SOLIS: An accurate IR/Vis line list for sulfur monoxide ($^{32}S^{16}O$) & UV photoabsorption and photodissociation cross section predictions

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Abstract:

We present a rovibronic IR/Vis line list for the transient diatomic sulfur monoxide ($^{32}S^{16}O$) computed through our variational code Duo using a semi-empirical spectroscopic model consisting of potential energy curves, spin-orbit curves, electronic angular momentum curves, (transition) dipole moment curves as well as other couplings. The underlying *ab initio* spectroscopic model of SO was taken from Brady et al. (2022) which was refined by fitting to a comprehensive experimentally derived set of energies of SO. To this end, an experimental set of 50106 transitions, 49613 of those being non-redundant, have been compiled through the analysis of 29 experimental sources. A self-consistent set of 8850 rovibronic energy levels for the $X^3\Sigma^-$, $a^1\Delta$, $b^1\Sigma^+$, $A^3\Pi$, $B^3\Sigma^-$, and $C^3\Pi$ electronic states has been generated with the MARVEL algorithm covering rotational and vibrational quantum numbers $J \leq 69$ and $v \leq 30$, respectively, and energies up to 52350.40 cm^{-1} (≥ 191 nm). A large gap in our network between 12300-20500 cm^{-1} exists due to lack of vibrational data for $X^3\Sigma^-$, $a^1\Delta$, and $b^1\Sigma^+$ with no coverage of the $c^1\Sigma^-$, $A'^3\Delta$, and $A''^3\Sigma^+$ states. Our refined spectroscopic model replicates the $X^3\Sigma^-$, $a^1\Delta$, $b^1\Sigma^+$, and $A^3\Pi$ MARVEL energies with a weighted root-mean-square error of 3.13×10^{-3} cm^{-1}, 1.08×10^{-3} cm^{-1}, 0.27 cm^{-1}, and 0.24 cm^{-1}. We have not currently refined the UV region of the spectroscopic model because of the many perturbations in the $B^3\Sigma^-$, and $C^3\Pi$ electronic state energies due to their overlapping potentials and large coupling. However, we present novel predicted UV absorption cross sections for the SO radical, highlighting specific wavelengths for its potential detection. Furthermore, we provide initial photodissociation cross sections, crucial for understanding SO's behavior in astrophysical environments, particularly the atmospheres of hot Jupiter exoplanets.

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Send to Tony & Jonathan before 10 April