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The 2020 release of the ExoMol database

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The 2020 release of the ExoMol database: molecular line lists for exoplanet and other hot atmospheres

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Abstract

The ExoMol database (www.exomol.com) provides molecular data for spectroscopic studies of hot atmospheres. While the data is intended for studies of exoplanets and other astronomical bodies, the dataset is widely applicable. The basic form of the database is extensive line lists; these are supplemented with partition functions, state lifetimes, cooling functions, Landé g-factors, temperature-dependent cross sections, opacities, pressure broadening parameters, k-coefficients and dipoles. This paper presents the latest release of the database which has been expanded to consider 80 molecules and 190 isotopologues totaling over 700 billion transitions. While the spectroscopic data is

concentrated at infrared and visible wavelengths, ultraviolet transitions are being increasingly considered in response to requests from observers. The core of the database comes from the ExoMol project which primarily uses theoretical methods, albeit usually fine-tuned to reproduce laboratory spectra, to generate very extensive line lists for studies of hot bodies. The data has recently been supplemented by line lists deriving from direct laboratory observations, albeit usually with the use of *ab initio* transition intensities. A major push in the new release is towards accurate characterisation of transition frequencies for use in high resolution studies of exoplanets and other bodies.

Keywords: infrared, visible, Einstein A coefficients, transition frequencies, partition functions, cooling functions, lifetimes, cross sections, k coefficients, Landé g-factors, pressure broadening

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1. Introduction

The ExoMol project was started in 2011 [1] with the purpose of providing molecular line lists for studies of exoplanets and other (hot) atmospheres. Besides data demands for exoplanets [2], other hot astronomical bodies with significant molecular content in their atmospheres include cool stars [3] and brown dwarfs [3, 4]. On Earth, similar spectroscopic data are required to study flames [5, 6], discharge plasmas [7], explosions [8] and the gases emitted from smoke stacks [9]. In addition, bodies in non-local thermodynamic equilibrium (non-LTE) such as comets and masers give observable emissions from highly excited states [10–12].

ExoMol data are proving very popular among the exoplanet atmospheric modellers owing to their extensive coverage of the molecular species and their completeness as function of both frequency and, very importantly, temperature. ExoMol data have been incorporated into many radiative transfer and retrieval codes including Tau-REx [13–15], Phoenix [16], NEMESIS [17], CHIMERA [18], HELIOS [19] and HELIOS-r2 [20], ATMO [21–23], ARCiS [24], ARTES [25], HyDRA [26], GENESIS [27], petitRADTRANS [28], PLATON [29], VSTAR [30, 31], BART [32] and Pyrat Bay [33]. In addition the ExoMol database has been used to support a variety of other studies. Examples including the analysis of gaseous ammonia in Jupiter [34], tentative detection of H_2S in Uranus [35], detection of CaO in meteors [36] and SiO in B[e] Supergiants [37], Late-type stars [38] or circumstellar environment [39]. Detections in the atmospheres of exoplanets are discussed below. More diverse applications include modeling laser analysis of Solar System objects [40, 41], isotope abundance quantification in stars [42], search for molecules highly sensitive to proton-to-electron mass ratio variation [43, 44], models of molecular steering [45, 46] , design of THz lasers [47], design of dark matter detection schemes [48] and the design of novel propulsion systems [49].

A number of diatomic molecules for which ExoMol provides extensive hot line

lists have been detected in sunspots. These include SiO [50], SiH [51], SH [52], BeH [53], VO [54], as well as MgH, MgO, TiO, C_2 and CaH which have all long been observed in sunspots [55]. In addition the spectrum of water is well-known in sunspots [56–60]; studies of water spectra in sunspots should be aided by the new POKAZATEL water line list [61] which is designed for studies at temperatures above 3000 K such as those encountered in solar umbra and penumbra.

ExoMol line lists have been published as a series in the journal Monthly Notices of the Royal Astronomical Society (see below) and a first data release in 2016 [62], henceforth ExoMol2016, provided full documentation for the ExoMol database which can be found at `www.exomol.com`. The basic form of the database is extensive line lists; these are supplemented with partition functions, state lifetimes, cooling functions, Landé g-factors, temperature-dependent cross sections, opacities, pressure broadening parameters, k-coefficients and dipoles. The ExoMol website also offers an extensive bibliography database on research literature on molecules relevant for ExoMol applications. So far the bibliography database contains 6709 sources.

Since ExoMol started there have been major changes in exoplanet science which have driven further expansion and development of the ExoMol database. The first is the discovery of rocky exoplanets orbiting so near to their host star that their surfaces are likely to be molten. The atmospheres of these planets are thought to contain a variety of species not considered previously [63–66]. Secondly higher temperature planets have been observed than anyone anticipated, the poster child for hot exoplanets is Kelt-9b which is thought to reach temperatures of 4000 K [67], hotter than most of the stars in our Galaxy! This has led to the need to construct line list for key species over an extended temperature range. Third is the development of Doppler-shift high resolution spectroscopy of exoplanets [68, 69] which has proved a powerful tool for detecting molecules but fails in the absence of highly accurate molecular line lists [70]. These develop-

ments have led us to both expand the range of molecules included in the database and to begin a systematic attempt to improve the accuracy of the line positions for the line lists contained in the database. Progress on both of these objectives is described below as well work on extending the coverage of the database into the ultraviolet.

