Icarus 226 (2013) 1673–1677

Contents lists available at SciVerse ScienceDirect

Icarus

journal homepage: www.elsevier.com/locate/icarus

Temperature-dependent molecular absorption cross sections for exoplanets and other atmospheres

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ARTICLE INFO

Article history:
Available online 14 August 2012

Keywords:
Atmospheres, Composition
Extrasolar planets
Infrared observations
Radiative transfer

ABSTRACT

Exoplanets, and in particular hot ones such as hot Jupiters, require very significant quantities of molecular spectroscopic data to model radiative transport in their atmospheres or to interpret their spectra. This data is commonly provided in the form of very extensive transition line lists. The size of these line lists is such that constructing a single model may require the consideration of several billion lines. We present a procedure to simplify this process based on the use of cross sections. Line lists for water, H_3^+, HCN/HNC and ammonia have been turned into cross sections on a fine enough grid to preserve their spectroscopic features. Cross sections are provided at a fixed range of temperatures and an interpolation procedure which can be used to generate cross sections at arbitrary temperatures is described. A web-based interface (www.exomol.com/xsecs) has been developed to allow astronomers to download cross sections at specified temperatures and spectral resolution. Specific examples are presented for water and ammonia.

1. Introduction

With the growing realization that many, probably most, stars support exoplanets, developing the means to systematically characterize the atmospheres of these planets has become a major scientific priority (Tinetti et al., 2012a). Given the likely complex chemistry of these atmospheres and the elevated temperature that is found in the most observable planets, there is a significant demand for spectroscopic data on the probable exoplanet atmospheric constituents.

Recently we have launched a new project, called ExoMol (see www.exomol.com), with the aim of providing molecular transition data appropriate for exoplanet models which are reliable over a wide range of temperatures (Tennyson and Yurchenko, 2012). The ExoMol project involves constructing line lists of spectroscopic transitions for key molecules which are valid over the entire temperature and wavelength domain that is likely to be astrophysically important for these species. Especially for polyatomic molecules, these line lists can become very large with hundreds of millions (Harris et al., 2006; Barber et al., 2006; Voronin et al., 2010; Tashkun and Perevalov, 2011) or even billions (Yurchenko et al., 2011) of individual transitions needing to be characterized and stored. A complete linelist for methane, for which so far only a preliminary version is available (Warmbier et al., 2009), can be expected to be even larger. Indeed potential line lists for larger species, such as higher hydrocarbons, for which spectroscopic data is needed for exoplanetary research, are likely to be so large as to potentially make their use impractical.

Molecular line lists are being actively used to model the spectra of exoplanets (e.g. Beaulieu et al., 2011) and cool brown dwarfs with similar temperatures (e.g. Lucas et al., 2010; Cushing et al., 2011). However, sampling billions of individual transitions to model relatively low resolution astronomical spectra is probably not necessary in many cases. An alternative approach is to represent the molecular absorptions as cross sections generated at an appropriate resolution and temperature. The advantage of this approach is that the data handling issues related to dealing with large data sets largely disappear. The disadvantage is that cross sections are inflexible – a particular cross section set is only valid for a single state of temperature and pressure. Cross sections are therefore often regarded as a second choice compared to maintaining a full line list (Rothman et al., 2009).

In this paper we develop a strategy whereby cross sections are provided for the user in a flexible fashion without significant loss of accuracy or the specificity of using a complete line list. To this end we have provided a web application which, starting from very high resolution cross sections generated for each molecule at a range of temperatures, can provide cross sections at a temperature and resolution specified by the user. Of course this approach is based on the implicit assumption of local thermodynamic equilibrium (LTE) and any non-LTE treatment will continue to have to rely on the explicit use of transition line lists. So far, these cross sections do not consider collisional broadening effects and are therefore, at their highest resolution, appropriate for the zero pressure limit only.

