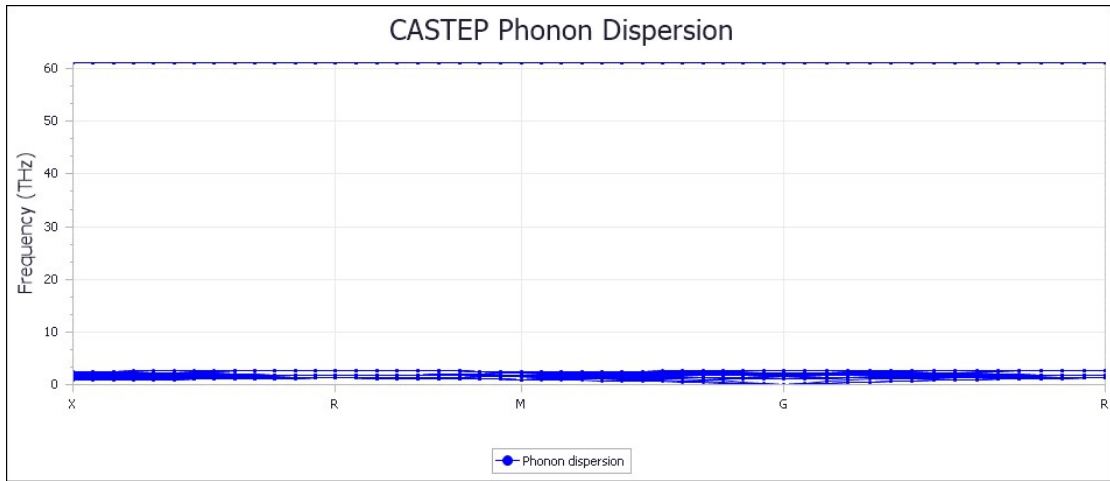
^e State Key Laboratory of Solidification Processing, Northwestern Polytechnical
University, Xi'an 710072, China

* Corresponding author. Email: zhushenghai@hotmail.com

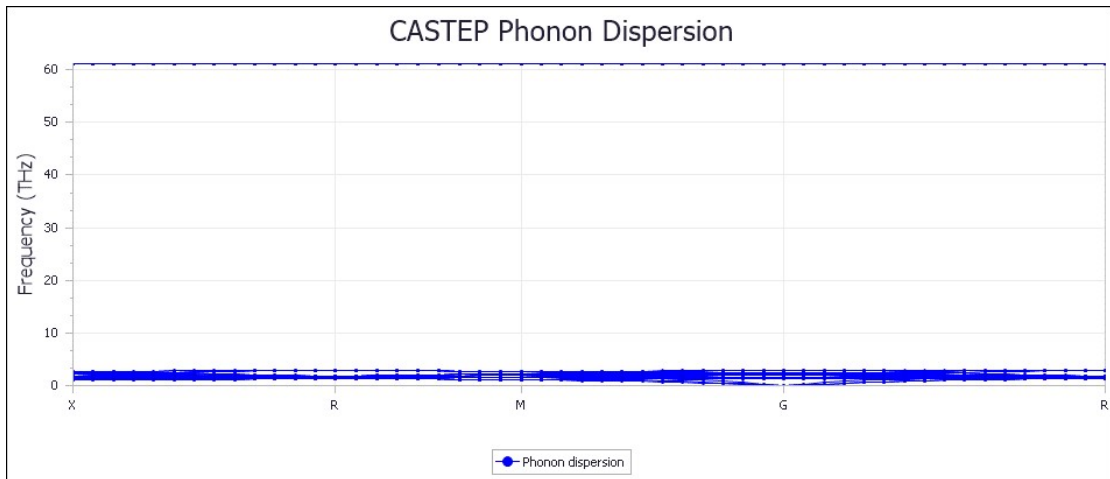
† Corresponding author. Email: qijunliu@home.swjtu.edu.cn



