

Abstract Submitted
for the DAMOP19 Meeting of
The American Physical Society

First-Principles Molecular Spectra of Air MARK ZAMMIT, JEFFERY LEIDING, Los Alamos National Laboratory — Comprehensive and highly accurate rovibronic spectral measurements of air molecules are critical to the modeling of low-temperature plasmas and air in extreme conditions. However, with the lack of experimental data, first-principles approaches are key to generating complete molecular line lists. Here, we will discuss the methodology employed for the accurate calculation of molecular rovibronic states, and present emission and equation of state results for NO, which forms in significant abundance in air under extreme conditions.

Mark Zammit
Los Alamos National Laboratory

Date submitted: 31 Jan 2019

Electronic form version 1.4