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0019-1035/$ - see front matter © 2012 Elsevier Inc. All rights reserved.
http://dx.doi.org/10.1016/j.icarus.2012.07.028

The line lists for water (Barber et al., 2006; Voronin et al., 2010), H_3^+ (Neale et al., 1996; Sochi and Tennyson, 2010), HCN/HNC (Harris et al., 2002, 2006, 2008) and ammonia (Yurchenko et al., 2011) were used to generate cross sections for these species. For concreteness, this work uses the main water isotopologue, $H_2{}^{16}O$, as its working example. Water is known to be a key species in exoplanetary atmospheres and the BT2 line list has been used in studies of exoplanets (Tinetti et al., 2007, 2010a,; Swain et al., 2009; Baraffe et al., 2010; Shabram et al., 2011; Barman et al., 2011; Tessenyi et al., 2012) as well in a large variety of planetary (Bykov et al., 2008; Chesnokova et al., 2009; Bailey, 2009), astrophysical (Warren et al., 2007; Dello Russo et al., 2004, 2005; Burgasser et al., 2008; Barber et al., 2009; Lyubchik et al., 2007; Banerjee et al., 2005) and, indeed, engineering (Kranendonk et al., 2007; Lindermeir and Beier, 2012) studies which generally focus on the radiative transport by hot water. The BT2 line list was used as part of the recently updated HITEMP database (Rothman et al., 2010). In that work, the size of the line list was reduced using a technique based upon importance sampling at a range of key temperatures. In practice the number of water lines in HITEMP remains large, over 100 million.

The calculation of opacities and other spectral properties due to water vapour at these elevated temperatures can therefore become onerous, and so we present here pre-calculated absorption cross sections for a range of temperatures between 296 K and 3000 K, binned to different resolutions. The highest resolution cross sections are suitable for modelling low-density environments where only Doppler broadening contributes to the line width whereas by binning to a wavenumber grid spacing significantly larger than the pressure-broadened half-width, higher-density environments are described well by the calculated cross sections. However, no attempt is made to include contributions to the opacity from the water vapour continuum or water dimer absorption.

2. Method

The high-resolution cross section is calculated on an evenly-spaced wavenumber grid, $\tilde{\nu}_i$, defining bins of width $\Delta\tilde{\nu}$. Only Doppler broadening is considered so each absorption line has a Gaussian shape (Fig. 1):

$$f_G(\tilde{\nu};\tilde{\nu}_{0:j},\alpha_j)=\sqrt{\frac{\ln 2}{\pi}}\frac{1}{\alpha_j}\exp\left(-\frac{(\tilde{\nu}-\tilde{\nu}_{0:j})^2\ln 2}{\alpha_j^2}\right), \tag{1}$$

where the line centre position is $\tilde{\nu}_{0:j}$ and the Doppler half-width at half-maximum,

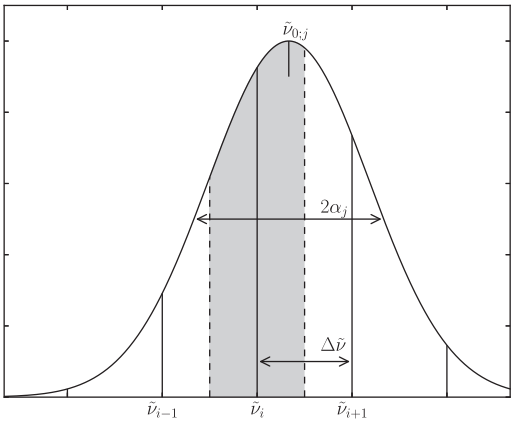

Fig. 1. The calculation of the absorption cross section in a wavenumber bin centred on $\tilde{\nu}_i$ due to a single line. The integrated line intensity within the shaded region, of width $\Delta\tilde{\nu}$, contributes to σ_{ij}.

$$\alpha_j=\sqrt{\frac{2k_BT\ln 2}{m}}\frac{\tilde{\nu}_{0:j}}{c}, \tag{2}$$

at temperature T for a molecule of mass m.

