



The ExoMol pressure broadening diet: H₂ and He line-broadening parameters

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ABSTRACT

In a variety of astronomical objects including gas giant (exo-)planets, brown dwarfs and cool stars, molecular hydrogen and helium are the major line broadeners. However, there is currently no systematic source for these parameters, particularly at the elevated temperatures encountered in many of these objects. The ExoMol project provides comprehensive molecular line lists for exoplanet and other hot atmospheres. The ExoMol database has recently been extended to provide additional data including temperature-dependent, pressure-broadening parameters. Here we assemble H₂ and He pressure-broadening datasets for the molecules H₂O, NH₃, SO₂, CH₄, PH₃, HCN and H₂CO using available experimental and theoretical studies.

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1. Introduction

Pressure broadening has a significant effect on the radiative transport through atmospheres. It is known to be important in the atmospheres of astronomical bodies such as hot Jupiter exoplanets and brown dwarfs [1–4] but the parameters necessary to characterize the effects of pressure on the spectral lines are not well known. For molecular absorbers the situation is complicated by the sheer number of lines, typically many billions for a single species, which contribute to the absorption. Furthermore such data that does exist largely probes room temperature.

The ExoMol project provides comprehensive lists of transitions (line lists) for molecules which are thought to be important in the atmospheres of exoplanets and other hot astronomical objects such as brown dwarfs and cool stars [5]. As part of a recent expansion of the ExoMol data structure [6], pressure broadening parameters have been incorporated into the ExoMol database. In this context, pressure broadening parameters refers to the Lorentzian half-width γ and its temperature dependence expressed as an exponent n (defined in Section 2). Currently ExoMol is considering broadening by air (or N₂), “self”, H₂ and He. Air and self broadening parameters are systematically provided by the HITRAN database [7] so in the absence of other sources those are taken from HITRAN 2012 [8] and simply expressed in ExoMol format. For ExoMol species not present in HITRAN, air- (or N₂) and self-broadening parameters will be taken from the literature where available. As such this article focuses on the creation of pressure broadening datasets for molecules perturbed by H₂ and He. There is no systematic source of parameters for broadeners H₂ and He,

although HITRAN is starting to include them [9], so we have to treat each system on a case-by-case basis. This article details the current ExoMol “diet” for H₂ and He pressure broadening parameters for several molecules of planetary interest. Underlying line lists for each of these molecules, H₂O [10–13] NH₃ [14–16], SO₂ [17], CH₄ [18,19], PH₃ [20,21], HCN [22–25] and H₂CO [26], are already available. Here we provide the necessary parameters to account for pressure broadening by H₂ and He for each of these species. As the methodology used here relies heavily on previous data, available experimental and theoretical data for each of these species are discussed below.

2. Pressure broadening file

ExoMol provides Lorentzian half-widths and temperature-dependent exponents in the new ExoMol format as a `.broad` file. The file is explained in detail in the recent ExoMol database paper, Tennyson et al. [6], hence only the main points are highlighted here.

The Lorentzian half-width of a spectral line specified by two parameters at temperature T and pressure P can be calculated as:

$$\gamma(T) = \gamma_{\text{ref}} \times \left(\frac{T_{\text{ref}}}{T} \right)^n \times \left(\frac{P}{P_{\text{ref}}} \right) \quad (1)$$

where n is the temperature-dependence exponent, $T_{\text{ref}} = 296$ K and $P_{\text{ref}} = 1$ bar. Values of γ_{ref} and n , differentiated by quantum number assignment, are given in the `.broad` file. The `.broad` file has a hierarchical structure, presenting experimental and theoretical parameters assembled from the literature with their full or partial quantum number assignments. Parameters with full quantum assignments are presented first. Additional semi-

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empirical parameters are determined by compiling all experimental and theoretical parameters as a function of J'' , the total rotational quantum number of the lower level of the transition, and computing an average value for each J'' . No attempt was made to construct fits to the available data, we simply compute a straight average. To avoid introducing additional error, no extrapolation is attempted beyond the J''_{max} for which data are available. These semi-empirical parameters are presented last in the `.broad` file, with their J'' assignment. More accurate methods for estimating line widths from available data, such as the energy difference method [27], recently applied to H₂O broadened by H₂/He [28], could be used to determine improved semi-empirical parameters. However this would require detailed calculations for each species considered and is hence beyond the scope of the current work.

3. Sources of parameters

Sources used in the creation of the current H₂ and He `.broad` files are discussed below.

3.1. H₂O

A number of works, including those discussed in our recent article [28], have provided pressure broadening parameters for broadening of H₂O by H₂ and/or He.

