The Importance of Accurate Molecular Spectroscopy for Characterising Exoplanetary Atmospheres

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Calculating Spectral Line Profiles

We have investigated the current methods for computing line profiles, specifically whether to use a Voigt profile when considering pressure broadening in exoplanetary atmospheres. A Voigt profile is a convolution of the Gaussian profile from thermal broadening and the Lorentzian profile from pressure broadening. Due to the the sheer volume of spectral lines that require broadening the calculation of a Voigt profile must be accurate and extremely quick. We have tested Voigt functions from [5] and [3] and found that, in temperature and pressure regimes for hot Jupiters, computing the Voigt profile with a complex Faddeeva function gives accurate results.

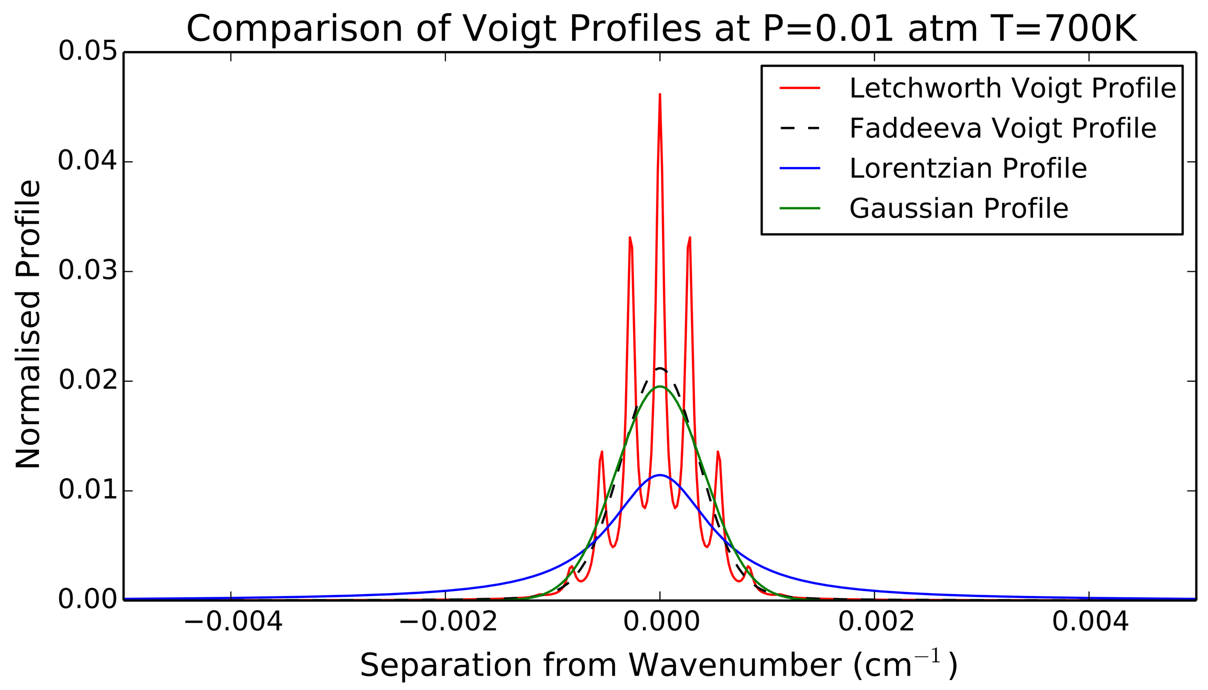


Figure 1: Different Voigt profile estimates showing that the method estimating the Voigt profile using Gauss-Hermite Quadrature from [3] gives an unrealistic estimate.

We have compared Lorentzian, Gaussian and Voigt profiles to judge whether a full calculation of the Voigt profile is necessary, instead of choosing a simpler Lorentzian profile. The results in Figure 2 show that, particularly for exoplanetary atmospheres, a Voigt profile is needed.