Of course ExoMol is not the only database providing spectroscopic data for atmospheric studies. For the Earth's atmosphere, databases HITRAN [71–73] and GEISA [74, 75] provide comprehensive and validated datasets for approximately 50 key molecules. However, these databases are designed for studies at room temperature and below and do not contain the necessary data for adequately calculating radiative transport in hot bodies. The HITEMP database was constructed to extend HITRAN to higher temperatures. The latest, 2010, release [76] only contained data on 5 molecules (OH, NO, CO, H_2O and CO_2) and improved hot line lists are available for all these molecules; an update to HITEMP is currently in progress [77–79]. Other relevant databases include TheoReTS [80], which contains hot line lists for 8 polyatomic molecules, and Kurucz's compilation of data, which is very complete for atomic sources but contains data only on about ten diatomic molecules [81] all of which are covered by ExoMol, usually to higher accuracy. The MoLLIST data base of Bernath and co-workers [82] contains empirically derived line lists for about 20 diatomic species. These line lists have recently been incorporated into the ExoMol database [83], see Table 2 below. Databases of hot molecular spectra for other specialised applications include those for combustion [6, 84] and studies of laser-induced plasmas [85]. ExoMol line lists together with data from other sources will serve as the main data source for exoplanet stands planned for the upcoming space missions Ariel and JWST.

The methodology [65, 86–91] and software [92, 93] developed and used by the ExoMol project has been extensively documented elsewhere. Here we will only

consider those aspects which impinge on the new ExoMol2020 release.

2. Database coverage

The ExoMol project aims at complete coverage of the spectroscopic properties of molecules which are deemed to be important in hot astrophysical environments. Coverage concerns (a) the molecular species considered, including isotopologues; (b) the spectroscopic and thermodynamic properties considered; (c) the frequency range considered and (d) the upper temperature range for which the data are reasonably complete. Both the required temperature and frequency range completeness are to some extent a judgement on what is required for astronomical and other studies.

Unlike ExoMol2016, the ExoMol2020 database essentially provides a complete dataset for modelling hot atmospheres. While new species are still being added, commonly at the request of users, the database now contains molecular data for 80 molecules and covers the key molecules thought to be important for exoplanetary studies. In many cases there is more than one line list for a given isotopologue. For this reason it is our practice to name each line list, including (unnamed) ones we have imported from other sources. In the case of multiple line lists the ExoMol website provides a recommended line list for the given species. This recommendation is for studies of hot atmospheres; other available line lists may be more suitable for room temperature studies.

For ease of understanding we have divided the description of line lists provided into three tables. Tables 1 and 2 summarise the molecules for which data are provided by ExoMol and give the characteristics of the line list in each case. Table 1 details line lists which have been formally published as part of the ExoMol project while Table 2 shows line lists imported from other sources which have been recast in the ExoMol format (see Wang *et al* [83] for example); these line

lists are fully integrated into the database. Table 3 lists the main extra line lists available through the ExoMol website; this table is not comprehensive but the other line lists available on the ExoMol website and not listed in Table 1 – 3 are largely of historic interest only.

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

Paper	Molecule	$N_{\rm iso}$	$T_{\rm max}$	$N_{\rm elec}$	$N_{\rm lines}$ [a]	DSName		Reference
I	BeH	1	2000	1	16 400	Yadin		Yadin et al. [94]
I	MgH	3	2000	1	10 354	Yadin	✔	Yadin et al. [94]
I	CaH	1	2000	1	15 278	Yadin	✔	Yadin et al. [94]
II	SiO	5	9000	1	254 675	EJBT	✔	Barton et al. [95]
III	HCN/HNC	1[a]	4000	1	399 000 000	Harris	✔	Barber et al. [96]
IV	CH_4	1	2000	1	34 153 806 005	YT34to10	✔	Yurchenko and Tennyson [97], Yurchenko et al. [98]
V	NaCl	2	3000	1	702 271	Barton	✔	Barton et al. [99]
V	KCl	4	3000	1	1 326 765	Barton	✔	Barton et al. [99]
VI	PN	2	5000	1	142 512	YYLT	✔	Yorke et al. [100]
VII	PH_3	1	1500	1	16 803 703 395	SAlTY	✔	Sousa-Silva et al. [101]
VIII	H_2CO	1	1500	1	10 000 000 000	AYTY	✔	Al-Refaie et al. [102]
IX	AlO	4	8000	3	4 945 580	ATP	✔	Patrascu et al. [103]
X	NaH	2	7000	2	79 898	Rivlin	✔	Rivlin et al. [104]
XI	HNO_3	1	500	1	6 722 136 109	AlJS	✔	Pavlyuchko et al. [105]
XII	CS	8	3000	1	548 312	JnK	✔	Paulose et al. [106]
XIII	CaO	1	5000	5	21 279 299	VBATHY	✔	Yurchenko et al. [107]
XIV	SO_2	1	2000	1	1 300 000 000	ExoAmes	✔	Underwood et al. [108]
XV	H_2O_2	1	1250	1	20 000 000 000	APTY	✔	Al-Refaie et al. [109]
XVI	H_2S	1	2000	1	115 530 3730	AYT2	✔	Azzam et al. [110]
XVII	SO_3	1	800	1	21 000 000 000	UYT2	✔	Underwood et al. [111]
XVIII	VO	1	2000	13	277 131 624	VOMYT	✔	McKemmish et al. [112]
XIX	$H_2{}^{17,18}O$	2	3000	1	519 461 789	HotWat78	✔	Polyansky et al. [113]
XX	H_3^+	1[b]	3000	1	11 500 000 000	MiZATeP	✔	Mizus et al. [114]
XXI	NO	6	5000	2	2 281 042	NOName	✔	Wong et al. [115]
XXII	SiH_4	1	1200	1	62 690 449 078	OY2T	✔	Owens et al. [116]
XXIII	PO	1	5000	1	2 096 289	POPS	✔	Prajapat et al. [117]
XXIII	PS	1	5000	3	30 394 544	POPS	✔	Prajapat et al. [117]
XXIV	SiH	4	5000	3	1 724 841	SiGHTLY	✔	Yurchenko et al. [118]
XXV	SiS	12	5000	1	91 715	UCTY	✔	Upadhyay et al. [119]
XXVI	NS	6	5000	1	3 479 067	SNaSH	✔	Yurchenko et al. [120]
XXVI	HS	6	5000	1	219 463	SNaSH		Yurchenko et al. [120]
XXVII	C_2H_4	1	700	1	60 000 000 000	MaYTY	✔	Mant et al. [121]
XXVIII	AlH	3	5000	3	40 000	AlHambra	✔	Yurchenko et al. [122]
XXIX	CH_3Cl	2	1200	1	166 279 593 333	OYT	✔	Owens et al. [123]
XXX	$H_2{}^{16}O$	1[c]	5000	1	5 745 071 340	POKAZATEL	✔	Polyansky et al. [61]
XXXI	C_2	3	5000	8	6 080 920	8states	✔	Yurchenko et al. [124]
XXXII	MgO	5	5000	5	72 833 173	LiTY	✔	Li et al. [125]
XXXIII	TiO	5	5000	13	59 000 000	Toto	✔	McKemmish et al. [126]
XXXIV	PH	1	4000	2	65 055	LaTY	✔	Langleben et al. [127]
XXXV	NH_3	1[d]	1500	1	16 900 000	CoYuTe	✔	Coles et al. [128]
XXXVI	SH	2	3000	2	572 145	GYT	✔	Gorman et al. [129]
XXXVII	HCCH	1	2000	1	4 347 381 911	aCeTY	✔	Chubb et al. [130]
XXXVIII	SiO_2	1	3000	1	32 951 275 437	OYT3	✔	Owens et al. [131]
XXXIX	CO_2	1	3000	1	7 996 570 390	UCL-4000	✔	Yurchenko et al. [132]
XL	H_3O^+	1	1500	1	2 089 331 073	eXeL	✔	Yurchenko et al. [133]

