DETERMINING CONSISTENT AND ACCURATE LINE POSITIONS FOR THE AMES-296K OCS IR LINE LIST

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For those IR line lists semi-empirically computed for polyatomic molecules using their potential energy surfaces (PES) refined with high-resolution experimental data, their line position accuracy typically falls within 0.01 - 0.05 cm^{-1}. It is preferable to enhance these line lists with more accurate line positions derived from experiments and/or Effective Hamiltonian models. However, this task is not straightforward and heavily relies on the specific molecule, mainly contingent upon the consistency and accuracy of the data available. Recently, we have tried to improve the Ames-296K IR line list[b] for carbonyl sulfide (σ_{rms}=0.007 cm^{-1}) by utilizing HITRAN data (for 6 isotopologues), MARVEL level set (for the primary isotopologue 622)[c], and high-resolution experiments. In order to minimize the impact of various inconsistencies, less accurate data, and even errors identified in the data, we opted to implement state-specific adjustments on Effective Hamiltonian model-based levels and the original rovibrational levels computed variationally on the Ames-1 PES refinement. In this talk, we will present our discoveries ranging from better-than-expected agreements to enlightening discrepancies, explain the reasoning and intricacies behind the adjustments, and discuss remaining issues and future enhancements. It is worth noting that matching to a global Effective Hamiltonian model (when available) would be a distinct and more challenging scenario. The new Ames-296K OCS line list includes an estimate of uncertainty for each updated line position.

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[b]https://huang.seti.org/OCS/ocs.html

[c]Even Xu & Jonathan Tennyson (2023) Mol. Phys, e2279694