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Molecular line shape parameters for exoplanetary atmospheric applications

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Abstract.

We describe the recent updates to the ExoMol database regarding the molecular spectral line shapes. ExoMol provides comprehensive molecular line lists with a special emphasis on the applications involving characterization of hot atmospheres such as those found in exoplanets and cool stars. Among important requirements of such applications are (i) the broadening parameters for hydrogen and helium dominating atmospheres and (ii) very broad ranges of temperature and pressures. The current status of the available line shape data in the literature, demands from the exoplanetary community and their specific needs are discussed.

1. Introduction

Molecules in the atmospheres of exoplanets, and similar astronomical objects such as brown dwarfs, are observed at pressures approaching atmospheric and therefore display pronounced pressure effects in their spectra [1, 2, 3]. There is, however, a severe lack of data appropriate for reproducing these pressure effects.

The ExoMol project provide extensive line lists for a large range of molecules, mostly related to the atmospheric retrievals for exoplanets and cool stars [4]. The selection of molecules and the spectroscopic coverage in ExoMol are dictated by the requirements from these applications. A major requirement is that the line lists must be sufficiently complete to be applicable for high temperatures specific for atmospheres of most of these objects [5]. Spectroscopic data for almost 40 molecules are currently covered by the ExoMol database, including diatomic, triatomic, tetratomic and two pentatomic species. The available line lists were generated both by ExoMol and other groups, see Table 1.

Recently we have undertaken a major upgrade of the ExoMol database [6]. The upgrade was motivated by the growing role of ExoMol as a major provider of the hot spectroscopic line lists for atmospheric retrievals from exoplanetary observations. The most important modifications include: (i) introduction of application programming interface (API); (ii) line shape parameters; (iii) cooling functions; (iv) radiative life times [7] and Landé g-factors [8]. In this contribution the new line shape data provided by ExoMol are discussed.

2. Requirements for the line shape parameters from the exoplanetary applications.

It is widely recognized that Voigt profiles only provide an approximate solution, especially for high resolution atmospheric studies [116]. However Voigt profiles are in widespread use and



Table 1. Molecular line lists included in the ExoMol database and Voigt line shape parameters when available.

Molecule	Reference	Broadener	Molecule	Reference	Broadener
AlO	[9]		HD ⁺	[10]	
BeH	[11]		HeH ⁺	[12]	
CaH	[11]		HNO ₃	[13]	Air
CaH	[14]		KCl	[15]	
CaO	[16]		LiH	[10]	
CH	[17]		LiH ⁺	[10]	
CH ₄	[18]	Air, He, H ₂ , CH ₄	MgH	[11]	
CN	[19]		MgH	[20]	
CP	[21]		NaCl	[15]	
CrH	[22]		NaH	[23]	
CS	[24]	Air, CS	NH	[25]	
FeH	[26]		NH ₃	[27]	Air, H ₂ , He, NH ₃
H ₂ CO	[28]	Air, He, H ₂ , H ₂ CO	PH ₃	[28]	Air, He, H ₂ , PH ₃
H ₂ O	[29]	Air, H ₂ , He, H ₂ O	PN	[30]	
H ₃ ⁺	[31]		ScH	[32]	
HCl	[33]	Air, H ₂ , He, HCl	SiO	[34]	
HCN/HNC	[35]	Air, He, H ₂ , HCN	TiH	[36]	
SO ₂	[37]	Air, He, H ₂	SO ₃	[38]	
H ₂ S	[39]		H ₂ O ₂	[40]	
VO	[41]				
H ₃ ⁺	[42]				

are easily computed [117, 118, 119]; they are therefore uniformly used to represent pressure broadening effects in exoplanetary models and hence in the ExoMol database.

Table 1 illustrates the coverage of the broadening parameters in ExoMol, which is also a reflection of the current status in the field. Below we list the main factors affecting the development of the line shapes for the exoplanetary applications.

- (i) The dominant species in gas giant planets such as hot Jupiter atmospheres are H₂ and He, often at high pressure [120]. However most of the line shapes parameters available in the literature are for the air (or N₂) as the main broadener and motivated by the terrestrial applications. Even though the needs for the line shapes broadened by H₂ and He have been recently recognized by HITRAN [121], the corresponding line shape data is still incomplete [122, 2].
- (ii) The large size of the line lists in ExoMol, which consist of tens of billions of lines for larger molecules, make it practically impossible to populate the whole database with accurate, line-by-line line shape parameters, experimental or theoretical. Only simple and very approximate models (e.g. based only on one quantum number J'') can afford productions of the data on such a large scale. However even simple models do not exist for most of the species in question, especially for H₂ and He as broadeners.
- (iii) The high temperatures ($T > 1000K$) of hot Jupiters, and other exoplanets of current interest [123], require line profiles for a large range of rotation and vibration excitations over extended temperature ranges. It is considered to be important to model at least the rotational (J) dependence of the line widths broadened by H₂ [120].
- (iv) There is no agreement on the value of the line wing cut-off to be used when computing Voigt profiles. On one hand, it is imperative to use a reasonable cut-off distance in order to speed

Table 2. Voigt parameters available in the literature and used in the ExoMol database.