Paper Number in series published in Mon. Not. R. Astron. Soc.

$N_{\rm iso}$ 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 isotope.

✔ indicates line list recommended for studies of hot atmospheres.

[a] The Larner line list for $H^{13}CN/HN^{13}C$ due to Harris et al. [134] is recommended.

[b] The ST line list for H_2D^+ due to Sochi and Tennyson [135] is recommended,.

[c] The VTT line list for HDO due to Voronin et al. [136] is recommended.

[d] There is a room temperature $^{15}NH_3$ line list due to Yurchenko [137].

Table 2: Datasets not created as part of the ExoMol project but included in the ExoMol database.

Molecule	$N_{\rm iso}$	$T_{\rm max}$	$N_{\rm elec}$	$N_{\rm lines}$	DSName		Reference	Methodology
H_2	1	10000	1	4712	RACPPK	✔	Roueff et al. [138]	Ab initio
CH	1	5000	4	52201	MoLLIST	✔	Masseron et al. [139]	Empirical
NH	1	5000	1	12150	MoLLIST	✔	Brooke et al. [140, 141], Fernando et al. [142]	Empirical
OH	1	5000	2	54276	MoLLIST	✔	Brooke et al. [143]	Empirical
AlCl	2	5000	1	20245	MoLLIST	✔	Yousefi and Bernath [144]	Empirical
AlF	1	5000	1	40490	MoLLIST	✔	Yousefi and Bernath [144]	Empirical
OH^+	1	5000	2	12044	MoLLIST	✔	Hodges and Bernath [145], Hodges et al. [146]	Empirical
CaF	1	5000	6	14817	MoLLIST	✔	Hou and Bernath [147]	Empirical
MgF	1	5000	3	8136	MoLLIST	✔	Hou and Bernath [148]	Empirical
KF	1	5000	2	10572	MoLLIST	✔	Frohman et al. [149]	Empirical
NaF	1	5000	1	7884	MoLLIST	✔	Frohman et al. [149]	Empirical
LiCl	1	5000	4	26260	MoLLIST	✔	Bittner and Bernath [150]	Empirical
LiF	1	5000	2	10621	MoLLIST	✔	Bittner and Bernath [150]	Empirical
MgH	2	5000	1	14179	MoLLIST	✔	GharibNezhad et al. [151]	Empirical
TiH	1	5000	3	181080	MoLLIST	✔	Burrows et al. [152]	Empirical
CrH	1	5000	2	13824	MoLLIST	✔	Chowdhury et al. [153]	Empirical
FeH	1	5000	2	93040	MoLLIST	✔	Wende et al. [154]	Empirical
HF	2	5000	1	7956	Coxon-Hajig	✔	Coxon and Hajigeorgiou [155]	Empirical
HCl	4	5000	1	2588	HITRAN	✔	Li et al. [156]	Empirical
CP	1	5000	2	28752	MoLLIST	✔	Ram et al. [157]	Empirical
CN	1	5000	3	195120	MoLLIST	✔	Brooke et al. [158]	Empirical
C_2	1	5000	2	47 570	MoLLIST		Brooke et al. [159]	Empirical
CaH	2	5000	1	6000	MoLLIST	✔	Li et al. [160], Shayesteh et al. [161]	Empirical
N_2	1	10000	4[a]	7 182 000	WCCRMT	✔	Western et al. [162]	Empirical
SiO	1	5000	3	6 67 814	Kurucz-SiO		Kurucz [81]	Empirical
ScH	1	5000	6	1 152 827	LYT	✔	Lodi et al. [163]	Ab initio
LiH	1	12000	1	18 982	CLT	✔	Coppola et al. [164]	Ab initio
LiH^+	1	12000	1	332	CLT	✔	Coppola et al. [164]	Ab initio
CO	9	9000	1	752 976	Li2015	✔	Li et al. [165]	Empirical
HeH^+	4	9000	1	1430	ADSJAAM	✔	Amaral et al. [166]	Ab initio
HD^+	1	9000	1	10285	ADSJAAM	✔	Amaral et al. [166]	Ab initio
HD	1	9000	1	5939	ADSJAAM	✔	Amaral et al. [166]	Ab initio
CH_3F	1	300	1	139 188 215	OYKYT	✔	Owens et al. [167]	Ab initio
AsH_3	1	300	1	3 600 000	CYT18	✔	Coles et al. [168]	Ab initio
P_2H_2[b]	2	300	1	10 667 208 951	OY-Trans	✔	Owens and Yurchenko [169]	Ab initio
P_2H_2[b]	2	300	1	11 020 092 365	OY-Cis	✔	Owens and Yurchenko [169]	Ab initio
PF_3	1	300	1	68 000 000 000	MCYTY	✔	Mant et al. [170]	Ab initio
CH_3	1	1500	1	2 058 655 166	AYYJ	✔	Adam et al. [171]	Ab initio
BeH	3	5000	2	592308	Darby-Lewis	✔	Darby-Lewis et al. [172]	ExoMol
CO_2	13	4000	1	298 323 789	Ames-2016		Huang et al. [173, 174]	ExoMol-like
SiH_2	1	2000	1	254 061 207	CATS	✔	Clark et al. [175]	ExoMol
YO	1	5000	6	3520133	SSYT	✔	Yurchenko et al. [176]	Ab initio