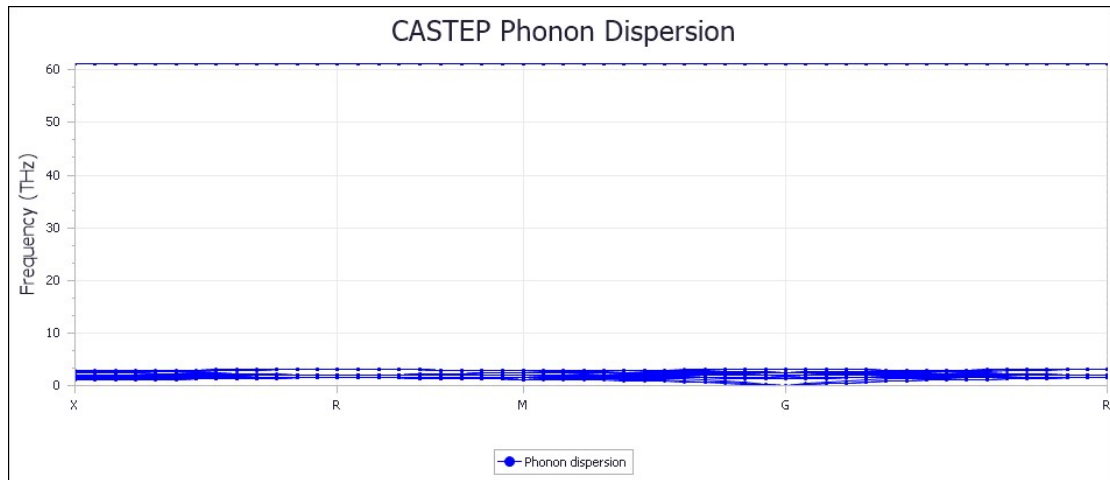
α -N₂ with $Pa\bar{3}$ at 0 GPa



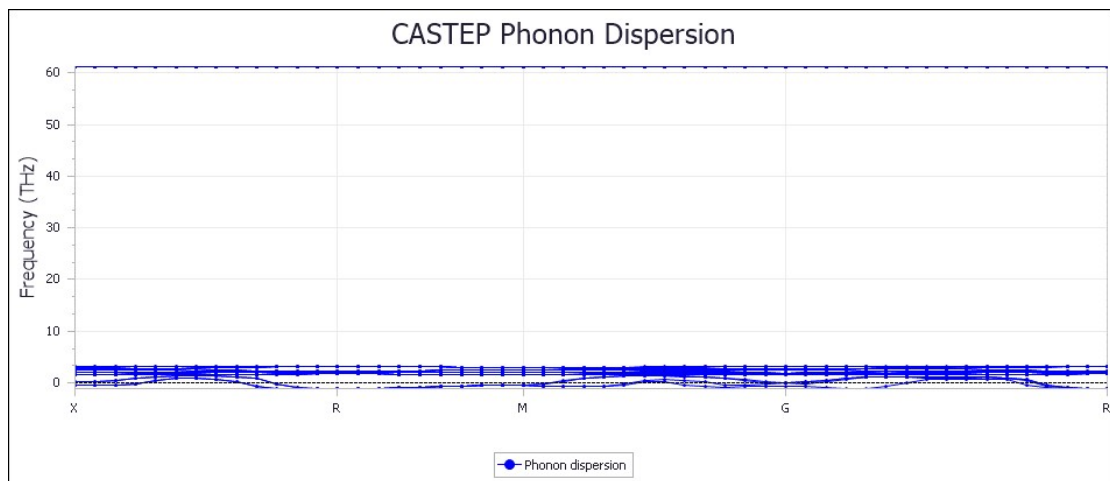
α -N₂ with $Pa\bar{3}$ at 0.1 GPa



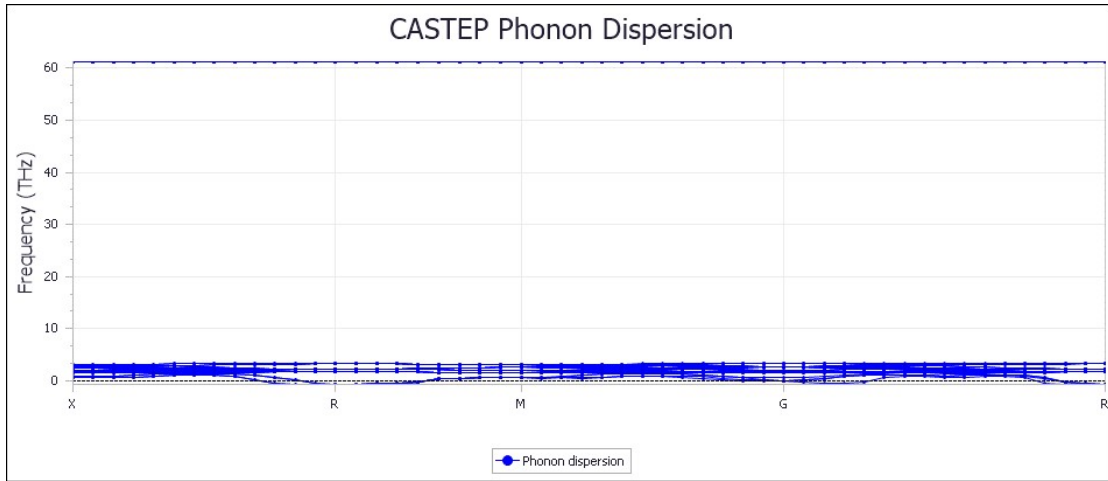
$\alpha\text{-N}_2$ with $Pa\bar{3}$ at 0.2 GPa



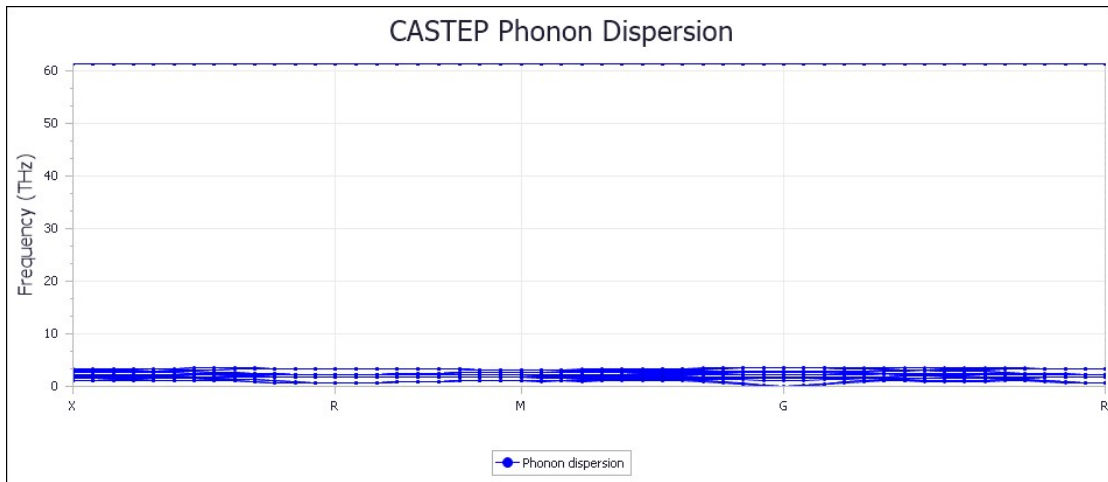
$\alpha\text{-N}_2$ with $Pa\bar{3}$ at 0.3 GPa



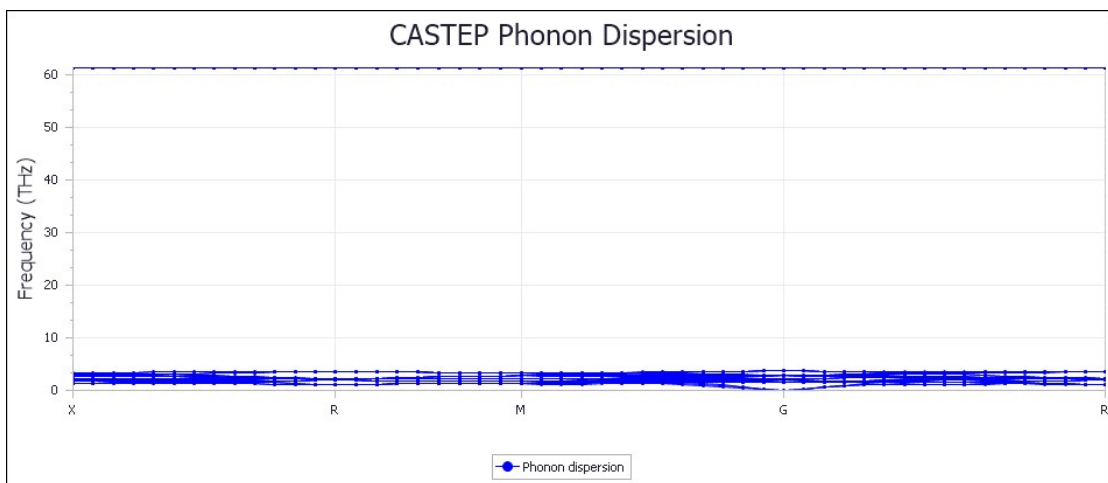
$\alpha\text{-N}_2$ with $Pa\bar{3}$ at 0.4 GPa



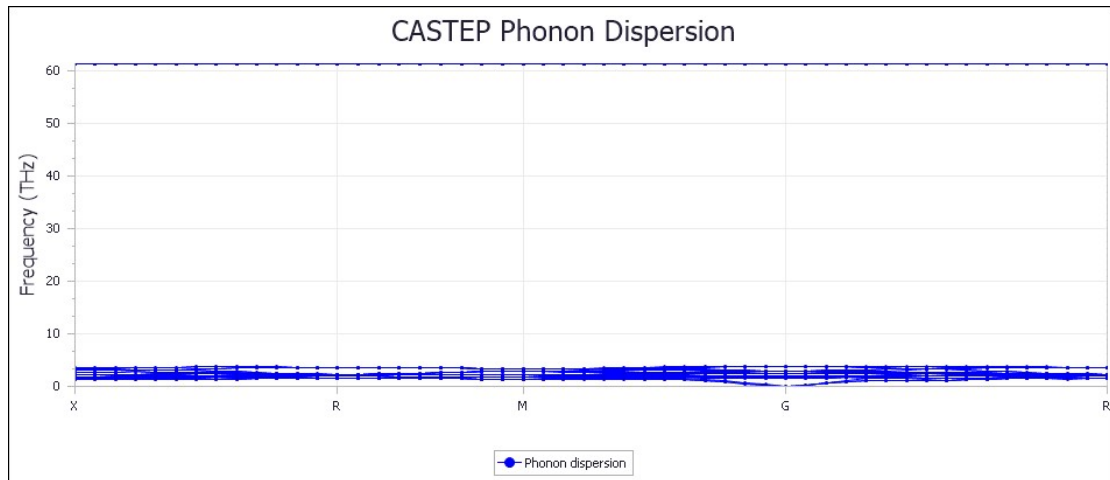
$\alpha\text{-N}_2$ with $Pa\bar{3}$ at 0.5 GPa