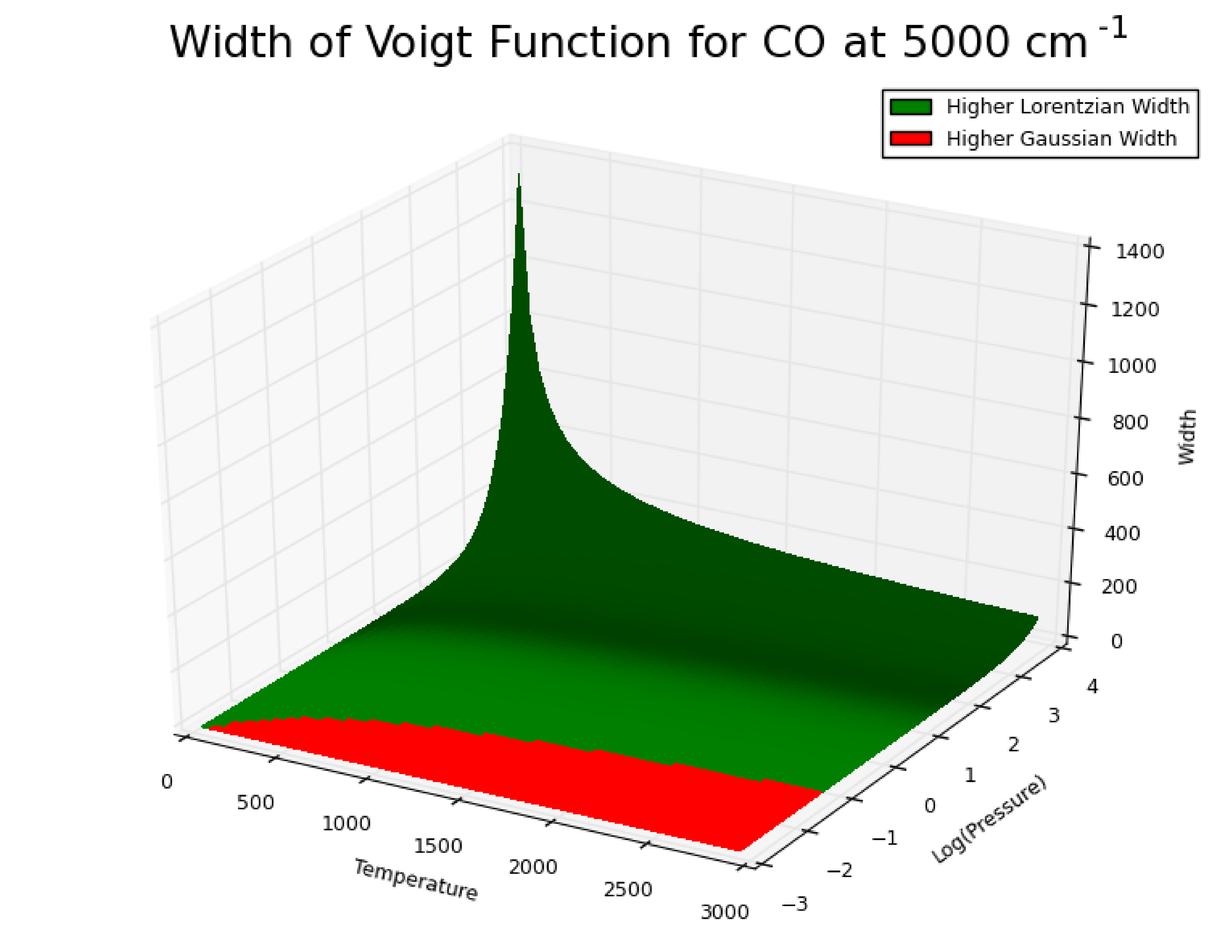
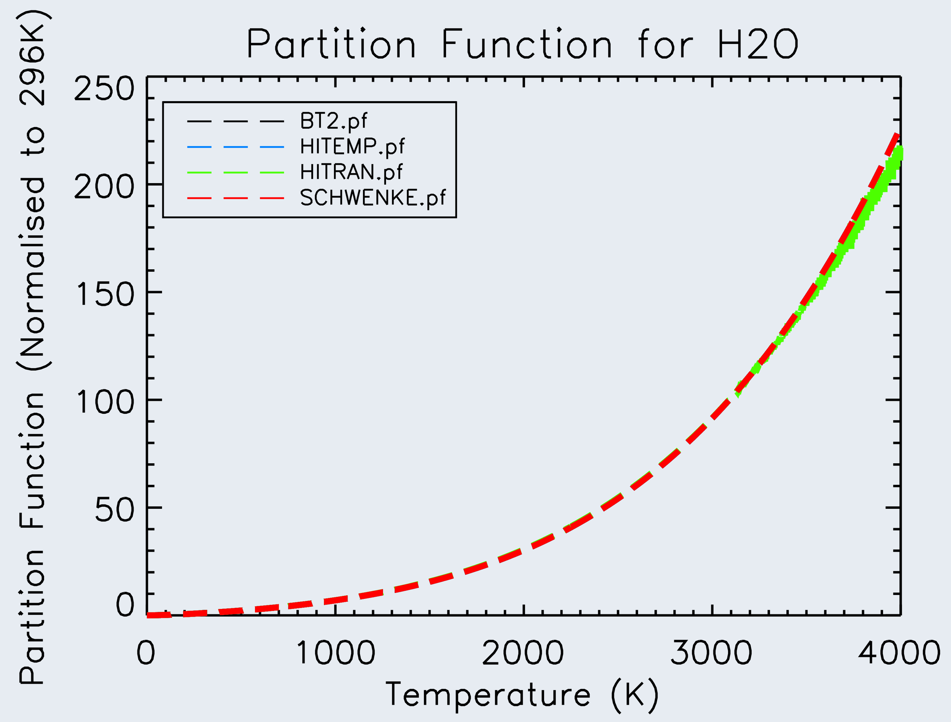