$N_{\rm iso}$ 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 isotope.

✔ indicates line list recommended for studies of hot atmospheres.

[a] The WCCRMT line list considers triplet states only.

[b] There are separate line lists for cis and trans P_2H_2.

Table 3: Supplementary datasets available from the website.

Molecule	$N_{\rm iso}$	$T_{\rm max}$	$N_{\rm elec}$	$N_{\rm lines}$	DSName		Reference	Methodology
H_3^+	2^a	4000	1	3 070 571	NMT		Neale et al. [177]	ExoMol
H_2O	2^b	3000	1	505 806 202	BT2		Barber et al. [178]	ExoMol
NH_3	2^c	1500	1	1 138 323 351	BYTe		Yurchenko et al. [179]	ExoMol
HeH^+	4	10000	1	1 431	Engel		Engel et al. [180]	Ab initio
HD^+	1	12000	1	10 119	CLT		Coppola et al. [164]	Ab initio
CO_2	13	300	1	161944	Zak		Zak et al. [181, 182, 183]	ExoMol
CO_2	1	4000	1	628 324 454	CSSD-4000		Tashkun and Perevalov [184]	Empirical
H_2O	1	300	1		WAT_UV296	[185]	ExoMol	

$N_{\rm iso}$ 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 isotope.

3. Individual line lists

An overview of the line lists in the ExoMol database is given in Fig. 1.

One general issue is that Medvedev and co-workers [165, 186] identified a numerical problem with the intensities of high overtone transitions computed with the standard compilation of the diatomic vibration-rotation program Level [187]. Our diatomic line lists computed with Level or Duo [188] have been adjusted to remove transitions affected by this issue. Medvedev *et al.* [189] recently identified similar issues with triatomic systems but tests suggest that in practice our triatomic line lists seem largely unaffected by the problem.

Below we consider some of the line lists presented in the ExoMol database and listed in Tables 1 and 2. We restrict our discussion to issues not covered in the ExoMol2016 release or the original publications. We start by considering the 42 molecules for which line lists have been created as part of the ExoMol series as listed in Table 1.

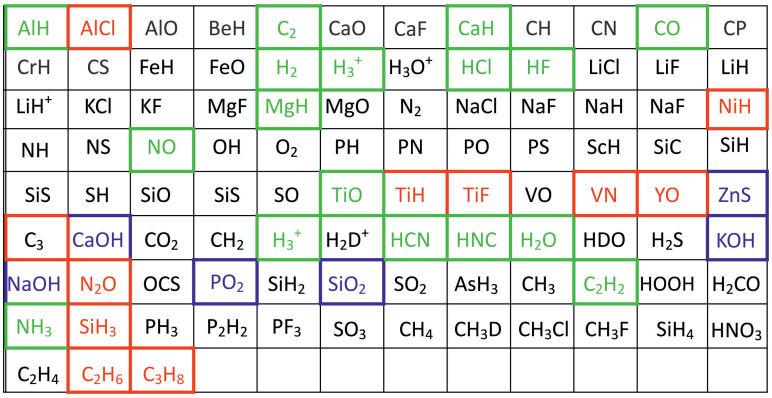

Figure 1: Molecular line lists: red indicates line lists in progress, blue corresponds to the line lists suggested for molecules specific for hot rocky exoplanets and green indicates line lists which contain data applicable for high resolution.

3.1. Diatomics

3.1.1. AlH, paper XVIII

There is a new AlHambra line list for AlH [122]. A MARVEL (measured active rotational-vibrational energy levels [190]) project was performed as part of this project meaning that many transitions are predicted with experimental accuracy. The AlHambra line list has been updated to give the uncertainty in the energy in the states file which allows users to determine the uncertainty in a given transition wavenumber.

3.1.2. AlO, paper IX

No change. The APTY line list was recently used to make a detection of AlO in an exoplanet atmosphere, the ultra-hot Jupiter exoplanet WASP-33 b [191] and hot Jupiter exoplanet WASP-43 b [192].

