

Computing highly accurate spectroscopic line lists for characterization of planetary atmospheres: CO₂ and SO₂ line lists needed for modeling Venus

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Over the last decade, it has become apparent that the most effective approach for determining highly accurate rotational and rovibrational line lists for molecules of interest in planetary atmospheres and other astrophysical environments is through a combination of high-resolution laboratory experiments coupled with state-of-the art *ab initio* quantum chemistry methods. The approach involves computing the most accurate potential energy surface (PES) possible using state-of-the art electronic structure methods, followed by computing rotational and rovibrational energy levels using an exact variational method to solve the nuclear Schrödinger equation. Then, reliable experimental data from high-resolution experiments is used to refine the *ab initio* PES in order to improve the accuracy of the computed energy levels and transition energies. From the refinement step, we have been able to achieve an accuracy of approximately 0.015 cm⁻¹ for rovibrational transition energies, and even better for purely rotational transitions. This combined “experiment / theory” approach allows for determination of essentially a complete line list, with hundreds of millions of transitions, and having the transition energies and intensities be highly accurate. Our group has successfully applied this approach to determine highly accurate line lists for NH₃, CO₂ and isotopologues, and SO₂ and isotopologues. Here I will report our latest results for CO₂ and SO₂ including all isotopologues. Comparisons to the available data in HITRAN2012 and other available databases will be shown, though we note that our line lists for SO₂ are significantly more complete than any other databases. Since it is important to span a large temperature range in order to model the spectral signature of Venus as well as exoplanets, we will demonstrate how the spectra change on going from low temperatures (100 K) to higher temperatures (500 K to 1500 K).