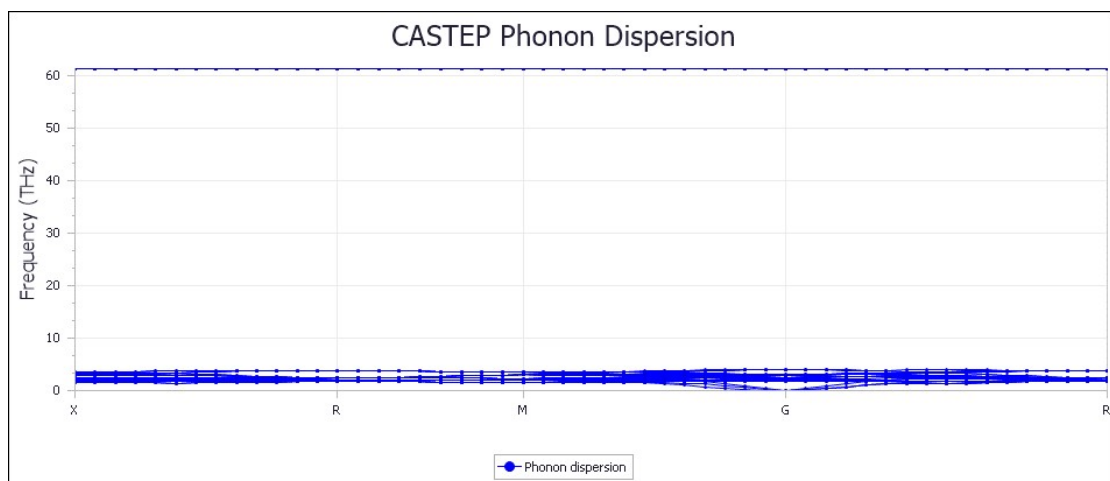
$\alpha\text{-N}_2$ with $Pa\bar{3}$ at 0.6 GPa



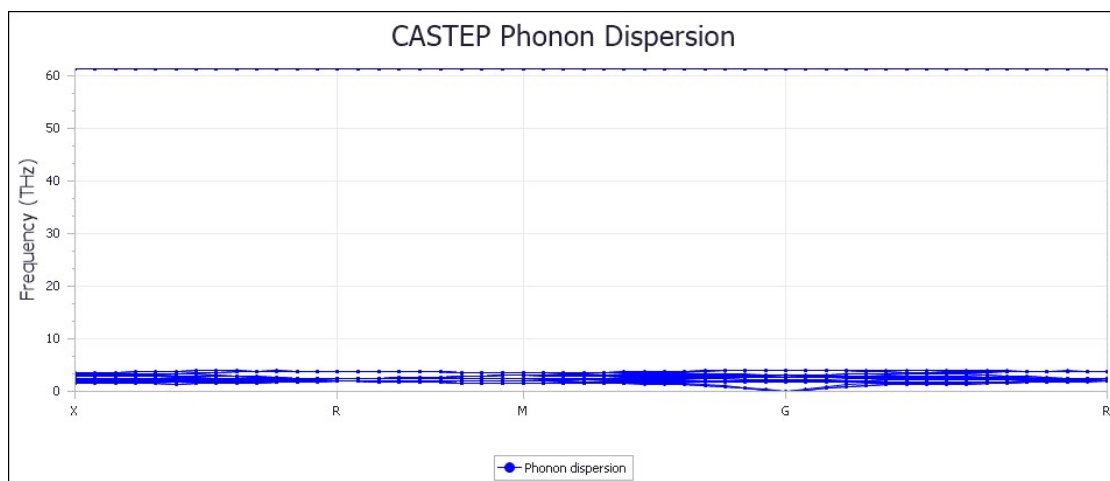
$\alpha\text{-N}_2$ with $Pa\bar{3}$ at 0.7 GPa