3.1.3. BeH, paper I

The BeH "Yadin" line list was one of the first constructed by ExoMol [94]; however, the line list only included transitions within the X $^2\Sigma^+$ ground electronic

state. Recently Darby-Lewis et al. [172] constructed line lists for BeH, BeD and BeT which consider both the ground and first excited (A $^2\Pi$) states. At the same time Darby-Lewis *et al.* performed a MARVEL analysis and used their empirical levels in the fit. The Darby-Lewis line list is therefore more accurate and more extensive than the Yadin one which it replaces in the ExoMol database and is therefore recommended. Yadin is still available on the website though renamed to Yadin-BeH in order to avoid conflict with the "Yadin" line lists for MgH and CaH, which remain to be recommended for the IR region.

3.1.4. C_2, paper XXXI

There are two new line lists for C_2 in the ExoMol2020 release: ExoMol 8state [124] and the empirical MoLLIST [159]. The MoLLIST line list only considers the much-observed Swan band while 8state covers the 8 band systems which interconnect the 8 lowest electronic states of C_2. As 8state uses empirical MARVEL energy levels [193] where available it should be as accurate as MoLLIST for the Swan band. Use of 8state is therefore recommended. Since MoLLIST line lists are recommended for other molecules and in order to avoid conflicts with the 'recommended' flag for 8states, the C_2 MoLLIST line list is now referenced to as MoLLIST-C2 on ExoMol.

An update of the C_2 MARVEL data has just been completed [194]; this has been used to improve the 8state energies and hence transition wavenumbers. This latest version includes uncertainties in the states file.

3.1.5. CaH, Paper I

The "Yadin" CaH line list only considers transitions within the X $^2\Sigma^+$ ground electronic state [94]. MoLLIST provides a rovibronic line list for the $X\,^2\Sigma^+$–$X\,^2\Sigma^+$, $A\,^2\Pi$–$X\,^2\Sigma^+$, $B\,^2\Sigma^+$–$X\,^2\Sigma^+$ and E $^2\Pi$ – X $^2\Sigma^+$ systems due to Li et al. [160], Shayesteh et al. [161], Ram et al. [195]. Both line lists are included in the

ExoMol database; work is in progress on creating a single unified line list which will extend the range of rovibronic transitions considered. In the meantime both line lists are recommended.

3.1.6. CaO, Paper XIII

No change.

3.1.7. CS, Paper XII

No change. We note that a line list for CS has also recently been supplied by Hou and Wei [196] and Xing et al. [197] have extended consideration to rovibronic transitions for the lowest, A $^1\Pi$ – X $^1\Sigma^+$, allowed electronic band.

3.1.8. KCl, Paper V

No change

3.1.9. MgH, Paper I

The ExoMol "Yadin" line list for MgH only considers transitions within the X $^2\Sigma^+$ ground electronic state [94]. MoLLIST provides a rovibronic line list containing A $^2\Pi$ – X $^2\Sigma^+$ and B′ $^2\Sigma^+$ – X $^2\Sigma^+$ transitions due to GharibNezhad et al. [151]. Both line lists are included in the ExoMol database; work is in progress on creating a single unified line list which will extend the range of rovibronic transitions considered. In the meantime both line lists are recommended.

3.1.10. MgO, Paper XXXII

There is a new LiTY line list for MgO [125].

3.1.11. NaCl, Paper V

No change.

3.1.12. NaH, Paper X

No change.

3.1.13. NO, XXI

There is a new NOName line list for NO [115]. This line list was constructed using a combination of standard ExoMol and empirical methodologies, and also included a MARVEL project. Its transition frequencies should therefore be close to experimental accuracy. NOName has largely been adopted for the new release of HITEMP [77].

NOName only covers transitions between levels which lie within the X $^2\Pi$ ground electronic state of NO. A new line list which includes ultraviolet rovibronic transitions of NO is currently being constructed.

3.1.14. PH, Paper XXXIV

There is a new LaTY line list for PH [127].

3.1.15. PN, Paper VI

No change. An extended line list covering visible and ultra violet (UV), accompanied by a MARVEL project is currently in progress.

3.1.16. PO, Paper XXIII

There is a new POPS line list for PO [117].

3.1.17. PS, Paper XXIII

There is a new POPS line list for PS [117].

3.1.18. SH, Paper XXXVI

There are two new ExoMol line lists for SH: SNaSH [120] which only covers transitions within the X $^2\Pi$ ground electronic state of SH and the newer GYT line list of Gorman et al. [129]. GYT considers both transitions within X $^2\Pi$ and vibronic transitions in the A $^2\Sigma^+$ – X $^2\Pi$ band system. As GYT also improves the accuracy of the X state transitions, it is recommended for all applications.

The SNaSH SH line list is also renamed to SNaSH-SH in order to avoid a conflict and retained only for completeness.

3.1.19. SiO, Paper II

The ExoMol SiO line lists only consider transitions within the X $^1\Sigma^+$ ground electronic state [95]; these line lists have been widely used including a recent determination of isotopologue ratios in Arcturus [198]. For this release of ExoMol, an empirical and less accurate SiO line list by Kurucz [81] covering the X–X, A–X and E–X electronic bands was added. Given the importance of SiO for lava planets [65], construction of a comprehensive (accurate and complete) rovibronic line list for SiO covering both IR and ultraviolet would be useful.

3.1.20. SiH, Paper XXIV

There is a new SiGHTLY line list for SiH [118].

3.1.21. SiS, Paper XXV

There is a new UCTY line list for SiS [119].

3.1.22. SN, Paper XXVI

There is a new SNaSH line list for SN [120].

3.1.23. TiO, Paper XXXIII

There is a new Toto line list for TiO [126]. The line list for the main isotopologue (^{48}Ti^{16}O) used empirical energies from an associated MARVEL study [199] while the energy levels of other isotopologues were improved using the procedure of Polyansky et al. [113]. The Toto line list has been updated to give MARVEL uncertainties, where available, in the States file. For other states the uncertainties were estimated as follows: 1 cm^{-1} for all levels in vibronic states that contain levels determined by MARVEL, 10 cm^{-1} for levels in those electronic states who

excitation energy (T_e/T_0) is known from experiment and 100 cm^{-1} for all other levels.

