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The ExoMol pressure broadening diet: H_2 and He line-broadening parameters

Emma J. Barton, C. Hill, M. Czurylo, H.Y. Li, A. Hyslop, Sergei N. Yurchenko, Jonathan Tennyson *

Department of Physics and Astronomy, University College London, London WC1E 6BT, UK

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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 H_2 and He pressure-broadening datasets for the molecules H_2O, NH_3, SO_2, CH_4, PH_3, HCN and H_2CO using available experimental and theoretical studies.

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 N_2), "self", H_2 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 N_2) 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 H_2 and He. There is no systematic source of parameters for broadeners H_2 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 H_2 and He pressure broadening parameters for several molecules of planetary interest. Underlying line lists for each of these molecules, H_2O [10–13] NH_3 [14–16], SO_2 [17], CH_4 [18,19], PH_3 [20,21], HCN [22–25] and H_2CO [26], are already available. Here we provide the necessary parameters to account for pressure broadening by H_2 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:

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

where n is the temperature-dependence exponent, $T_{\mathrm{ref}} = 296$ K

* Corresponding author.

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and P_{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-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 H_2O broadened by H_2/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 H_2 and He `.broad` files are discussed below.

3.1. H_2O

A number of works, including those discussed in our recent article [28], have provided pressure broadening parameters for broadening of H_2O by H_2 and/or He.

For the H_2O-H_2 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 H_2O - 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 H_2O - H_2 and Refs. [33,30–32,38,35,37,34,41–45] for H_2O - 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 H_2 or He respectively. This represents an average of all experimentally derived n values in each case.

3.2. NH_3

A summary of H_2 and He pressure broadening parameter sources for NH_3 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 NH_3 - H_2 and [53–60,68,61] for NH_3 - He are presented in the `.broad` files with rotational assignments only.

Temperature dependence of H_2 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 NH_3 - He widths. For all other line broadening the average n value of 0.37 is used.

3.3. SO_2

As with NH_3, broadening of SO_2 by H_2 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 SO_2 lines perturbed by H_2. The derived temperature exponents from [71] average to roughly 0.75, hence this is used as a default n value.

For SO_2 - 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 H_2 and He pressure broadening coefficients so all parameters are presented in the `.broad` files with rotational assignments.

3.4. CH_4

The CH_4 - H_2 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 CH_4 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 H_2 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 CH_4 - H_2 and Refs. [73–80] for CH_4 - He are presented in the `.broad` files with rotational and vibrational assignments. Default temperature exponents of 0.5 and 0.35 for H_2 and He coefficients respectively are used where necessary.

3.5. PH_3

Like NH_3, the H_2 and He pressure broadening parameters for PH_3 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 PH_3 - H_2 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 PH_3 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 PH_3 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).

Table 1
`31P-1H3__H2.broad`: Extract of PH_3 - H_2 broad file: portion of the file (upper part); field specification (lower part).

a1	0.1342	0.760	4	4
a1	0.1167	0.640	6	6
a1	0.1279	0.690	7	0
a1	0.1301	0.660	7	1
…				
a0	0.1052	0.741	1	
a0	0.1157	0.715	2	
a0	0.1174	0.734	3	
a0	0.1166	0.744	4	
…				

Field	Fortran format	C format	Description
code	A2	%2s	Code identifying quantum number set following J''*
γ_{ref}	F6.4	%6.4f	Lorentzian half-width at reference temperature and pressure in cm^{-1}/bar
n	F5.3	%5.3f	Temperature exponent
J''	I7	%7d	Lower J-quantum number
K''	I2	%2d	Lower rotational quantum number

* Code definitions: a1 = parameters presented as a function of J'' (compulsory) and K''; a0 = parameters presented as a function of J'' (compulsory).

Table 2
`31P-1H3__He.broad`: Extract of PH_3 - He broad file: portion of the file (upper part); field specification (lower part).

a1	0.0526	0.300	6	0
a1	0.0539	0.300	6	1
a1	0.0523	0.300	7	0
a1	0.0535	0.300	7	3
…				
a0	0.0602	0.300	1	
a0	0.0584	0.300	2	
a0	0.0589	0.300	3	
a0	0.0574	0.300	4	
…				

Field	Fortran Format	C format	Description
code	A2	%2s	Code identifying quantum number set following J''*
γ_{ref}	F6.4	%6.4f	Lorentzian half-width at reference temperature and pressure in cm^{-1}/bar
n	F5.3	%5.3f	Temperature exponent
J''	I7	%7d	Lower J-quantum number
K''	I2	%2d	Lower rotational quantum number

* Code definitions: a1 = parameters presented as a function of J'' (compulsory) and K''; a1 = parameters presented as a function of J'' (compulsory) and K''.