Molecule	Broadener	Reference
H ₂ O	H ₂	[43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55]
H ₂ O	He	[56, 57, 58, 59, 60, 43, 44, 45, 48, 49, 61, 52, 53, 54]
H ₂ O	Air	[62, 63, 64, 65, 66, 67]
H ₂ O	H ₂ O	[62, 63, 68, 69, 70]
CH ₄	H ₂	[71, 72, 73, 74]
CH ₄	He	[75, 76, 77, 73]
CH ₄	Air	[78, 79, 80]
CH ₄	CH ₄	[81, 82, 79]
NH ₃	H ₂	[83, 84, 85, 86]
NH ₃	He	[83, 84, 85, 86]
NH ₃	Air	[87, 88, 86]
NH ₃	NH ₃	[87, 89, 90, 91, 92, 93]
PH ₃	H ₂	[94, 89, 90, 92]
PH ₃	He	[95, 89, 90, 92]
PH ₃	Air/N ₂	[95, 96, 97]
PH ₃	PH ₃	[96, 97, 98, 99]
H ₂ CO	H ₂	[100]
H ₂ CO	He	[100]
H ₂ CO	N ₂	[101]
H ₂ CO	H ₂ CO	[101]
SO ₂	H ₂	[102]
SO ₂	He	[102, 103]
SO ₂	Air	[102, 103]
HCN	Air/N ₂	[104, 105, 106]
HCN	HCN	[105, 107]
HCN	H ₂	[108]
HCN	He	[108]
HCl	N ₂	[109]
HCl	HCl	[110]
HCl	H ₂	[111]
HCl	He	[112, 109]
CS	Air	[113]
CS	CS	[114]
HNO ₃	Air	[115]

up the line-by-line calculations of the molecular opacities. On the other hand, the choice of the cut-off is known to effect the results at high pressures. Common practices include a fixed cut-off (e.g. 25 cm⁻¹ or 100 cm⁻¹ [120]), variable cut-off depending on pressure P (e.g. min(25 P ; 100) cm⁻¹ [85]) or proportional to the line (half-)width (e.g. 500 widths [3]). The importance of folding back the truncated wings to ensure that the strength of the profile is conserved [85] is also considered in certain circumstances.

- (v) Efficient computational algorithms for the Voigt evaluations [117, 124] as well as the sampling method [125] are required when billions of lines are involved.

Some progress in estimating H₂ and He pressure-broadening parameters for water at elevated temperatures [50, 126] which are assumed to appropriate not only for our H₂¹⁶O line lists [29, 127] but also those for H₂¹⁷O and H₂¹⁸O [128].

In practice it is computationally prohibitive to perform radiative transport calculations on hot exoplanets line-by-line. Therefore the models either use precomputed cross sections, such as is done by τ -Rex [28, 129], or tables of k -coefficients, as done by the NEMISIS [130]. This means that appropriate values are precomputed on a grid of temperatures and pressures as inputs to such codes. Progress has been made recasting very large line lists, such as that for methane, into a background quasi-continuous pressure-independent cross section which can be combined with a full pressure-dependent treatment of the stronger lines [131, 132]. This approach would appear to provide a practical way forward.

3. Conclusion

We are in the advanced stages of developing a diet for pressure broadening of molecules present in exoplanetary atmospheres and those of other hot astronomical objects. A full discussion of this problem will be given elsewhere [133].

Pressure broadening data is urgently needed for atmospheric studies (retrievals) of exoplanets and cool stars. There is huge demand on the comprehensive solutions of the line shape problems for most of the molecules important for exoplanetary studies. The ExoMol database is arguably the main source of opacities for hot species important for modeling these atmospheres, where we have created a structure for depositing and curating any molecular data important for spectroscopic properties of hot atmospheric and other gaseous environments. We invite the molecular data producers to contribute to this database. The line shape data is especially important as the line parameters are missing or incomplete for the H₂-rich atmospheres even for the most important absorbers. Exoplanetary atmospheric retrieval is a hot topic at the moment with a lot of interest from the society, which makes it a good place to be for an expert in the molecular line profiles. The lack of data, a strong demand from the field and interest from the public is a very attractive mixture for work in this direction to be properly recognized and rewarded.

We also invite the community to visit and test the new ExoMol database at www.exomol.com. Any feedback will be greatly appreciated.

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