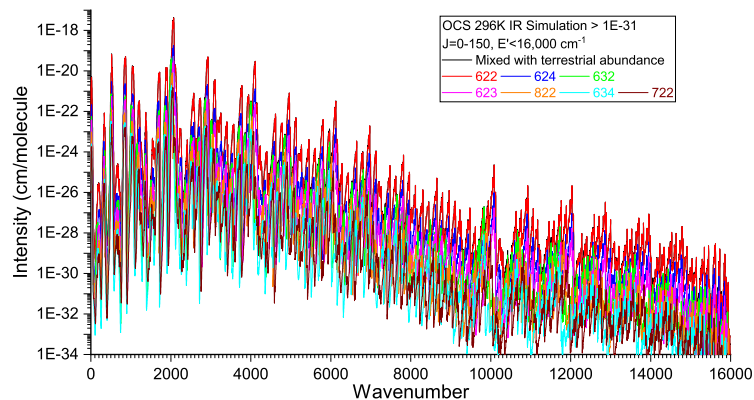


AMES-1 296K IR LINE LISTS FOR OCS ISOTOPOLOGUES

XINCHUAN HUANG, *Carl Sagan Center, SETI Institute, Mountain View, CA, USA*; DAVID SCHWENKE, *MS 258-2, NAS Facility, NASA Ames Research Center, Moffett Field, CA, USA*; TIMOTHY J. LEE, *Space Science and Astrobiology Division, NASA Ames Research Center, Moffett Field, CA, USA*.



To fill in the OCS data gaps in IR databases, Ames-1 296K IR line lists are reported for OCS isotopologues in the range of 0 - 16,000 cm⁻¹, with line intensity cut off at 1E-30 cm/molecule.^a Seven isotopologues (622,624,632,623,822,634,and 722) are included in a "natural" OCS line list with their terrestrial abundances. The Ames-1 potential energy surface (PES) for OCS was refined using selected HITRAN data and band origins up to 13,952 cm⁻¹(with reduced weight). It can reproduce most HITRAN levels with $\sigma_{rms} < 0.01$ cm⁻¹, except a few bands of the main isotopologue: 5002, 4112 and 9110. The Ames-1 dipole moment surface (DMS) was fit from extrapolated

CCSD(T)/aug-cc-pV(T,Q,5+d)Z dipoles, with fitting $\sigma_{rms} = 5.8E-7$ a.u. for 1862 points in 0 - 20,000 cm⁻¹. In general, the Ames-1 296K intensity finds good agreement with experiment and HITRAN. Agreements for bands >10,000 cm⁻¹ are also reasonable. In future, we need to identify the source of discrepancies observed in the Ames-1 vs Expt/HITRAN comparisons, and focus on higher energy and higher temperature line lists. See <http://huang.seti.org> for latest update.

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