ROVIBRONIC INFRARED AND VISIBLE LINE LIST FOR O_2

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The increasingly frequent observations of hot, rocky, Earth-like exoplanets make the production of hot high-resolution line lists for geo-chemically relevant species all the more important. Furthermore, molecular oxygen (O_2) is a critical biosignature molecule in atmospheric exoplanet retrievals and plays an important role in many chemical processes.

Ab initio spectroscopy of the O_2 molecule is uniquely challenging due to the fact that dipole transitions are forbidden within the three lowest lying electronic levels of, and thus transitions in infrared and visible regions are due solely to higher order electric quadrupole and magnetic dipole moments. Nonetheless, accurate line lists for these spectral regions are vital for astronomical applications.

We present results of MRCI calculations on the the $X^3\Sigma_g^-$, $a^1\Delta_g$, $b^1\Sigma_g^+$ and $d^1\Pi_g$ states, and related spin-orbit, and electric quadrupole couplings. Using the Duo program we then obtain a variational solution to the rovibronic Schrödinger equation, and perform empirical refinement of the energy levels by fitting a Morse/Long-range potential energy curve, along with spin-orbit and spin-spin coupling functions. We also discuss ongoing and future work for the magnetic dipole moment transitions.