Figure 2: Regions where a Gaussian is wider and a Lorentzian is wider in temperature and pressure space. Any region near the boundary is where a Voigt profile is necessary. However a Voigt profile is always advised due to the wide Lorentzian wings.

Comparing Partition Functions

In this work we aim to test all of the basic inputs in the generation of cross sections from line lists. One aspect of this investigation is partition functions, the functions that determine the scaling of line intensity. We find that for water there are many well known partition functions that match up quite well. However there are discrepancies, particularly at high temperatures around 3000K and above. This is also true for other molecules. We are currently investigating whether the discrepancies in the partition functions give noticeably different cross sections at the high temperatures needed for hot Jupiters.



Cross Sections for Future Instruments

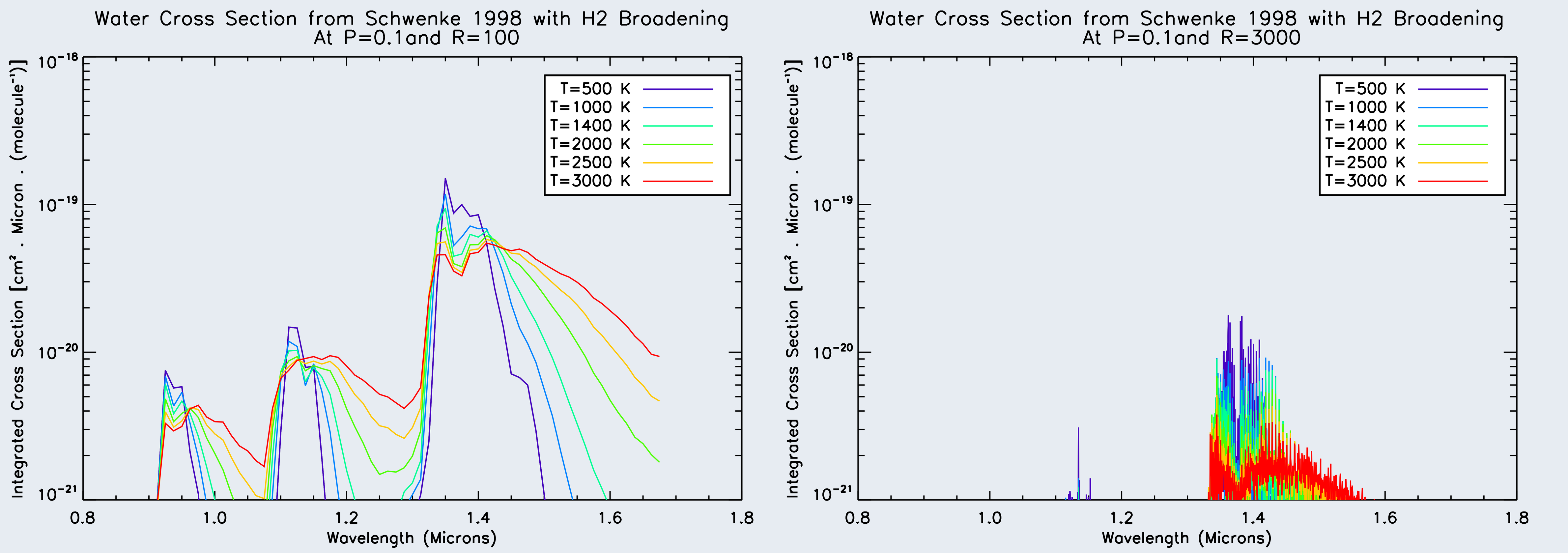


Figure 3: Comparison of cross sections at different temperatures for an HST and JWST-like resolution at a pressure of 0.1 atm in the range of the G102 (blueward) and G141 (redward) grisms. At these resolutions the differences introduced from pressure broadening are within $\leq 1\%$.