For the H₂O-H₂ system experimental Lorentzian half-widths for hundreds of lines at room temperature have been derived by Refs. [29–34]. The temperature dependence of the collision induced widths for select lines has been investigated by a handful of studies [34–37]. Theoretically determined pressure broadened widths and their temperature dependence are also available from Gamache, Lynch & Brown [38], Faure et al. [39], Drouin & Wisenfeld [40] and Barton et al. [28].

Studies [33,30–32,38,35,37,34,28] also reported Lorentzian half-widths for the H₂O - He system, although the most extensive work has been performed recently by Petrova and co-workers [41–43], and Solodov & Starikov [44,45]. In addition Refs. [46–49] measured room temperature line widths and Goyette & De Lucia [50] and Godon & Bauer [51] studied temperature dependence.

Parameters from Refs. [29–34] for H₂O - H₂ and Refs. [33,30–32,38,35,37,34,41–45] for H₂O - He are presented in the `.broad` file with their vibrational and rotational assignments. Barton et al. [28] neglected vibrational dependence as it was found to change the calculated widths by only a few percent, hence these parameters come with rotational assignments only.

For pressure broadened widths with no explicitly determined temperature dependence, a constant value of $n=0.6$ or 0.3 is used for broadening by H₂ or He respectively. This represents an average of all experimentally derived n values in each case.

3.2. NH₃

A summary of H₂ and He pressure broadening parameter sources for NH₃ was included in the recent article by Wilzewski et al. [9]. The pressure broadened parameters show strong rotational dependence, but apparently no vibrational dependence. Therefore parameters from numerous studies [52–67] for NH₃ - H₂ and [53–60,68,61] for NH₃ - He are presented in the `.broad` files with rotational assignments only.

Temperature dependence of H₂ line width coefficients was carefully assessed by Nemtchinov et al. [52]. n values derived by [52] average to 0.59, this value is used for widths with no explicitly determined temperature dependence.

Refs. [54,56–59] reported data for the temperature dependence

of a subset of NH₃ - He widths. For all other line broadening the average n value of 0.37 is used.

3.3. SO₂

As with NH₃, broadening of SO₂ by H₂ and He was summarised recently by Wilzewski et al. [9].

Cazzoli and Puzzarini [69] and Sumpf et al. [70] measured line broadening coefficients at room temperature while Ball et al. [71] explored the temperature dependence of SO₂ lines perturbed by H₂. The derived temperature exponents from [71] average to roughly 0.75, hence this is used as a default n value.

For SO₂ - He Wilzewski et al. [9] discount data from Sumpf et al. [70] on the basis that it disagrees with other measurements performed by Cazzoli and Puzzarini [69] and Tasinato et al. [72]. We follow the same approach and present results from Cazzoli and Puzzarini [69], Tasinato et al. [72] and, in the case of temperature dependence, Ball et al. [71]. The derived temperature exponents from [71] average to roughly 0.64, hence this is used as a default n value.

Overall the data indicates no vibrational dependence of the H₂ and He pressure broadening coefficients so all parameters are presented in the `.broad` files with rotational assignments.

3.4. CH₄

The CH₄ - H₂ broadening parameters for different vibrational bands have been explored in Refs. [73–78]. Varanasi and Chudamani [74,77] in particular examined the temperature dependence of line width coefficients, the average of their derived n roughly equates to the classical value of 0.5.

He broadening of CH₄ lines has received a similar treatment from Refs. [73–80]. Again Varanasi and Chudamani [74,77] derived temperature exponents, this time with an average of 0.35.

The pressure broadening H₂ and He parameters appear to vary with vibrational and rotational quantum numbers in a non-systematic way, though there is an overall trend of decreasing Lorentzian half-width with increasing rotational quantum number. As such line widths from Refs. [73–78] for CH₄ - H₂ and Refs. [73–80] for CH₄ - He are presented in the `.broad` files with rotational and vibrational assignments. Default temperature exponents of 0.5 and 0.35 for H₂ and He coefficients respectively are used where necessary.

3.5. PH₃

Like NH₃, the H₂ and He pressure broadening parameters for PH₃ Refs. [81–87] exhibit strong rotational dependence, but apparently no vibrational dependence. However, the molecule has not been studied quite as extensively in this context.

For PH₃ - H₂ line broadening coefficients from [81–85] are presented in the `.broad` file. Where no temperature exponent is available from the literature, a value of 0.75, recommended by Kleiner et al. [87], is used.

Refs. [81–83] also observed PH₃ spectra in the presence of He. Line broadening coefficients from these sources and Salem et al. [86] are presented in the `.broad` file. Where no temperature exponent is available from the literature a value of 0.35, an average of values reported by Levy, Lacome & Tarrago [81], is used.

Table 1 gives an extract from the ExoMol broadening file for PH₃ which is designed to be used with either of the available line lists [20,88]. Figs. 1 and 2 compare our model with room-temperature measurements of phosphine broadening (Table 2).

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