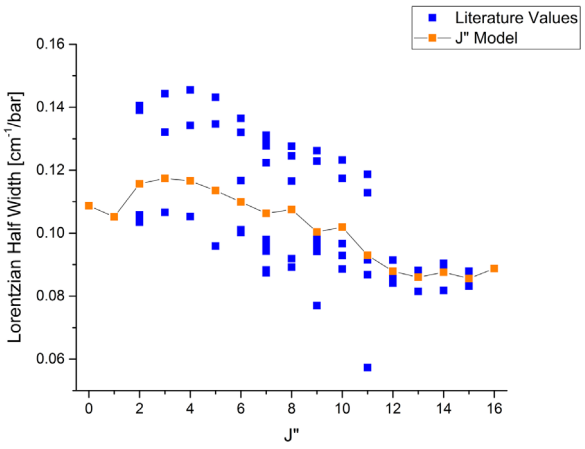

Fig. 1. Comparison of PH_3 - H_2 broadening coefficients from peer reviewed sources and semi-empirical parameters determined as a function of J'' at 296 K.

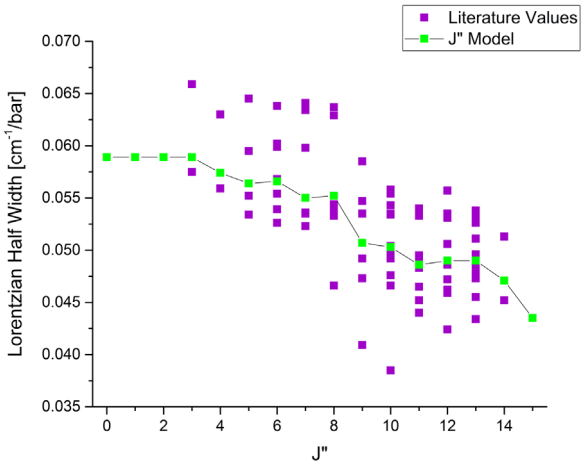

Fig. 2. Comparison of PH_3 - He broadening coefficients from peer reviewed sources and semi-empirical parameters determined as a function of J'' at 296 K.

3.6. HCN

Only three studies [89–91] have determined line widths for HCN perturbed by H_2 and/or He. All three focused on l-type doublet transitions in the bending vibrational state (0 1^1 0) having $5 \leq J \leq 10$.

Mehrotra et al. [89] and Charron, Anderson & Steinfeld [90] examine both HCN -H_2 and HCN - He systems, while Cohen and Wilson [91] studies HCN in the presence of noble gases.

No obvious trend with quantum numbers is observed for either broadener, see Fig. 3. Hence measured line widths ($5 \leq J \leq 10$) are presented in the `.broad` files with their rotational and vibrational assignments. For the semi-empirical model, an average of the measured H_2 or He widths respectively is given for $J < 5$.

All studies were performed at room temperature hence the classical value of n, 0.5 [92], is used as the temperature exponent in all cases.

3.7. H_2CO

To the best of our knowledge only one study [93] provides H_2/He pressure broadened widths. Nerf [93] measured self, H_2 and He line broadening coefficients for 12 rotational transitions of H_2CO at room temperature. These measurements, for J=1, 2, 3, 6 and 9, are presented in the `.broad` files with their rotational assignments (including K_a and K_c). No obvious trend with quantum numbers is observed for either broadener, see Fig. 4. For the semi-empirical model, an average of the measured H_2 or He widths respectively is given for J=0, 4, 5, 7 and 8.

As with HCN, the classical value of n, 0.5 [92], is used as the temperature exponent in all cases.

3.8. Mixtures

Only rarely will the data presented here be used in an atmosphere composed of a single species. It is therefore important to know how to treat broadening by a mixture of gasses. As constructed, each `.broad` file provides pressure broadening parameters for a single broadener. Lorentzian halfwidths for a mixed environment can then be generated using a generalized broadening parameter:

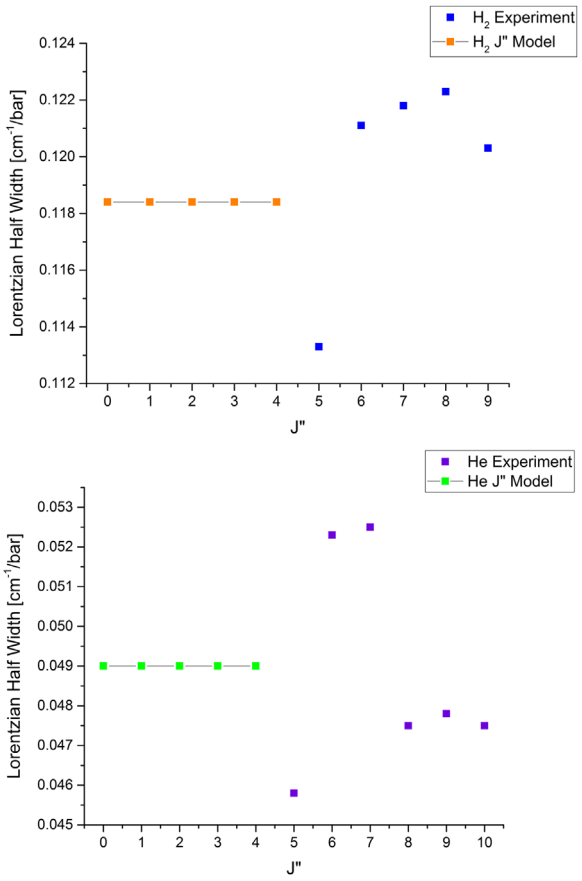

Fig. 3. Measured HCN - H_2/He broadening coefficients at 296 K and averaged values used for $J \leq 5$ in the semi-empirical model. The observations display no obvious trend with J''.

