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Comparison of line-by-line and band-model calculations of methane absorption in outer planet atmospheres.

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Abstract

Recent improvements in the measurement of methane absorption lines at wavenumbers in the region between 4800 cm^{-1} and 7700 cm^{-1} have greatly increased the number of lines with known ground-state energies, the number of weak lines, and the number of lines observed at low temperatures. This has made it possible to create a low-temperature line list that allows modeling near IR spectra of Titan using line-by-line calculations instead of band models [1]. Here, we compare current band models with line-by-line calculations, both to assess the behavior of band models, and to identify remaining issues with line-by-line calculations when applied to outer planet atmospheres.

1. Introduction

Ideally, line-by-line (LBL) calculations should be capable of defining the true dependence of absorption on temperature, pressure, and path length, provided sufficient numbers of lines are characterized to allow computation of all but a tiny fraction of the total absorption. The key parameters are the frequency, ground-state energy, and pressure-broadened line widths. In addition, because at high pressures window regions can be affected by the tails of nearby strong lines, it becomes necessary to know the line shape function in the far wing region, sometimes several hundred cm^{-1} from the center of the line. Furthermore, the temperature dependence of the pressure broadened line width is also needed. Unfortunately not all of this information is available for every line in the line databases. In many cases, line widths are assumed to be constant, and far-wing line shapes need to be constrained by observations. Thus, it is not immediately obvious whether our current improved line data bases will actually be better than band models, even in regions where there are sufficiently many lines. Where LBL calculations can be verified they provide the tremendous advantage of high spectral resolution that cannot be matched by band models.

2. Band models

A big improvement in near-IR modeling of Uranus was obtained using the band model of Irwin et al. 2006 [5, 2]. However, this band model is based on laboratory measurements that must be significantly extrapolated to reach outer planet conditions of temperature, pressure, and path length. Observations by the Descent Imager/Spectral Radiometer (DISR) during the Huygens Probe descent to the surface of Titan provided a new constraint on band models, though it was of lower resolution than the 10 cm^{-1} of the band models, and was limited to wavelengths less than 1.6 μm. Using this constraint as well as other constraints, including lab and HST observations, an improved band model was constructed by Karkoschka and Tomasko [3], providing significantly increased window absorption lacking in the Irwin et al. band model.

3. Line lists

To address deficiencies of the Bailey et al. [1] compilation, we made a number of additions and modifications. The most important were to (1) replace lines in the 6165-6750 cm^{-1} range with line data from [6], (2) add lines from [4] in the 1.28 μm transparency region, and (3) incorporate both room-temperature and 80 K lines to allow a wider range of utility. Compared to HITRAN 2008 our line list provides much better coverage of low strength lines and has much better information on ground-state energies for the lines at shorter wavelengths, as shown in Fig. 1.

4. Transmission comparisons

Fig. 2 compares the two band models with line-by-line calculations using our augmented line list (red) and the HITRAN 2008 line list (blue). For these conditions the two band models are in close agreement, and the augmented line list provides vast improvements over HITRAN between 5000 cm^{-1} and 7900 cm^{-1}. The disagreements between LBL and band models in the

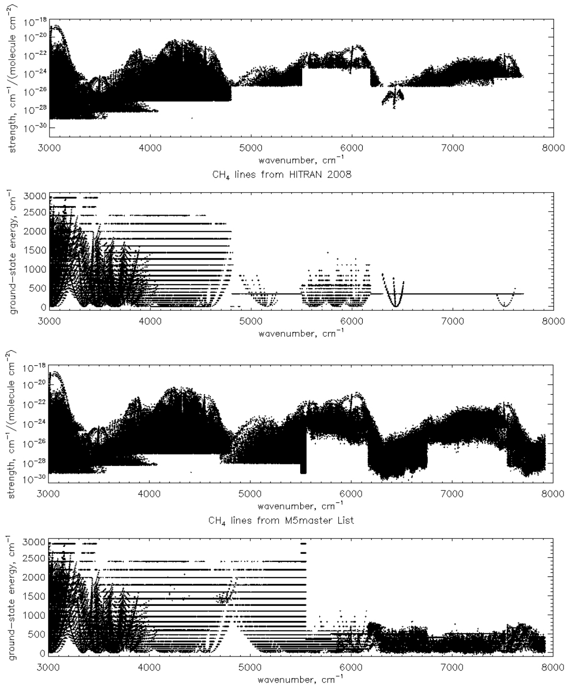

Figure 1: HITRAN 2008 line strength and groundstate energies for all CH_4 isotopologues (top) compared to our augmented line list (bottom).

5000-5500 cm^{-1} region is likely due to the absence CH_3D line data in this region, while the band models do account for CH_3D absorption. For Uranus conditions temperatures are lower and path lengths are much longer, resulting in disagreements between band models in the more transparent regions, but generally good agreement between KT2009 and our LBL calculations. All models agree well in the strong bands. Under Saturn conditions ammonia fills in the transparent regions, and the presence of methane in greater abundance in the stratosphere (no cold trap) produces some disagreement in the strong bands, where significant opacity is here reached at fairly low pressures. Similar comments apply to Jovian conditions.

5. Summary and Conclusions

New measurements of line strengths and ground-state energies have made line-by-line calculations competitive with band models for outer planet applications to wavelengths as short as 1.26 μm, but more work is needed to characterize CH_3D lines in the 4500 - 6000 cm^{-1} region, and in several other regions, including near 3 μm and 2.08 μm, where apparently more weak lines are needed to properly characterize these regions

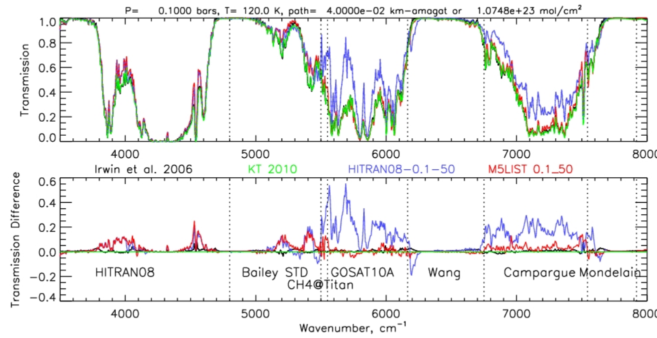

Figure 2: Comparison of transmissions in the Jovian atmosphere for a path of 0.04 km-am at T = 120 K and P = 0.1 bar (new LBL results in red, [4] in green).

of high transparency.

Acknowledgements

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