

TOWARDS AN ACCURATE INFRARED LINELIST FOR SO₂

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The "Best Theory + High-resolution Expt Data" strategy now extends from NH₃, CO₂ to SO₂ which is considered a "weed" in high resolution astronomical data analysis (such as for Herschel, SOFIA, and JWST). Refining a high quality ab initio potential energy surface (PES) with selected HITRAN data, we have made significant progress toward an accurate IR line list for SO₂. Similar to the situation for CO₂, we have achieved 0.01-0.02 cm⁻¹ accuracy for reliable line positions. Outliers in existing HITRAN models have been identified. Compared to CO₂, the SO₂ rovibrational energy levels are more difficult to converge. A pure, experimentally measured dataset (instead of HITRAN models) would greatly enhance the reliability of higher J/K and higher energy levels computed on the refined PES. An initial IR line list has been generated to test an ab initio dipole moment surface (DMS). Limitations, deficiencies, and future developments for both line positions and IR intensities will be discussed.