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HITEMP: Extensive molecular line lists for high-temperature exoplanet atmospheres

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Abstract

Characterizing exoplanet atmospheres at high temperatures requires the underlying data to be sufficiently accurate and complete. The high temperature molecular spectroscopic database, HITEMP, aims to provide line lists for use in the modelling of high-temperature environments, including the atmospheres of exoplanets. This work discusses the recent and ongoing updates to HITEMP (including CH_4), and outlines the future plan for inclusion of additional molecules. A brief discussion of broadening parameters will also be included.

1. Introduction

The HITRAN database [1] is a compilation of molecular spectroscopic parameters that can be used to model the radiative transfer of the Earth's atmosphere. However, using HITRAN for high-temperature applications (such as the modelling of hot-Jupiter atmospheres) can lead to an incomplete model.

The high temperatures observed for some exoplanets, brown dwarfs and stars significantly increases the amount of lines required to model their atmospheres. The HITEMP database [2] has therefore been developed to be used for high temperature environments. HITEMP2010 contains line parameters for five molecules (i.e., H_2O, CO_2, CO, NO, and OH). Since the publication of this work, there has been a significant increase in the amount of theoretical and experimental data, which allows the HITEMP database to be substantially updated and extended. Some molecules, originally omitted due to limited or inaccurate high temperature data, have now become important for the characterization of exoplanets, cool stars and brown dwarfs (e.g., CH_4).

An outline for the next major update of HITEMP will be presented, with a brief description of the aims and difficulties that will need to be addressed.

2. Proposed HITEMP outline

Compiling the HITRAN and HITEMP databases requires a collaborative effort throughout the spectroscopic community. In order to provide a sufficient number of hot bands important at higher temperatures, HITEMP data has been constructed from a combination of empirical, theoretical and semi-empirical studies. Figure 1 outlines the proposed molecules for the next update to the HITEMP database, with the corresponding lead groups and collaborations identified for each molecule.

3. Recent updates

The most recent additions to HITEMP include NO, NO_2, and N_2O [3]. The combination of each molecular data set will be discussed in detail. Furthermore, the recent updates for CO [4] will also be covered. These updates expand the total number of molecules included in HITEMP to seven. Work is already under-

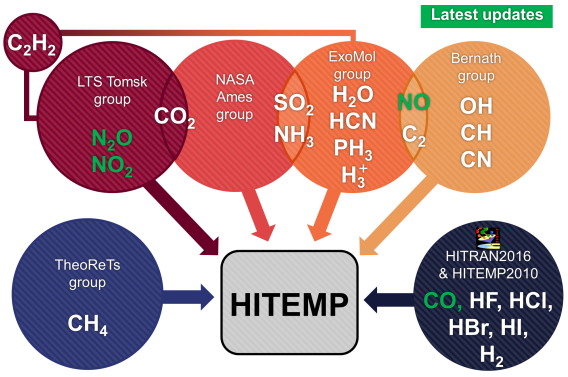

Figure 1: An overview of the proposed molecules to be included in the forthcoming HITEMP update. Those molecules that have been updated since HITRAN2010 are shaded green.

way on the construction of the CH_4 line list and the latest progress will be presented.

In addition, broadening parameters of relevance to exoplanet atmospheres will be discussed along with their inclusion into the HITRAN and HITEMP databases.

3.1. Validation steps

A crucial procedure when including data into the HITEMP (as well as HITRAN) database, is a careful validation of each set of molecular parameters. While discussing the updates for NO, NO_2, and N_2O, a number of examples will be shown where these validation steps highlight important and necessary corrections that are required before inclusion. Figure 2 includes a demonstration of the correction to the intensities necessary for the NOSD-1000 [5] semi-empirical line lists when compared to experimental observations [6].

4. Summary and conclusions

The HITEMP database is undergoing a major expansion, and now includes seven molecules. N_2O and NO_2 are new additions and join H_2O, CO_2 and OH, with NO and CO being updated. Further updates of HITEMP (of relevance to exoplanet atmospheres) are planned over the coming month/years. These updates include additional molecules (CH_4, SO_2, NH_3, HCN, C_2H_2, PH_3, C_2, CH, CN and H_3^+), molecules included from HITRAN2016 (HF, HCl, HBr, HI and H_2), as well as updates to the current HITEMP lists for H_2O, CO_2 and OH.

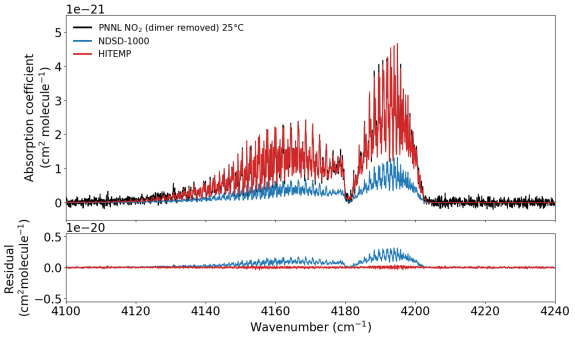

Figure 2: A comparison between absorption cross sections of NO_2 from experiment (PNNL) [6], NOSD-1000 [5] and HITEMP (this work). For this spectral region the HITEMP line list includes corrected intensities from NOSD-1000.

The considerable size of the HITEMP line lists mean that these data are available to download as static files. In the near future a more flexible structure will be introduced. To aid the useability of the large HITEMP line lists, the libraries for HAPI [7] are also undergoing significant updates. This includes a substantial speed improvement for line-by-line calculations, allowing the large HITEMP files to be employed more easily.

Access to both the HITRAN and HITEMP databases is freely available through the HITRAN website (https://hitran.org).

Acknowledgements

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