

HITRAN2020: Deciphering spectra from the Cytherean atmosphere. I. E. Gordon¹, F. M. Skinner¹, R. J. Hargreaves¹, R. Hashemi¹, L. S. Rothman¹, Center for Astrophysics | Harvard&Smithsonian (igordon@cfa.harvard.edu).

Introduction: The new era of remote and *in situ* spectroscopic sensing of the Venusian atmosphere has begun. New ESA and NASA missions to Venus will be equipped with high-resolution spectrometers targeting relevant molecular species. The HITRAN and HITEMP databases have traditionally been the sources of molecular opacities for interpreting spectra in the atmosphere of Venus and for creating suitable climate and photochemical models. Therefore, it is essential that the HITRAN project provides the best available spectroscopic parameters for the primary constituents and trace gases in the atmosphere of Venus. This refers not only to the “traditional” HITRAN parameters but also to the line-shape parameters due to the ambient pressure of CO₂. In addition to the half-widths and shifts of individual lines, the line-mixing needs to be accounted for due to the high pressure of CO₂ on the surface of the planet. Also relevant is collision-induced absorption. Moreover, these parameters need proper temperature dependence considering a wide range of temperatures encountered in the different layers of the planetary atmosphere. Some notable updates were made towards these goals in the HITRAN2020 release [1]. Still, more experimental and theoretical work is needed to be adequately prepared to improve the scientific output from the proposed missions *before they are launched*. In summary, a comprehensive overview of the important updates and remaining deficiencies in HITRAN relevant to the exploration of Venus will be provided.

Overview of HITRAN2020: The line-by-line lists for the majority of the HITRAN molecules were updated (and six new molecules added) in comparison with the previous compilation HITRAN2016 [2] that has been in use, along with some intermediate updates, since 2016. The extent of the updates ranges from updating a few lines of certain molecules to complete replacements of the lists and the introduction of additional isotopologues. The database now provides parameters beyond the traditional “.par” format (although it remains as a default output format), including non-Voigt line profiles for many gases; broadening by “planetary” gases, including CO₂ [3]; update of collision-induced absorption sets [4], etc.

We continue to take advantage of the modern structure and interface available at www.hitran.org and the HITRAN Application Programming Interface (HAPI) [5]. Both tools have been improved to work with the new edition.

Improvements relevant to Venus: Many of the improvements or additions enhance the applicability of the database for studies of Venus.

“New” molecules and isotopologues. Six molecules have been added to HITRAN for the first time, with line lists for SO and CS₂ directly relevant to Venus research. Moreover, the line lists of OCS and especially SO₂ were substantially improved and expanded (with respect to the previous edition) by incorporating additional bands and isotopologues. In particular, for SO₂, the ³³S¹⁶O₂ and ¹⁶O³²S¹⁸O, which will be targeted by the laser spectrometer on the DaVinci+ mission, were added to HITRAN for the first time.

In the case of CO₂ magnetic dipole, transitions have been added to the database for the first time and are expected to be observable on Venus. In the future, electric quadrupole transitions will be added as well.

Broadening by CO₂. Broadening parameters associated with the ambient pressure of CO₂ (and their temperature dependencies) were initially introduced in the HITRAN2016 edition for a number of molecules. These have been revised for some of the molecules (including CO, SO₂, and OCS), while line lists of more molecules now have these parameters. Effectively following molecules (and their isotopologues) have relevant parameters in HITRAN2020: N₂O, CO, SO₂, NH₃, HF, HCl, OCS, H₂CO, C₂H₂, and H₂S.

The self-broadening of the CO₂ lines has been updated recently and now also includes non-Voigt line shapes and both first order and full line-mixing parametrizations [6].

Future work: Many additional laboratory and theoretical spectroscopic investigations need to be carried out. In particular, for broadening by CO₂ for different molecules as, in many cases, crude semi-empirical models had to be employed. Algorithms for the far-wing modeling of lines broadened by CO₂ need to be developed.

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References:

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