

UPDATING THE CARBON DIOXIDE LINE LIST FOR THE HITEMP DATABASE

R. J. HARGREAVES, I. E. GORDON, L. S. ROTHMAN, *Center for Astrophysics | Harvard and Smithsonian, 60 Garden Street, Cambridge, MA 02138, USA*; **X. HUANG**, *NASA Ames Research Center, Moffett Field, CA 94035, USA*; *SETI Institute, 339 Bernado Avenue, Mountain View, CA 94043, USA*

The HITEMP database¹ (www.hitran.org/hitemp) was established to model the radiative transfer of high temperature gaseous environments and provides accurate line-by-line molecular spectroscopic parameters for eight molecules: H₂O, CO₂, N₂O, CO, CH₄, NO, NO₂, and OH. The addition and update of HITEMP line lists relies on the accuracy and completeness of state-of-the-art *ab initio* works. To account for molecular absorption at high temperatures, it is often necessary for these works to consider billions of individual transitions per isotopologue. This makes implementing full *ab initio* line lists in line-by-line calculations impractical for applications such as calculating the radiative transfer of stellar, brown dwarf, and exoplanetary atmospheres. When adding methane to the HITEMP database, a methodology² was developed to convert the intensity contribution of numerous weak transitions into a relatively small number of “effective” lines, thereby substantially reducing the size of the line list while retaining the absorption contribution.

The recently-published AI-3000K infrared line list for hot carbon dioxide³ contains over 36 billion transitions for the four most abundant CO₂ isotopologues, and has been shown to be accurate at high temperatures. AI-3000K provides an opportunity to extend the effective line approach developed for CH₄ in order to update the HITEMP line list of CO₂. This presentation will outline the development of the effective line methodology for CO₂, which reduces the total number of lines by 2 orders of magnitude. The CO₂ effective lines retain some quantum information that enables line broadening parameters to be applied to the HITEMP line list. The presentation will also include detailed validations against a series of high temperature experimental spectra.

¹Rothman, et al. *JQSRT*, **111**, 2139 (2010), doi:10.1016/j.jqsrt.2010.05.001

²Hargreaves, et al. *ApJS*, **247**, 55 (2020), doi:10.3847/1538-4365/ab7a1a

³Huang, et al. *JQSRT*, **392**, 111748 (2023), doi:10.1016/j.jms.2023.111748