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The ExoMol project: progress and perspectives

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Abstract

The ExoMol project aims to provide molecular line lists for exoplanets and other atmosphere with a particular emphasis on those atmospheres which are significantly hotter than the Earth's. ExoMol has now computed line lists for about 40 molecules including, in most cases, isotopologues. These are available at WWW.EXOMOL.COM. Key new line lists include ones for H_3^+, NO, C_2H_4 and a significantly improved one for hot water, as well as for a range closed and open shell diatomic molecules.

The ExoMol database underwent a major reformat and upgrade in 2016; it now provides information on a variety of topics including, of course, line lists, cross sections (generated from the same line lists), lifetimes and Landé g-factors. It now comprises 52 molecules (130 isotopologues). Our new flexible code ExoCross can rapidly generate cross sections even from huge line lists. ExoCross also allows facile conversion between ExoMol and HITRAN formats.

1. ExoMol data 2018

The need for extensive, high temperature spectroscopic data on molecules, many of whom do not occur in the Earth's atmosphere, has led to a number of systematic efforts to generate the molecular line lists required [1]. In particular, a number of groups have been progressively generating line lists for key molecules. These includes the TheoReTS [2] group (Reims/Tomsk), the NASA Ames team and our own ExoMol activity based in University College London, all of which used similar theoretical procedures discussed below, and an experimental initiative led by Bernath [3]. These activities have been significantly enhanced by the discovery of exoplanets and the requirement of extensive line lists to be used in exoplanet models and characterization [4, 5].

The ExoMol database comprises line lists for 52 molecules (130 isotopologues). Table 1 summarises the molecules for which line lists have been provided as part of the ExoMol project. Sources for line lists of other key species are also provided, many based on line lists from Bernath and co-workers, see [6].

Table 1: Datasets created by the ExoMol project and included in the ExoMol database [7].

Paper	Molecule	$N_{\rm iso}$	$T_{\rm max}$	$N_{\rm elec}$	$N_{\rm lines}$	DSName
I	BeH	1	2000	1	16,400	Yadin
I	MgH	3	2000	1	10,354	Yadin
I	CaH	1	2000	1	15,278	Yadin
II	SiO	5	9000	1	254,675	EJBT
III	HCN/HNC	1	4000	1	399,000,000	Harris
IV	CH_4	1	1500	1	9,819,605,160	YT10to10
V	NaCl	2	3000	1	702,271	Barton
V	KCl	4	3000	1	1,326,765	Barton
VI	PN	2	5000	1	142,512	YYLT
VII	PH_3	1	1500	1	16,803,703,395	SAITY
VIII	H_2CO	1	1500	1	10,000,000,000	AYTY
IX	AlO	4	8000	3	4,945,580	ATP
X	NaH	2	7000	2	79,898	Rivlin
XI	HNO_3	1	500	1	6,722,136,109	AIJS
XII	CS	8	3000	1	548,312	JnK
XIII	CaO	1	5000	5	21,279,299	VBATHY
XIV	SO_2	1	2000	1	1,300,000,000	ExoAmes
XV	H_2O_2	1	1250	1	20,000,000,000	APTY
XIV	H_2S	1	2000	1	115,530,3730	AYT2
XV	SO_3	1	800	1	21,000,000,000	UYT2
XVI	VO	1	2000	13	277,131,624	VOMYT
XIX	$H_2{}^{17,18}O$	2	3000	1	519,461,789	HotWat78
XX	H_3^+	1	3000	1	11,500,000,000	MiZATeP
XXI	NO	6	5000	2	2,281,042	NOName
XXII	SiH_4	1	1200	1	62,690,449,078	OY2T
XXIII	PO	1	5000	1	2,096,289	POPS
XXIII	PS	1	5000	3	30,394,544	POPS
XXIV	SiH	4	5000	3	1,724,841	SiGHTLY
XXV	SiS	12	5000	1	91,715	UCTY
XXVI	HS	6	5000	1	219,463	SNaSH
XXVI	NS	6	5000	1	3,479,067	SNaSH
XXVII	C_2H_4	1	700	1	49,841,085,051	MaYTY
XXVIII	AlH	3	5000	3	40,000	AlHambra
XXIX	CH_3Cl	2	1200	1	166,279,593,333	OYT
XXX	$H_2{}^{16}O$	1	5000	1	1,500,000,000	POPKAZATEL
XXXI	C_2	3	5000	8	6,080,920	8State
XXXII	MgO	3	5000	4	22,579,054	LiPTY

$N_{\rm iso}$: Number of isotopologues considered; $T_{\rm max}$: Maximum temperature for which the line list is complete; $N_{\rm elec}$: Number of electronic states considered; $N_{\rm lines}$: Number of lines, value is for the main isotopologue; DSName: Name of line list and of data set in ExoMol database [7].

Data for all these species, including cross sections, are available on the ExoMol website. A comprehensive status review of the molecular line lists in the ExoMol database in a form of an atlas of opacities, illustrating their spectroscopic coverage, main spectroscopic signatures as well as temperature dependence of the molecular opacities relevant for atmospheric studies of hot exoplanets and stars can be found in [6].

Figure 1 presents an example of temperature-dependent cross sections for three isotopologues of water computed using ExoMol line lists. The opaci-

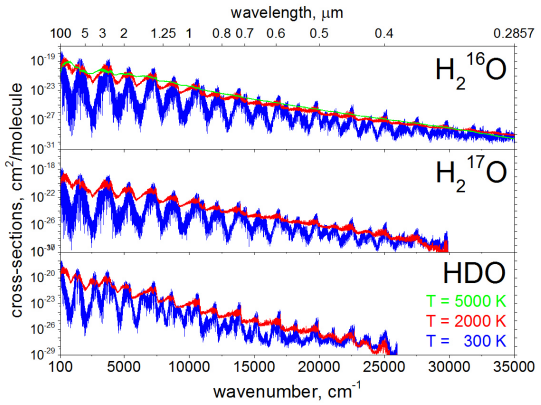

Figure 1: Cross sections for $H_2{}^{16}O$ from the POKAZATEL line list [9], $H_2{}^{17}O$ from the HotWat78 line list [10] and HDO from the VTT line list [11]. All cross sections are for 100% abundance, see [6].

ties are given for two reference temperatures, 300 K, 2000 K and 5000 K. For simplicity, we use a Doppler profile on a wavenumber grid of 1 cm^{-1}. A full atlas of ExoMol opacities can be found in [6]. The cross sections can be also obtained at higher resolutions (up to 0.01 $^{-1}$) using the cross sections App at www.exomol.com. The cross sections have been generated using the methodology by Hill et al. [8].

Compiling molecular opacity functions requires a large range of spectroscopic data on a large range of molecules. For many key species, there are now extensive line lists available that can be used to compute temperature-dependent opacity functions. This is a process of constant improvement and immediate improvements are indeed identified for several species discussed above. Recent observations have identified a whole new class of exoplanets with masses somewhat larger than the Earth's and orbits close to their host stars. These hot rocky super-Earths, lava planets or magma planets as they are variously known as are just beginning to be characterized [12], for which opacities are missing or incomplete [13].

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