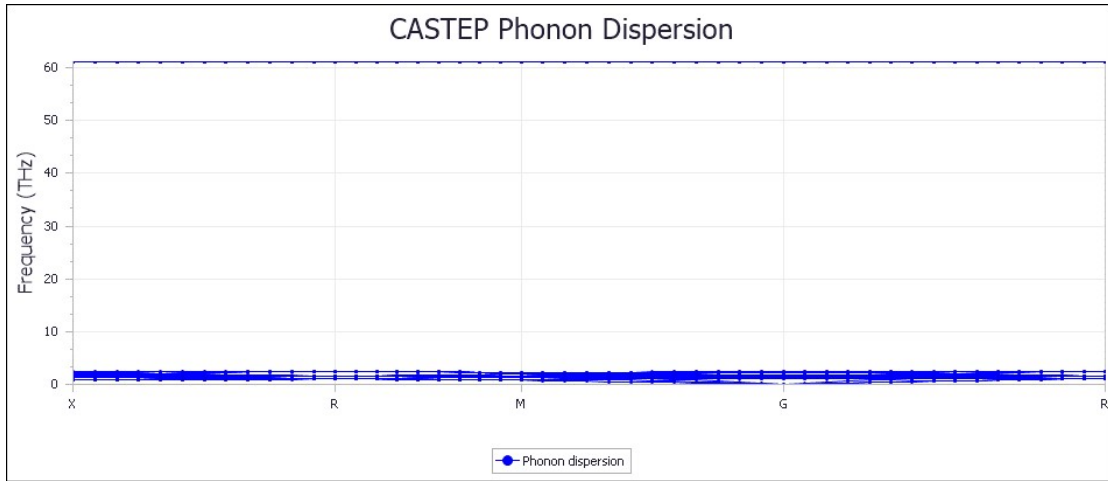
α -N₂ with $Pa\bar{3}$ at 0.8 GPa



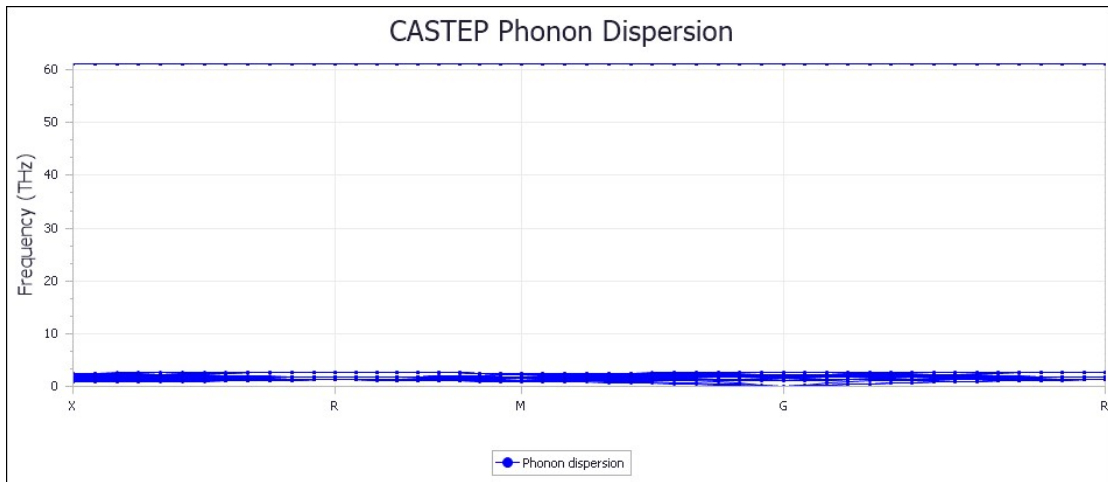
α -N₂ with $Pa\bar{3}$ at 0.9 GPa



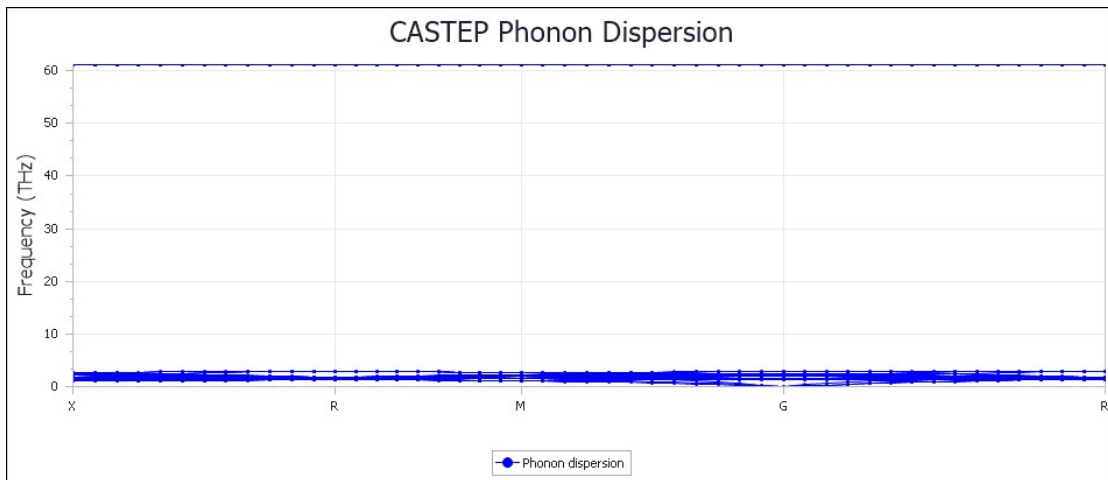
$\alpha\text{-N}_2$ with Pa^3 at 1 GPa



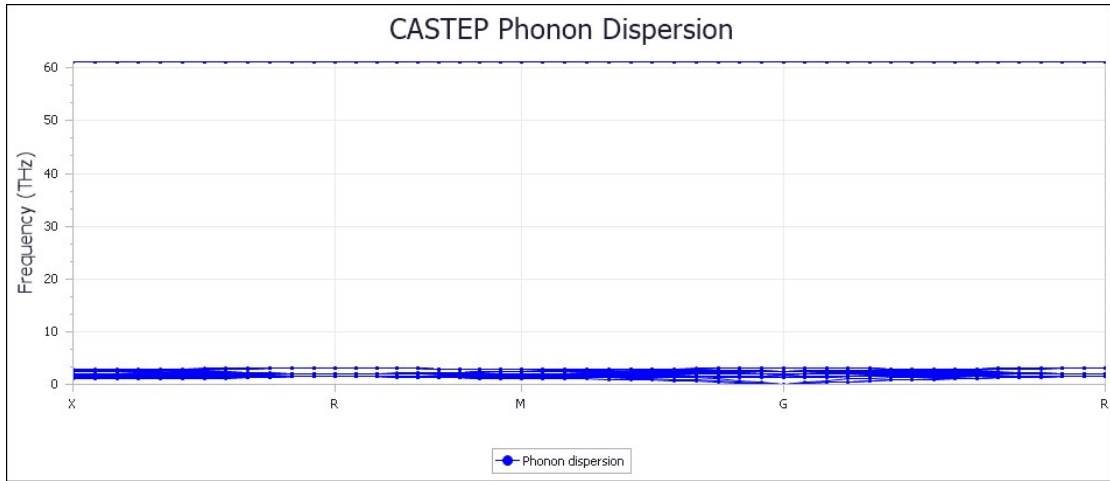
α -N₂ with $P2_13$ at 0 GPa



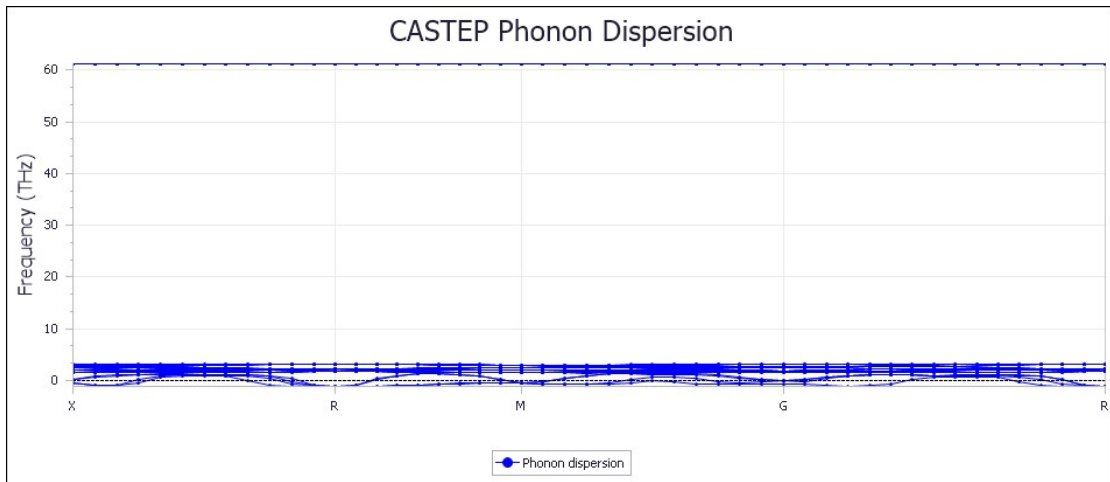
α -N₂ with $P2_13$ at 0.1 GPa