TiO is a particularly important species in the atmosphere of cool stars and has been detected in exoplanets [200, 201]. The Toto line list is significantly better at reproducing stellar spectra than the line lists due to Plez [202] and Schwenke [203] which it supersedes. Furthermore a recent study of Ti isotope abundances in two M-dwarf stars demonstrated the accuracy of the line lists for several isotopologues of TiO [42]. However, TiO remains a challenging system to treat using *ab initio* electronic structure methods (see McKemmish et al. [204]) and further work is required before there is a definitive line list for TiO.

3.1.24. VO, Paper XVIII

There is a new VOMYT line list for VO [112] which has been used to tentatively identify VO in the atmosphere of exoplanets [205, 206]. We note that VO spectra display particularly large splittings due to hyperfine effects as well as transitions which are only allowed due to these effects [207]. VOMYT does not include hyperfine effects in its spectroscopic model meaning that the line list unsuitable for high resolution studies. We plan to address this problem by both performing a hyperfine resolved MARVEL study and extending Duo to allow for hyperfine effects.

3.2. Triatomics

3.2.1. CO_2, Paper XXXIX

Line lists for hot CO_2 have been constructed by NASA Ames [173, 173] using methodologies similar to those employed by ExoMol. The CDSD-4000 hot line list due to Tashkun and Perevalov [184] and the room temperature line lists due to Zak et al. [181, 182, 183] are also available on the ExoMol website. The CDSD-4000 line list is based on the use of an effective Hamiltonian which tends to miss contributions from unobserved hot bands.

A new ExoMol line list UCL-4000 for CO_2 has been produced [132] using an accurate *ab initio* dipole moment surface (DMS) by Polyansky et al. [208] and empirical potential energy surface (PES) Ames-2016 by Huang et al. [209]; where possible computed energies have been replaced by empirical one derived from HITRAN. The UCL-4000 line list covers the wavenumber range 0–20000 cm^{-1} and should be applicable for temperatures up to 4000 K [132]. It is recommended for use in high temperature applications.

3.2.2. HCN/HNC, Paper III

The combined HCN/HNC ExoMol line list of Barber *et al* [96] made extensive use of empirical energy levels due to Mellau [210, 211]. This has enabled the line list to be successfully used in high-resolution Doppler spectroscopy studies of exoplanets [212–214].

3.2.3. H_2O, Papers XIX and XXX

Water is one of the most widely studied molecules and its spectrum has been detected in a variety of exoplanets, in many cases as the only clearly identifiable molecule [206, 215]. Good water line lists have been available for some time, in particular the Ames line list of Partridge and Schwenke [216] and the BT2 line list due to Barber et al. [178]. While BT2 was significantly more complete than Ames, the Ames line list was more accurate, particularly at infrared wavelengths. A new line list, known as POKAZATEL [61] has been generated by the ExoMol project. POKAZATEL is complete in the sense that it contains transitions between all bound rotation-vibration states in the molecule and thus is reliable for temperatures above 3000 K where the earlier line lists are not valid. POKAZATEL is also intrinsically more accurate than the Ames line list and, indeed, as many of its energy levels have been replaced by empirical energy levels generated using MARVEL [217], key transition frequencies are actually reproduced to

experimental accuracy. POKAZATEL should therefore be used in preference to the earlier line lists.

It has become apparent that the rotation-vibration spectrum of water is responsible for weak but observable near-UV absorption in the Earth's atmosphere [218]. The POKAZATEL line list, which used the *ab initio* LTP2001S DMS of Lodi et al. [219], appears to underestimate the strength of water absorption in the blue and near-UV. As a response to this Conway and co-workers have recently developed a more accurate global dipole moment surface [220]. Through a significant number of comparisons against high quality experimental and theoretical sources of spectroscopic data [221, 222], their results suggest there may be advantages of using their line lists in particular regions, primarily at short wavelengths. For this reason, a new room temperature $H_2{}^{16}O$ line list called WAT_UV296 [185] has been computed. This line list is available on the website and should be used for room temperature studies of spectra with $\lambda < 0.5$ μm. A high temperature companion to this line list will form the basis of the updated HITEMP database [79].

Polyansky et al. [113] provided the HotWat78 line lists for $H_2{}^{17}O$ and $H_2{}^{18}O$. The energy levels of this line list were improved using MARVEL energies [223, 224]. Furthermore, Polyansky et al. [113] developed a method which gives excellent isotopologue energy levels for states only observed for $H_2{}^{16}O$. Finally the VTT line list due to Voronin et al. [136] remains the recommended one for HDO; a new, improved HDO line list is currently under construction [225].

A new room temperature line list CKYKKY for H_2O containing electric quadrupole moments was computed using an *ab initio* quadrupole moment surface [226] and accurate empirical PES by Mizus et al. [227] with the variational program TROVE [228]. The energies were replaced by the H_2O IUPAC MARVEL values [217] or HITRAN values [229], if available.

3.2.4. H_2S, Paper XVI

There is a new ExoMol AYT2 line list for hydrogen sulphide due to Azzam et al. [110]. Since completion of this line list a MARVEL project has been performed for H_2S [230]; the AYT2 line list is being updated to use these improved energy levels.

3.2.5. H_3^+

The new ExoMol MiZATeP line list of Mizus et al. [114] replaces that of Neale et al. [177] (NMT). The new line list uses empirical energy levels from the MARVEL study of Furtenbacher et al. [231]. Astronomy makes wide use of H_3^+ line lists and is reliant on *ab initio* line intensities since no absolute line intensities have been measured in the laboratory, see Petrignani et al. [232]. This astronomical work on H_3^+ has recently been reviewed by Miller et al. [233]. The ST H_2D^+ line list due to Sochi and Tennyson [135] plus the newly generated $D_3{}^+$ and D_2H^+ line lists will be MARVELised and released in the near future.

