

SO₂ and CO₂ IR line lists for atmospheric modeling on Venus and Exoplanets

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Abstract. Highly accurate IR line lists are ready for 13 CO₂ isotopologues and 7 SO₂ isotopologues. Ames-296K IR lists carry 0.01 - 0.03 cm⁻¹ accuracy up to 13,000 cm⁻¹ for CO₂ and 5500 cm⁻¹ for SO₂, and 90-95% intensity agreement for most observable bands. Good for atmospheric modeling on Venus and Exoplanets.

Keywords. CO₂, SO₂, isotopologue, Infrared, line list, ab initio, highly accurate, modeling

Existing high-resolution IR databases are far from complete for many CO₂ minor isotopologues and all SO₂ isotopologues. Recently we presented Ames-296K line lists for 5 SO₂ symmetric isotopologues: 626, 636, 646, 666 and 828. For CO₂, we have reported Ames-296K and Ames-1000K IR line lists for 13 isotopologues, including symmetric species 626, 636, 646, 727, 737, 828, 838, and asymmetric species 627, 628, 637, 638, 728, 738. CO₂ line shape parameters were also determined for four different temperature ranges: Mars, Earth, Venus, and Higher temperature. General line position prediction accuracy is 0.01-0.03 cm⁻¹ for wavenumber range up to 5500 cm⁻¹ (for SO₂) or 13,000 cm⁻¹ (for CO₂). Predicted transition intensities usually agree with experimental measurements to 85-95% or better. With such prediction accuracies, these SO₂ and CO₂ IR line lists are the best available alternatives for those spectra gaps missing from spectroscopic databases such as HITRAN and CDMS. See DOI:10.1016/j.jqrsr.2014.05.015 and 10.1016/j.jms.2015.01.010 and references therein for details. Size-reduced line lists are available upon request or at <http://huang.seti.org>.

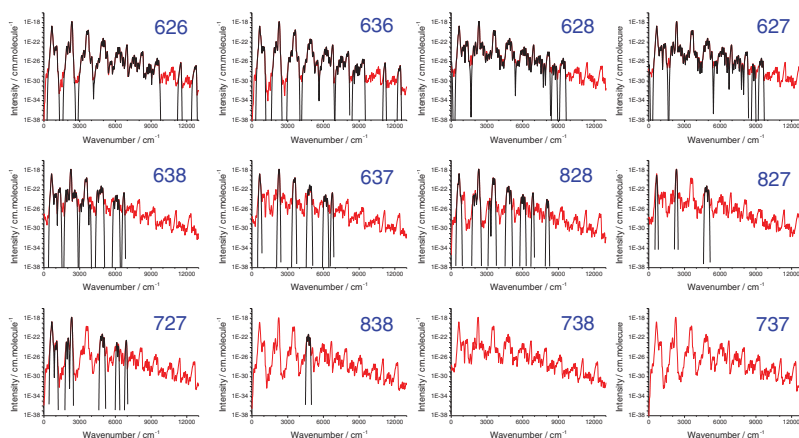


Figure 1. Ames-296K Line lists for 12 CO₂ isotopologues (red) vs. HITRAN2012 (black).