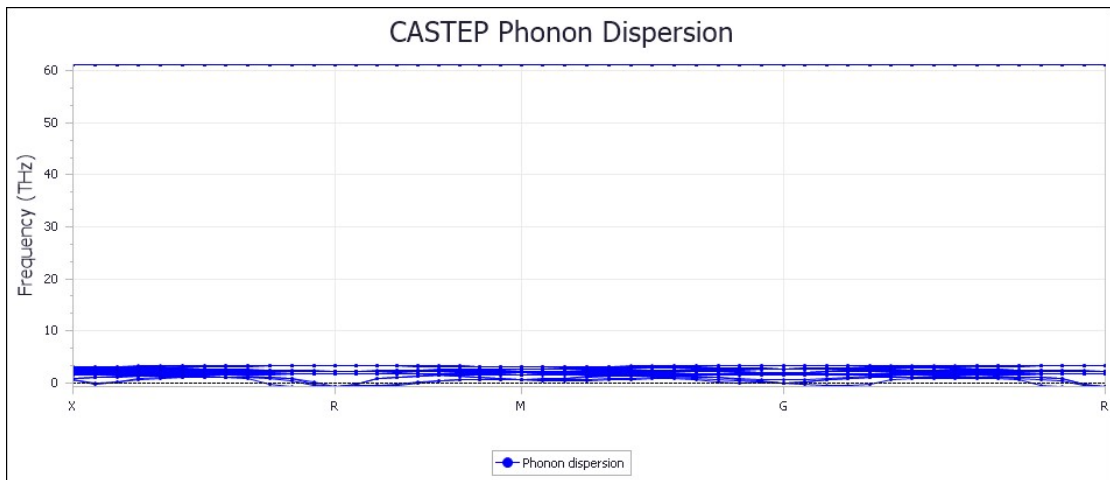
α -N₂ with $P2_13$ at 0.2 GPa



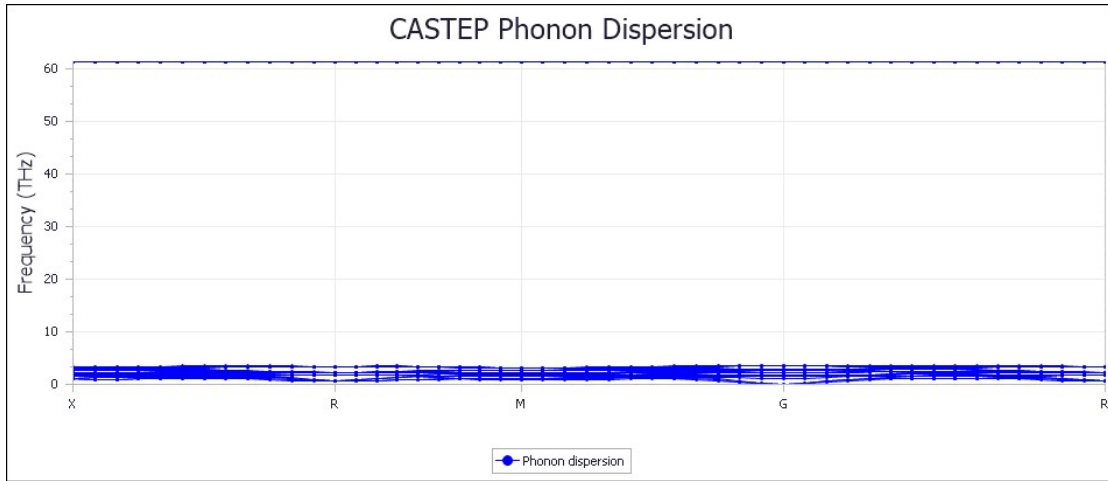
α -N₂ with $P2_13$ at 0.3 GPa



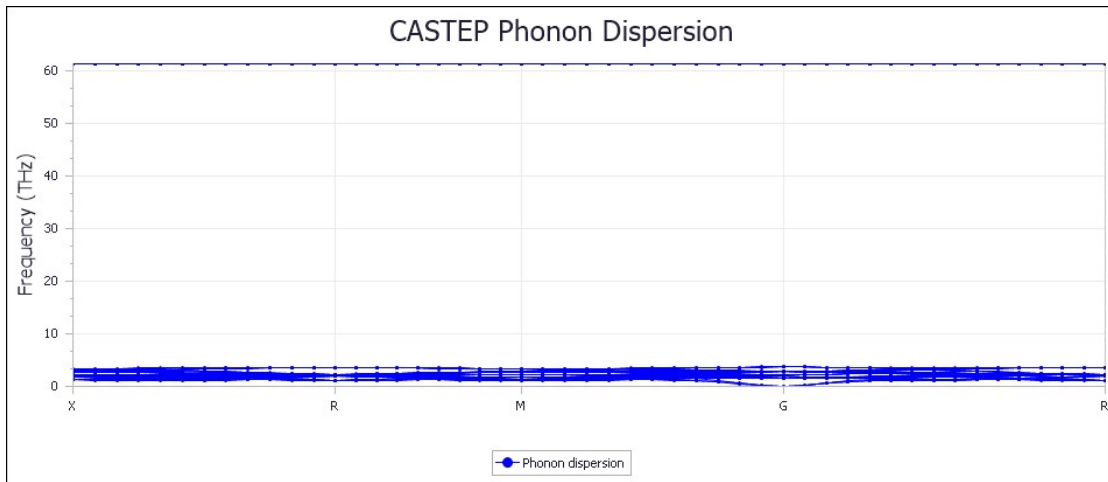
α -N₂ with $P2_13$ at 0.4 GPa



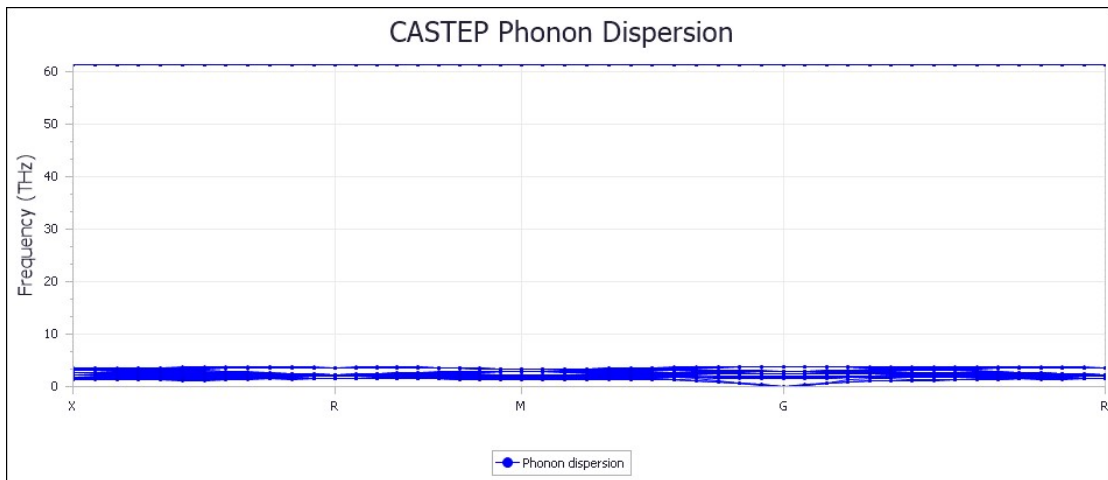
α -N₂ with $P2_13$ at 0.5 GPa



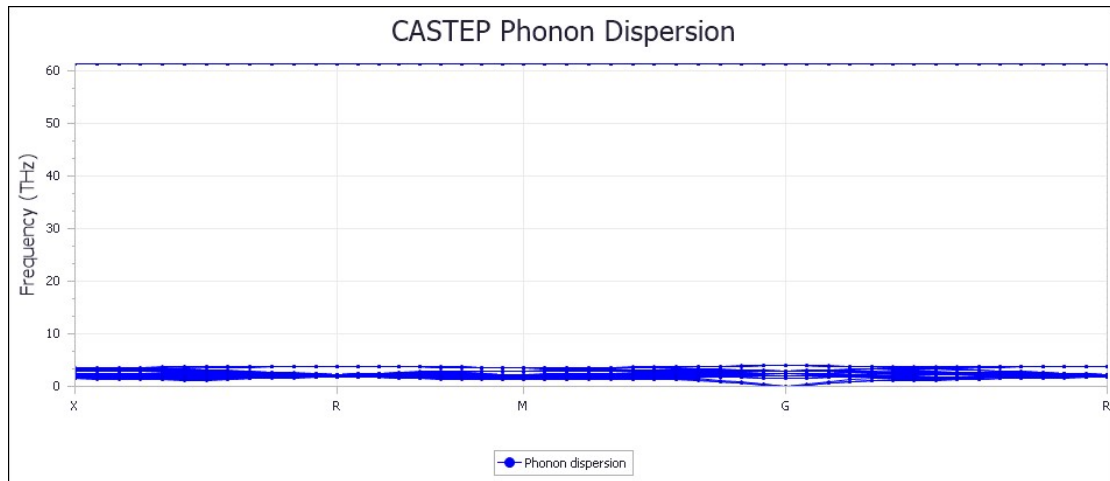
α -N₂ with $P2_13$ at 0.6 GPa



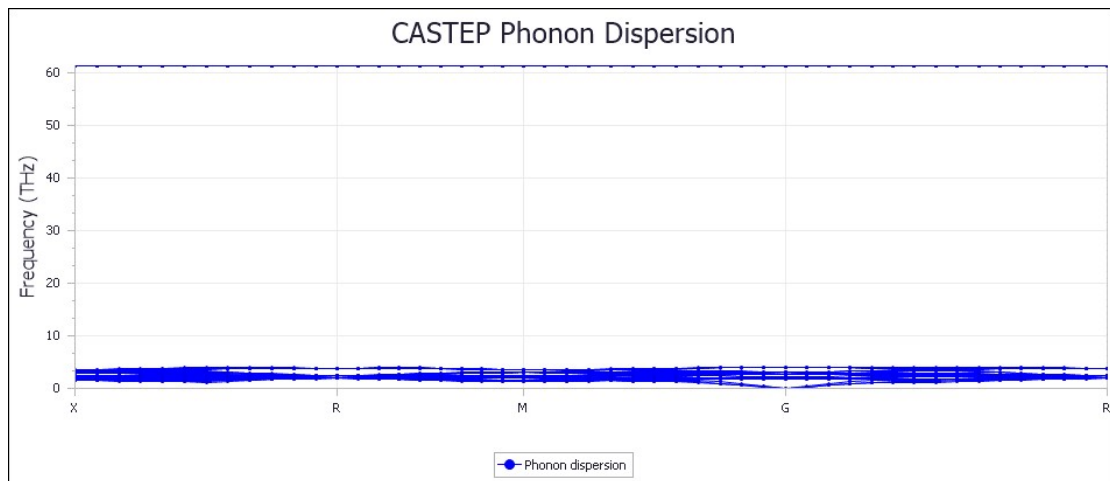
