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First-Principles Molecular Spectra of Air MARK ZAMMIT, JEFFERY LEIDING, JULIE JUNG, JAMES COLGAN, EDDY TIMMERMANS, 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. For the last five decades approximate approaches have been utilized to calculate comprehensive line lists of air molecules. Here we put these approximations to the test, comparing these results with our first principles state-of-the-art calculations for OH and NO, which form in significant abundance in air under extreme conditions. We will discuss the methods employed to calculate molecular rovibronic states, present emission spectra and equation of state results. By exploring the implications of emission spectra produced from approximate and state-of-the-art calculations we devise a ground-truth-oriented quantification of the line-list differences.

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