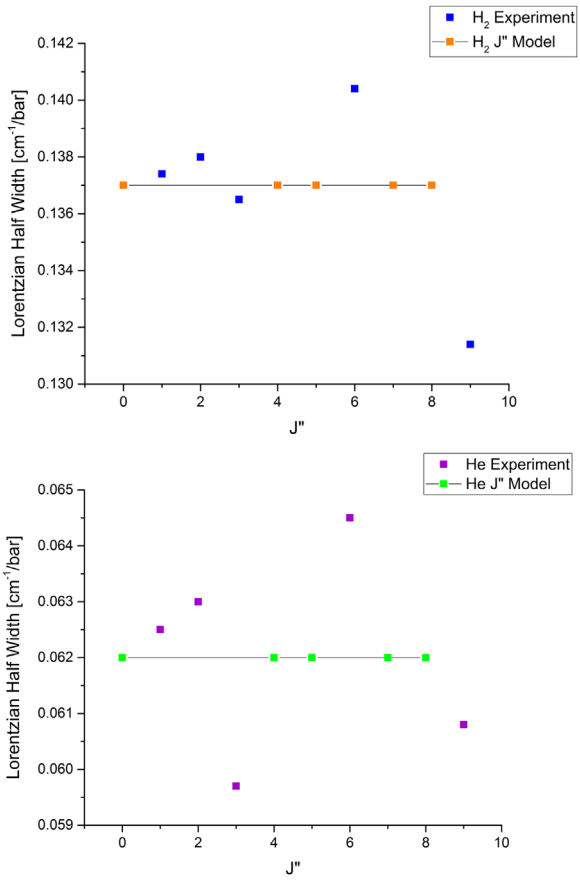

Fig. 4. Measured H_2CO - H_2/He broadening coefficients at 296 K and averaged values used for $J = 0, 4, 5, 7, 8$ in the semi-empirical model. The observations display no obvious trend with J''.

$$\gamma(T, P) = \sum_b \left(\frac{P_b}{P_{\text{ref}}}\right) \times \left(\frac{T_{\text{ref}}}{T}\right)^{n_b} \times \gamma_{\text{ref},} b. \tag{2}$$

where $\gamma_{\text{ref,b}}$ is the Lorentzian half-width due to a specific broadener in units cm^{-1}/bar (ExoMol convention), n_b is its temperature-dependence exponent and p_b is the partial pressure of the broadener.

Note that here and elsewhere, to convert from the units cm^{-1}/bar used by ExoMol to cm^{-1}/atm used by HITRAN requires γ to be mutiplied by 1.01325.

4. Conclusion

Lorentzian half-widths and temperature-dependence exponents have been collated for H_2O, NH_3, SO_2, PH_3, CH_4, HCN and H_2CO broadened by H_2 and He and presented in ExoMol format.

The `.broad` file for each molecule-broadener system contains experimental and/or theoretical parameters from the literature where available, and additional semi-empirical parameters determined as an average value for each J''. The files can be used to generate a complete, if mostly approximate, pressure broadening data set for each molecule-broadener system considered. Clearly further and improved parameters would be welcome.

Within the ExoMol data structure [6] the `.broad` file is associated with a particular molecule not a specific line list or isotopologue. This means that for molecule such as water, ammonia, phosphine and HCN, where more than one line list is available for the system, the broadening parameters can be associated with any of them. Similarly for water, ammonia and HCN line lists are available for more than one isotopologue, and the broadening file can automatically be associated with the isotopically-substituted species. This association makes the assumption that broadening parameters derived for the main isotopologue are valid for the minor species too; this assumption is widely made elsewhere, for example by the HITRAN database [8]. We note, however, that in some cases (e.g. HDO), isotopic substitution lowers the symmetry. Some databases, notably GEISA [94], choose to treat such isotopologues as separate species and the different vibrational modes certainly make it harder to transfer broadening parameters from the parent isotopologue (e.g. H_2O). This issue remains to be resolved in future work.

We note that many of the line lists considered here are very large and contain tens of billions of lines. Performing radiative transport calculations with the full line list and the use of pressure- and temperature-dependent line profiles is computationally daunting task. It has been suggested [95], that such a treatment is only really necessary for the strong lines while the background absorption (emission) can be treated as a quasi-continuum due to the many weak lines in the system. Tests performed on the using a new, enlarged methane line list with 34 billion lines suggest that it is indeed possible to obtain reliable spectral models with the explicit treatment of relatively few (about 18 million) lines [19]. In this case the remaining weak lines form a temperature-dependent continuum which is assumed to be independent of pressure. This reduces the explicit treatment of pressure-dependent lines to the "few" strong lines retained for full treatment. Broadening parameters for these can, of course, be taken from the diet presented here.

H_2 and He `.broad` files for additional molecules will be complied when data becomes available.

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