α -N₂ with $P2_13$ at 0.7 GPa



α -N₂ with $P2_13$ at 0.8 GPa

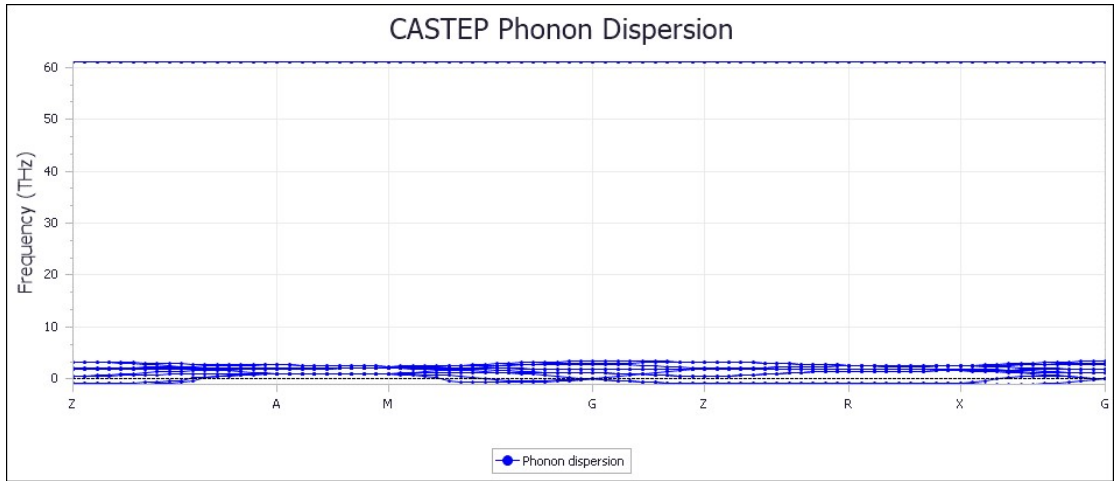


α -N₂ with $P2_13$ at 0.9 GPa

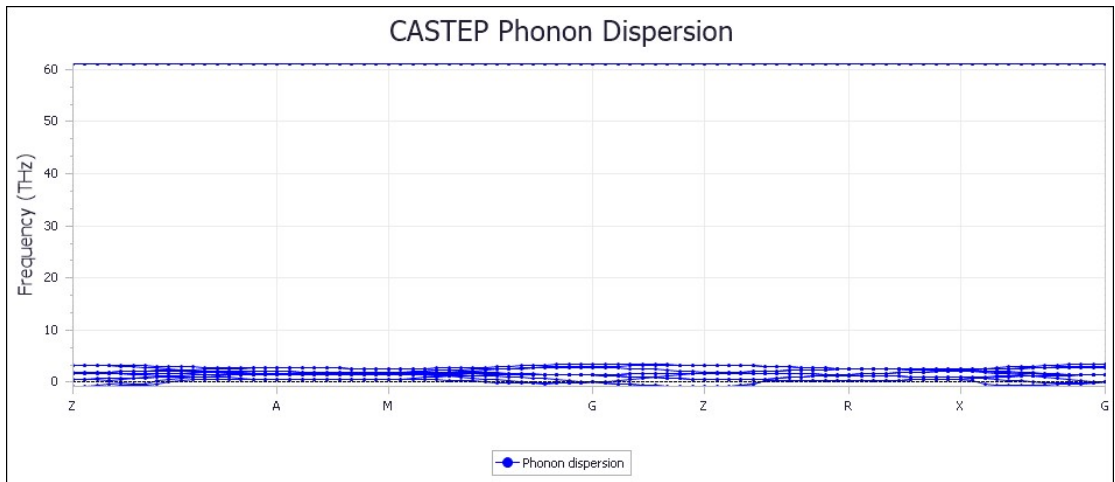


α -N₂ with $P2_13$ at 1 GPa

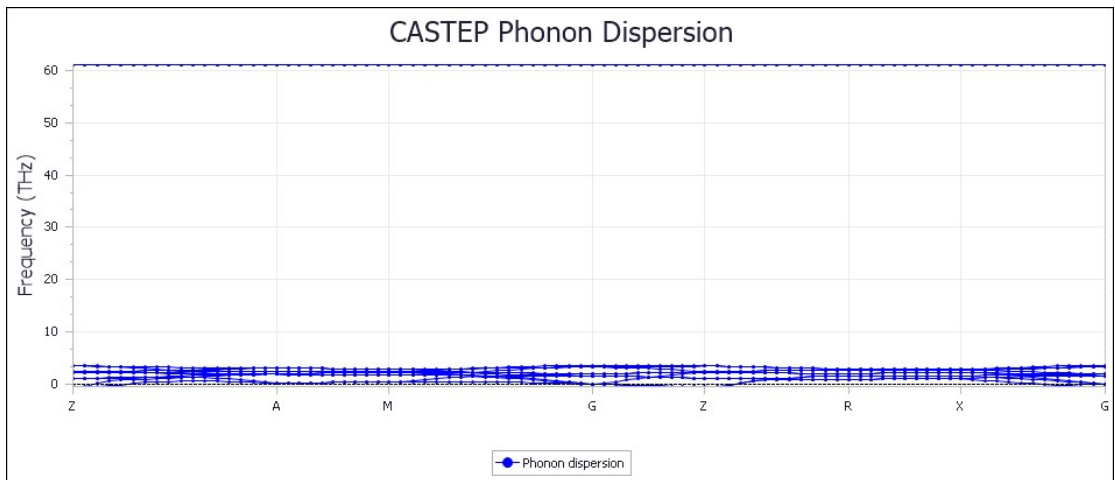
Figure S1 The complete individual phonon spectra of α -N₂ with (a) $Pa\bar{3}$ and (b) $P2_13$ space groups under pressure from 0 GPa to 1 GPa.



