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First-Principles Molecular Spectra for Air and Astrophysical Plasmas

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Comprehensive and highly accurate rovibronic spectral measurements of molecules are critical to the modeling of low-temperature plasmas. 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, equation of state and opacity results for H_2^+ , H_2 , NO , and OH , which form in significant abundance in astrophysical and air plasmas. We focus on the importance of electronic excited state transitions, which are generally difficult to model, and until recently were not included in many line-lists.