Conclusions

We are working towards an assessment of the differences that can be introduced to atmospheric models by cross sections and line lists, particularly at high temperatures for hot Jupiters. We are investigating the effects of pressure broadening on cross sections with respect to current and future instruments, particularly looking into the needs of JWST, CHEOPS and PLATO and which bands to observe in. We will also be investigating pressure broadening in the context of future very high resolution instruments.

Use in Observations

The goal of this work is to investigate the optimal bandpasses and resolutions for future instruments, but it can also be applied to the extraction of abundance measurements in current observations. Investigating the fundamentals of line lists and cross sections that are used in atmospheric models will give a representative picture of where errors are introduced in interpreting current observations. Figure 4 shows HST WFC3 data which is in the preliminary stages of reduction by our group. In the future we hope to use our investigation to find the most accurate cross sections, with pressure broadening included, to aid accurate abundance measurements from such spectra.

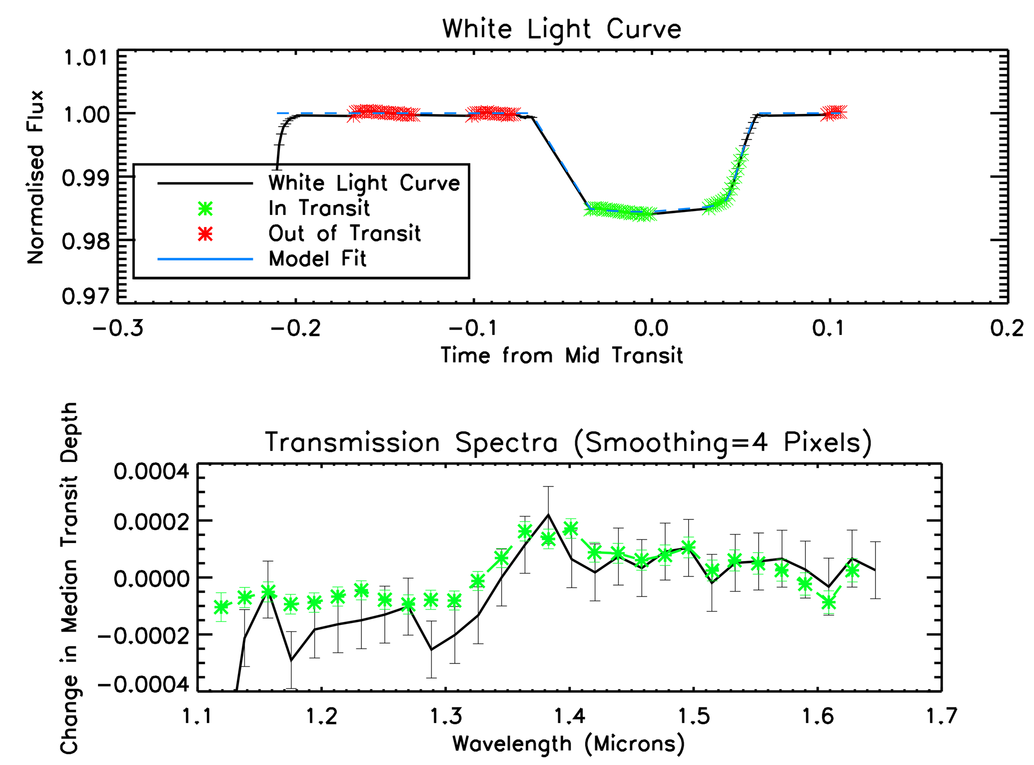


Figure 4: Figure showing on going work in the reduction of HST WFC3 data using the G141 grism. Transmission Spectrum (smoothed) of HD209458b. Green points show data from [1]. The work is on going and current results are in preliminary stages.

References

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