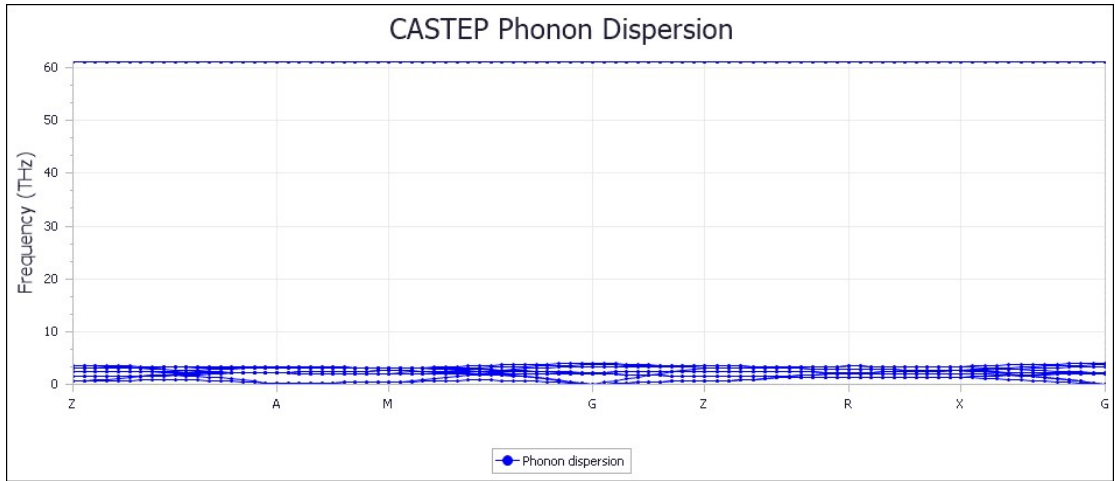
γ -N₂ at 0 GPa



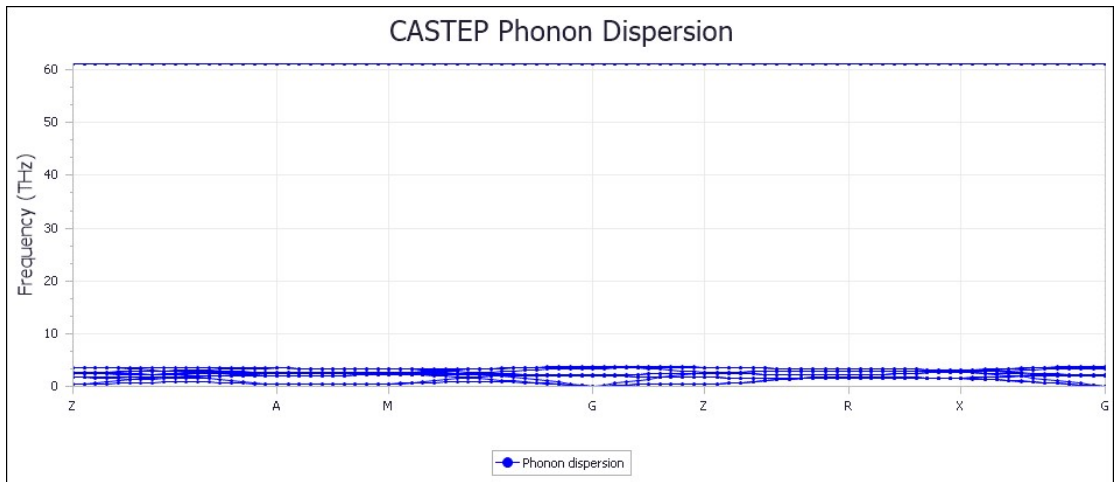
γ -N₂ at 0.1 GPa



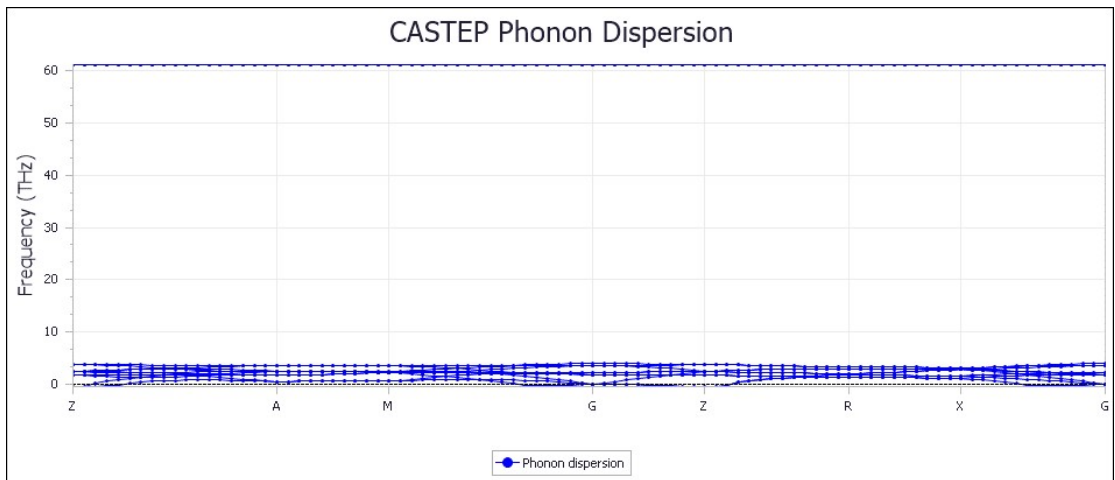
γ -N₂ at 0.2 GPa



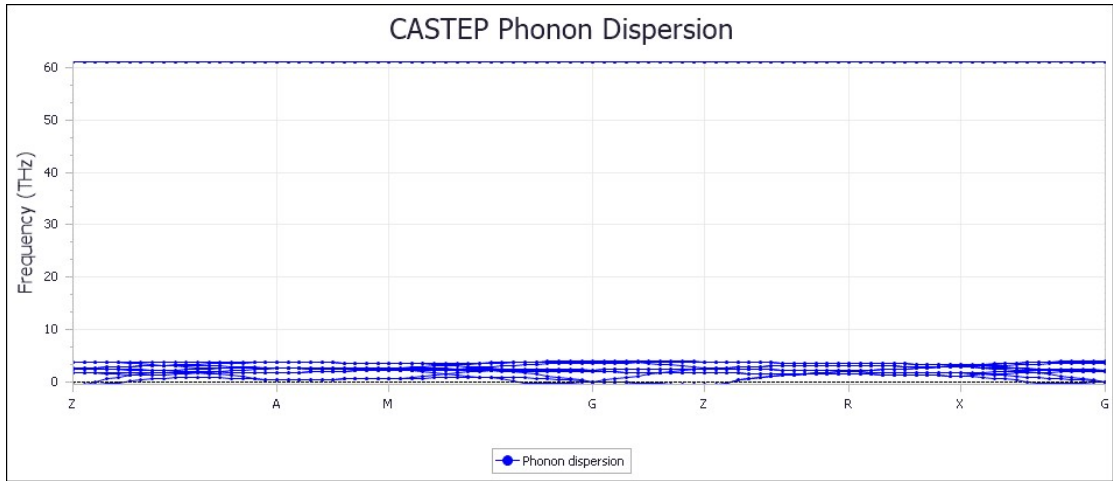
γ -N₂ at 0.3 GPa



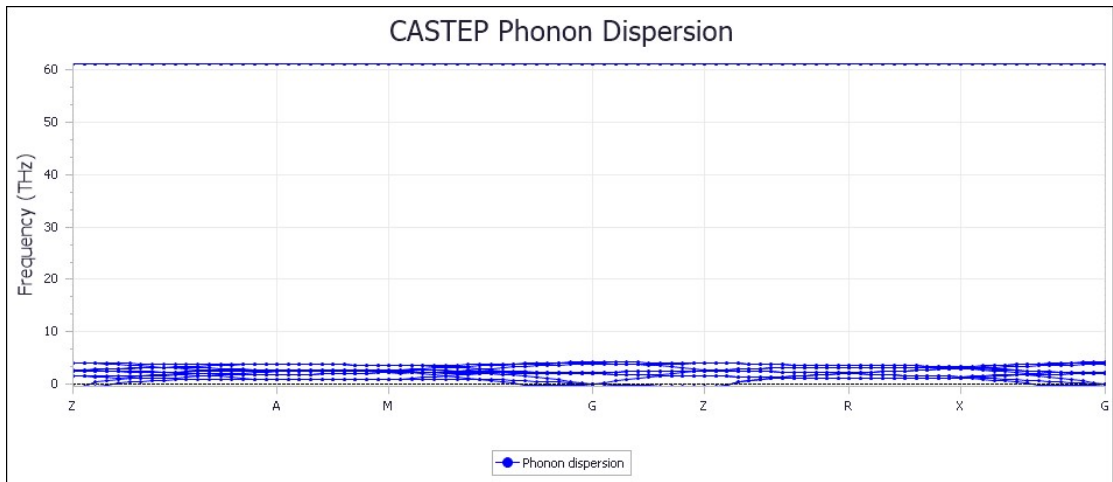
γ -N₂ at 0.4 GPa



