AMES-1 296K IR LINE LISTS FOR CS_2 ISOTOPOLOGUES

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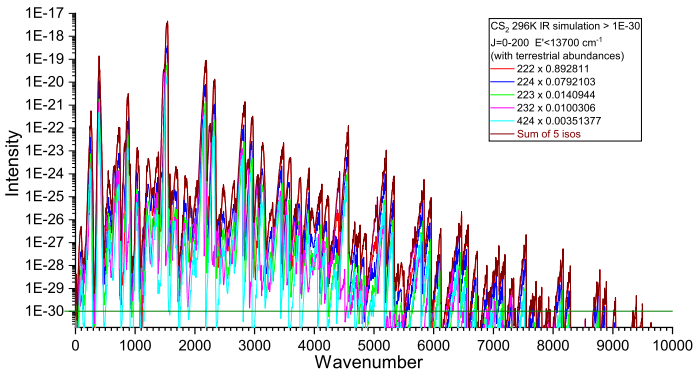

To fill in the CS_2 data gaps in IR databases, Ames-1 296K IR Line lists are reported in the range of 0 - 10,000 cm^{-1}, with line intensity cut off at 1E-30 cm/molecule.[a] Five most abundant isotopologues (222, 224, 223, 232, and 424) are included in a "natural" CS_2 combo list with their terrestrial abundances. The Ames-1 potential energy surface (PES) for CS_2 was refined using experimental levels compiled in Karlovets et al [JQSRT 258:1, 2021], with fitting σ_{rms}=0.02 cm^{-1}. The Ames-1 dipole moment surface (DMS) was fit from extrapolated CCSD(T)/aug-cc-pV(T,Q,5+d)Z dipoles, with fitting σ_{rms} = 5.2E-6 a.u. for 2416 points in 0 - 25,000 cm^{-1}. The "Ames-1 PES + Ames-1 DMS" intensity should be consistently reliable with better than 95% accuracy, but needs more experiment evaluation beyond a few strong peaks below 5000 cm^{-1}. Differences between Ames and HITRAN model extrapolations increase to 0.2-0.7 cm^{-1}at J=150. We plan to update the 222 line list with Tashkun's EH model levels [JQSRT 279:108072, 2022]. Future work may focus on states >10,000 cm^{-1}, the accuracy for J>100, and high density of states for high temperature line lists. See http://huang.seti.org for latest update.

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