The contribution to the cross section within each bin is a sum over contributions from individual lines:

$$\sigma_i=\sum_j\sigma_{ij}, \tag{3}$$

where

$$\sigma_{ij}=\frac{S_j}{\Delta\tilde{\nu}}\int_{\tilde{\nu}_i-\Delta\tilde{\nu}/2}^{\tilde{\nu}_i+\Delta\tilde{\nu}/2}f_G(\tilde{\nu};\tilde{\nu}_{0:j},\alpha_j)\mathrm{d}\tilde{\nu}, \tag{4}$$

$$=\frac{S_j}{2\Delta\tilde{\nu}}\left[\mathrm{erf}\left(x_{ij}^+\right)-\mathrm{erf}\left(x_{ij}^-\right)\right], \tag{5}$$

where erf is the error function and

$$x_{ij}^{\pm}=\frac{\sqrt{\ln 2}}{\alpha_j}\left[\tilde{\nu}_i\pm\frac{\Delta\tilde{\nu}}{2}-\tilde{\nu}_{0:j}\right], \tag{6}$$

are the scaled limits of the wavenumber bin centred on $\tilde{\nu}_i$ relative to the line centre, $\tilde{\nu}_{0:j}$, and the line intensity in units of $\mathrm{cm}^{-1}/(\mathrm{molecule\ cm}^{-2})$ is

$$S_j=\frac{A_j}{8\pi c}\frac{g_j'\mathrm{e}^{-c_2E_j''/T}}{\tilde{\nu}_{0:j}^2Q(T)}(1-\mathrm{e}^{-c_2\tilde{\nu}_{0:j}/T}). \tag{7}$$

Here, g_j' and E_j'' are the upper-state degeneracy and lower-state energy respectively, A_j is the Einstein A coefficient for the transition and $c_2\equiv hc/k_B$ is the second radiation constant. For $H_2{}^{16}O$, the molecular partition function, $Q(T)$, was obtained from the tabulated values of Vidler and Tennyson (2000).

Note that in the limit of $\Delta\tilde{\nu}\gg\alpha_j$, Eq. (4) reduces to

$$\sigma_{ij}\approx\frac{S_j}{\Delta\tilde{\nu}}\int_{-\infty}^{+\infty}f_G(\tilde{\nu};\tilde{\nu}_{0:j},\alpha_j)\mathrm{d}\tilde{\nu}=\frac{S_j}{\Delta\tilde{\nu}}, \tag{8}$$

whereas for $\Delta\tilde{\nu}\ll\alpha_j$,

$$\sigma_{ij}\approx S_jf_G(\tilde{\nu}_i;\tilde{\nu}_{0:j},\alpha_j). \tag{9}$$

However, the exact expression is used in all calculations of the cross sections presented in this work.

3. Results

The absorption cross section of $H_2{}^{16}O$ was calculated between 10 cm^{-1} and 30,000 cm^{-1} across the temperature range 296–3000 K (Table 1), using the wavenumber grid-spacing given in Table 2. Each region was calculated to overlap with its neighbours by at least 1 cm^{-1}, which we find is sufficient to avoid discontinuities when they are binned to a common grid-spacing.

For comparison with experimental spectra, low-resolution cross sections were produced by binning the high-resolution cross sections to the following fixed grid spacing across the entire wavenumber range: $\Delta\tilde{\nu}=0.01,0.1,1,10,100\ \mathrm{cm}^{-1}$. At these resolutions, the structure due to individual lines is lost and direct comparison can be made with, for example, the experimental water vapour cross sections of the PNNL database (Sharpe et al., 2004). Such a comparison for the $\Delta\tilde{\nu}=10\ \mathrm{cm}^{-1}$ resolution spectra is shown in

Table 1
Temperatures at which calculated $H_2{}^{16}O$ cross sections are provided.

296 K	400 K	500 K	600 K
700 K	800 K	900 K	1000 K
1200 K	1300 K	1400 K	1600 K
1800 K	2000 K	2200 K	2400 K
2600 K	2800 K	3000 K	