MARVEL ANALYSIS OF EXPERIMENTAL TRANSITION DATA AND REFINEMENT OF THE $^{32}S^{16}O$ SPECTROSCOPIC MODEL: THE IR/VIS LINE LIST

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We present a new rovibronic IR/Vis line list for the transient diatomic sulfur monoxide ($^{32}S^{16}O$) computed through our variational code DUO[1] 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)[2] 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[3] covering rotational and vibrational quantum numbers $J \leq 69$ and $\nu \leq 30$, respectively, and energies up to 52350.40 cm^{-1} ($\geq$ 191 nm). A large gap in our network between 12300–20500 cm^{-1} exists due to lack of vibrational data for $X\ ^3\Sigma^-$, $a\ ^1\Delta$, $b\ ^1\Sigma^+$ with no coverage of the $c\ ^1\Sigma^-$, $A\ ^{3\prime\prime}\Sigma^+$, and $A'\ ^3\Delta$ states. Our refined spectroscopic model represents the $X\ ^3\Sigma^-$, $a\ ^1\Delta$, $b\ ^1\Sigma^+$, and $A\ ^3\Pi$ MARVEL energies to a weighted root-mean-square error of 4.0×10^{-5} cm^{-1}, 1.5×10^{-6} cm^{-1}, 2.7×10^{-7} cm^{-1}, and 4.8×10^{-3} cm^{-1}. We do not refine the UV energies here because of the many perturbations in the $B\ ^3\Sigma^-$ and $C\ ^3\Pi$ energies due to their overlapping potentials and large coupling. We do not have data connecting the $B\ ^3\Sigma^-(\nu = 0)$ state which is required to model the perturbations correctly, and so we leave this to a future project.

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[2] doi:10.1039/D2CP03051A R. P. Brady, S. N. Yurchenko, G.-S. Kim, W. Somogyi and J. Tennyson, An *ab initio* study of the rovibronic spectrum of sulphur monoxide (SO): diabatic vs. adiabatic representation, *Phys. Chem. Chem. Phys.*, **24**, 24076 (2022)

[3] doi:10.1016/j.jms.2007.07.005 T. Furtenbacher, A. G. Császár and J. Tennyson, MARVEL: measured active rotational-vibrational energy levels, *J.Mol. Spectrosc.*, **245**, 115-125 (2007)

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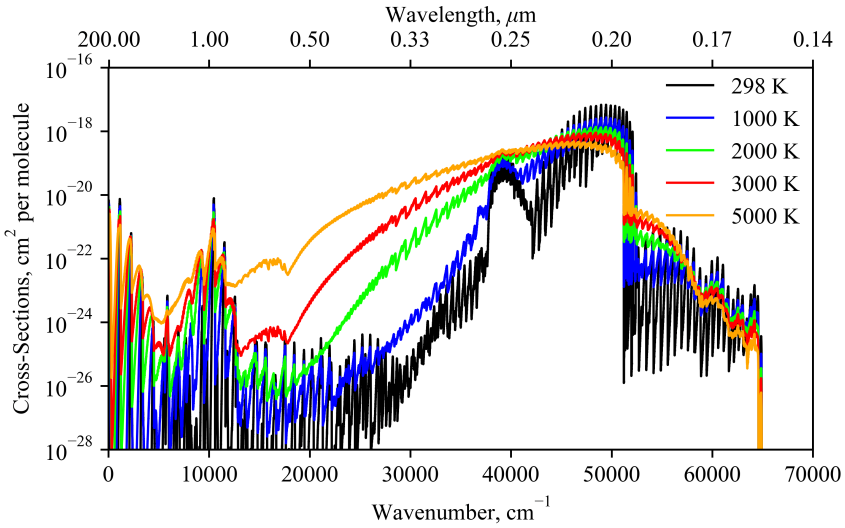
Wavelength, μm
200.00
1.00
0.50
0.33
0.25
0.20
0.17
0.14
Cross-Sections, cm^2 per molecule
10^{-16}
10^{-18}
10^{-20}
10^{-22}
10^{-24}
10^{-26}
10^{-28}
298 K
1000 K
2000 K
3000 K
5000 K
0
10000
20000
30000
40000
50000
60000
70000
Wavenumber, cm^{-1}