Photoionization of Molecular Species in the Atmosphere: Towards A Complete Air Opacity

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Radiative properties of heated air species are vital ingredients in detecting, modeling, and characterizing transport. This information can be utilized to describe the radiative energy transfer, collisional-radiative, radiation-hydrodynamic, and plasma kinetic models which are utilized to model spectra, energy transfer, and bulk-plasma transport in media such as the atmosphere. Ambient air at sea-level are composed primarily of N_2 and O_2, at 78% and 21%, respectively, with contributions from H_20, Ar, CO_2, Ne, He, CH_4, Kr, and N_20. The composition of air can change when heated, cooled, undergoes a strong shock, or is under vacuum. The main challenges of calculating accurate and complete molecular radiation data are with the modeling of excited electronic states of molecules for describing electronic processes, such as photoionization processes. Here we use *ab Initio* wavefunction and density functional theory methods to calculate photoionization cross-sections of diatomic molecules, such as O_2 and N_2. We compare computed cross-sections using Hartree-Fock and Kohn-Sham orbitals in the Gelius approximation to Dyson orbitals from EOM-CC calculations.