3.2.6. SO_2, Paper XVII

The ExoAmes line list for SO_2 [193] is unchanged since the ExoMol2016 release. However, a MARVEL set of energy levels for SO_2 are now available [234] and will be used to update ExoAmes in the near future.

3.3. Tetratomics

3.3.1. HCCH, Paper XXXVII

The new aCeTY line list for acetylene due to Chubb et al. [130] has recently been released. This line list already incorporated the MARVEL energies of Chubb et al. [235] and gives uncertainties in the energy levels as part of the States file.

3.3.2. H_2CO, Paper VIII

The AYTY formaldehyde line list [102] is in the process of being updated with empirical energy levels produced by a recent MARVEL study [236]; this will make the line list suitable for high resolution studies.

3.3.3. H_2O_2, Paper XV

There is a new ExoMol APTY line list for hydrogen peroxide [237]. We note because of difficulties with assigning spectra, even at room temperature HITRAN is very incomplete for H_2O_2. APTY should give complete coverage at infrared wavelengths. Recently APTY was used to suggest the importance of H_2O_2 as a greenhouse gas on oxidised Early Mars [238].

3.3.4. H_3O^+, Paper XL

A line list for the hydronium ion, H_3O^+, has recently been constructed [133] in response to a laboratory study by Bourgalais et al. [239] which suggested both that hydronium is likely to be a dominant molecular ion in gaseous exoplanets and that it should be detectable by upcoming space missions.

3.3.5. NH_3, Paper XXXV

A new ExoMol line list for ammonia called CoYuTe [128] has recently been completed. CoYuTe, which also uses MARVEL energy levels [188], is both more accurate and more extensive than the BYTe line list [179] it replaces. In particular, CoYuTe was found to provide a good model of the Jovian optical absorption spectrum due to ammonia [34] although with a shift in positions of the main bands. More laboratory work or analysis of existing laboratory work on the visible spectrum of ammonia will be required to resolve this issue. An illustration of the ammonia absorption cross sections computed using CoYuTe is given in Fig. 2.

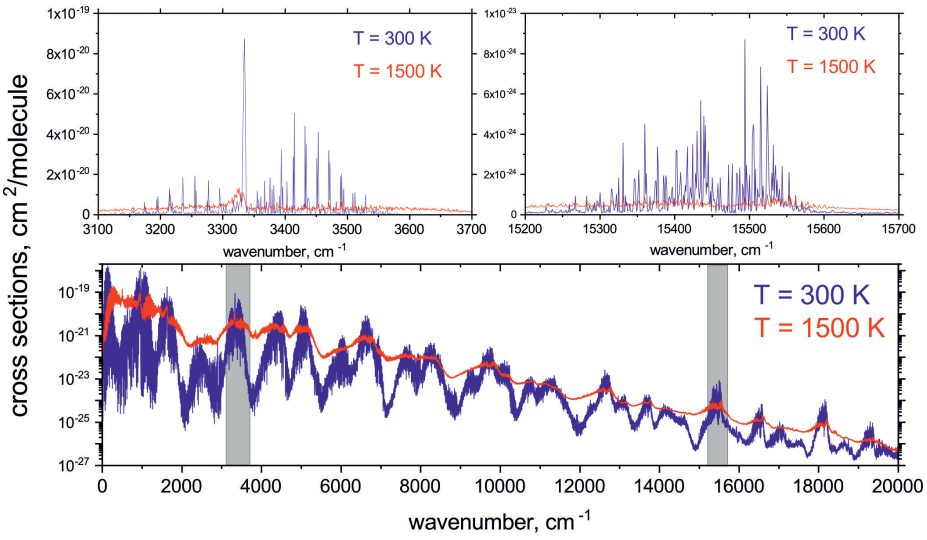

Figure 2: Absorption cross sections generated using the ExoMol line list CoYuTe for spectrum of NH_3 at $T = 300$ K and 2000 K, with the Doppler profile on a wavenumber grid of 1 cm^{-1}. The cross sections were computed using the ExoCross program, which is developed to work with two file line list structure adopted by ExoMol.

3.3.6. PH_3, Paper VII

No change. Sousa-Silva et al. [240] use the SAlTY PH_3 line list to assess the detectability of a possible PH_3 biosignature. A MARVEL project on the PH_3 experimental data is under way, which will improve the quality of the line positions in SAlTY.

3.3.7. SO_3, Paper XVII

There is a new UYT2 line list for SO_3 [111].

3.4. Pentatomics

3.4.1. CH_3Cl, Paper XXIX

There are new OYT line lists for methyl chloride [123] covering both major isotopes of chlorine.

3.4.2. CH_4, Paper IV

The ExoMol YT10to10 line list [97] has been extended to higher temperatures [98] to give the YT34to10 line list. However, at present the TheoReTS line list of Rey et al. [241] is the most accurate methane line list available and is recommended for detailed studies. This line list forms the basis of the very recent update to HITEMP [78].

The importance of methane and the huge number of lines required to accurately represent the opacity of hot methane [31] has led to this system being the primary focus of studies aimed at compacting these lines into a more manageable form [98, 242, 243]. This issue is discussed in section 5.3.2.

3.4.3. HNO_3, Paper XI

No change. We note that, like H_2O_2, because of difficulties with assigning spectra even at room temperature, HITRAN is very incomplete for nitric acid. The AlJS line list gives complete coverage at infrared wavelengths.