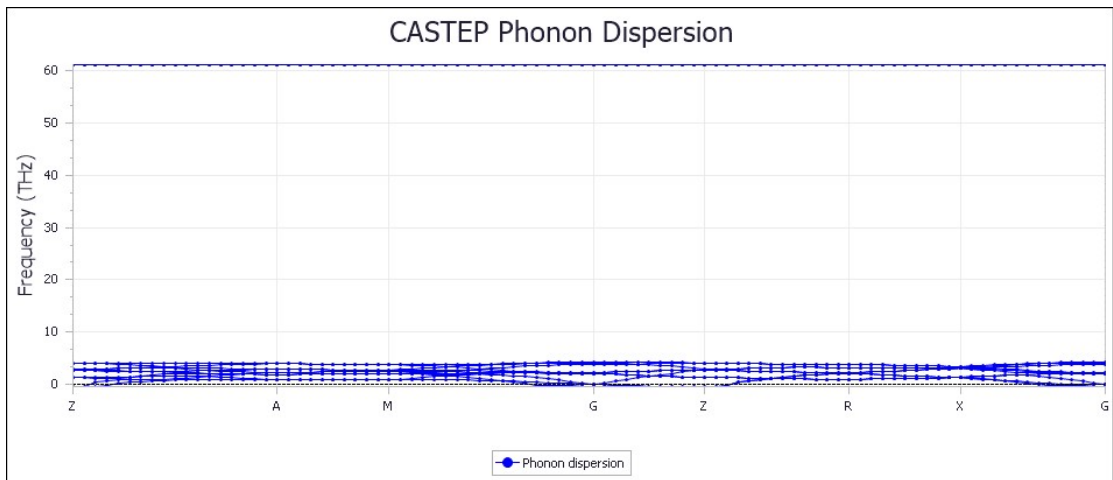
γ -N₂ at 0.5 GPa



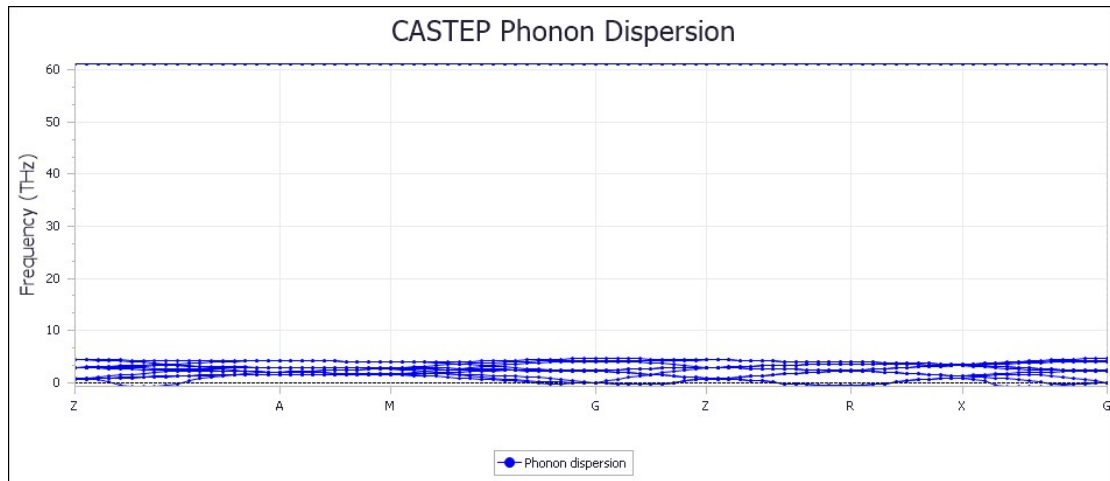
γ -N₂ at 0.6 GPa



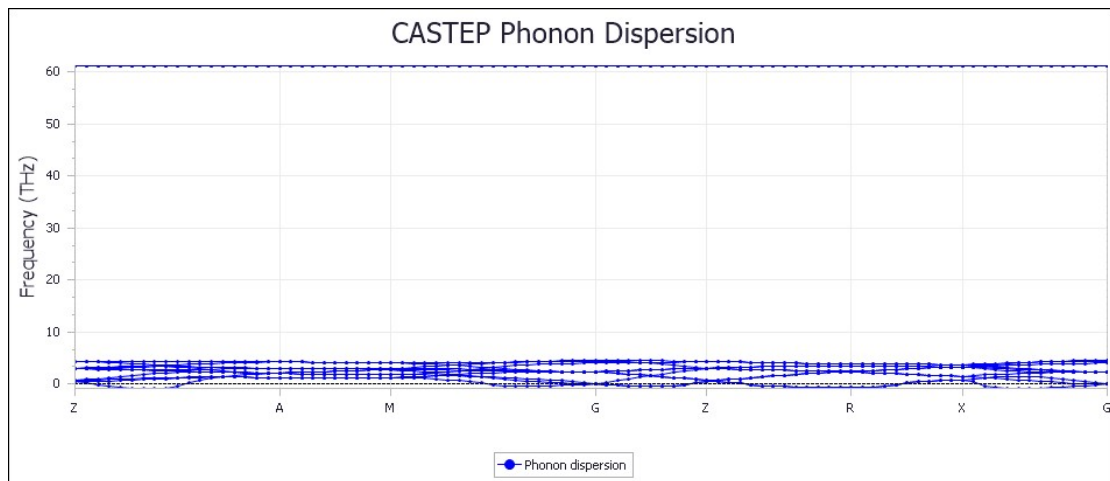
γ -N₂ at 0.7 GPa



γ -N₂ at 0.8 GPa



γ -N₂ at 0.9 GPa



γ -N₂ at 1 GPa

Figure S2 The complete individual phonon spectra of γ -N₂ under pressure from 0 GPa to 1 GPa.