Abstract Submitted
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First-Principles Molecular Spectra of Air[1] JEFFERY LEIDING, MARK ZAMMIT, Los Alamos National Laboratory — Comprehensive and high-accuracy experimental spectroscopy data for the rovibronic states of air molecules are critical to modeling of 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 opacity and equation of state results for nitric oxide (NO), which forms in significant abundance in air under extreme conditions.

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