3.4.4. SiH_4, Paper XXII

There is a new OY2T line list for silane [116].

3.5. Larger molecules

3.5.1. C_2H_4, Paper XXVII

There is a new MaYTY line list for ethylene [121].

3.6. MoLLIST species

A number of diatomic species have line lists provided by the MoLLIST website [82]. These have been incorporated into the ExoMol database, which now includes empirically-derived line lists for the following species [83]: CH [139]; NH [140–142]; OH [143]; AlCl [144]; AlF [144]; OH^+ [145, 146]; CaF [147]; MgF [148]; KF and NaF [149]; LiCl and LiF [150]; MgH [151]; TiH [152]; CrH [153]; FeH [154]; CP [157]; CN [158]; and CaH [160, 161]. See Table 2 for further details.

3.7. HITRAN

In general the line lists contained in the HITRAN database [229] do not provide the temperature coverage needed for astrophysical applications. However, for a few diatomic species very extensive line lists have been constructed. The line lists presented by Li et al. [156] for HCl and Li et al. [165] for CO are both valid over an extended temperature range and have been included in the ExoMol database.

The HF line list from Li et al. [244] and Coxon and Hajigeorgiou [155] is also adopted directly from HITRAN.

3.8. N_2

The empirical WCCRMT nitrogen molecule line list of Western et al. [162] is somewhat unusual in that it only considers transitions between excited, triplet states of the molecule. However, N_2 is an important molecule with very limited spectral signature at long wavelengths and WCCRMT may prove useful in hot or irradiated, usually non-LTE environments. For the partition function of N_2 the ground electronic state data from TIPS [245] were used.

3.9. HD, HD^+, HeH^+

One and two electron diatomics are important primordial species and may well play a role elsewhere. Recently Amaral et al. [166] created new line lists using high level *ab initio* procedures. These line lists have been included in the database with the name ADSJAAM. In particular the ADSJAAM line lists for HeH^+ and HD supersedes those due to Engel et al. [180] and Coppola et al. [164], respectively.

3.10. H_2

A new external line list RACPPK by Roueff et al. [138] for the ground electronic state of H_2 was converted to the ExoMol format. The line list contains

a combination of electric quadrupole and magnetic dipole transitions computed from first principles.

3.11. Other ab initio line lists

A number of other *ab initio* line lists are also available. In general *ab initio* line lists are only accurate for systems with very few electrons. The CLT line lists for LiH and LiH^+ due to Coppola et al. [164] fall into the few-electron category and should be reliable. The other *ab initio* line lists provided, namely those for ScH [163], CH_3F [167], AsH_3 [168], P_2H_2 [169], PF_3 [170], CH_3 [171] and YO [176] must be regarded as intrinsically less accurate than other line lists provided by the database. In the case of YO, work is in progress aimed at producing an empirical line list based on available experimental data. P_2H_2 occurs as two distinct isomers, the cis and trans forms. Separate line lists are provided for cis-P_2H_2 and trans-P_2H_2.

3.12. SiH_2

A new line list for SiH_2 [175] has been recently constructed in its ground electronic state using the standard ExoMol technology [93]. The set of experimental data or their quality were, however, very limited which may affect the quality of the hot bands, which basically has to rely on the quality of the *ab initio* PES.

3.13. NiH

Empirical line lists for three isotopologues of NiH (^{58}NiH, ^{60}NiH, ^{62}NiH) known as HRV. These line lists were constructed by Vallon et al. [246] and Harker et al. [247]. However, at present these line lists are not available in ExoMol format or accessible through the API.

3.14. Partition functions

The temperature dependent partition functions for most of the ExoMol line lists are computed using the corresponding energy levels as collected in the States files as

$$Q(T) = \sum_i g_{\rm ns}^{(i)} J_i(J_i+1) \exp\left(-\frac{c_2 \tilde{E}_i}{T}\right), \quad (1)$$

where $g_{\rm ns}^{(i)}$ is the state dependent nuclear statistical weight, J_i is the total angular momentum of the state i, c_2 is the second radiation constant (K cm) and $\tilde{E}_i$ is the corresponding energy term value (cm^{-1}). ExoMol uses the HITRAN convention [248], where the entire, integer $g_i = g_{\rm ns}^{(i)} J_i(J_i+1)$ factors are explicitly included.

Some of the line lists in the ExoMol database do not provide sufficiently complete sets states for a proper evaluation of the molecular partition functions. For example, most of the MoLLIST line lists are constructed from or based on the measured data only and therefore can be severely incomplete. In these cases the partition functions are either taken from external sources, such as the TIPS database [245], generated using the empirical expansions, such as by Irwin [249], Sauval and Tatum [250], Irwin [251], Barklem and Collet [252] or extrapolated using simplified models [253]. The external partition functions often include the $g_{\rm ns}^{(i)}$ factors in the astrophysical convention (see, e.g. Pavlenko et al. [198]) and therefore have to be transformed to the HITRAN convention.

We strongly recommend that users use these partition functions rather than attempting to compute their own using the ExoMol States files. These States files are not constructed with a view to delivering reliable partition functions and in a number of cases use of them has been found to lead to problems.

3.15. VUV sections

A section is provided based on measured ultraviolet cross sections for key species. For many molecules their ultraviolet spectrum is a mixture of line and

quasi-continuum absorption which cannot be represented as a line list. The new VUV section will provide temperature-dependent absorption cross sections. Recent results suggest the VUV absorption by H_2O enhances the production of OH, which plays an important molecule in atmospheric chemistry of exoplanetary atmospheres [254]. Currently, the VUV cross sections are provided for H_2O, H_2, CO_2, SO_2, NH_3, H_2CO and C_2H_4 measured by Fateev's lab at the Danish Technical University (DTU) [255] and for CO_2 by Venot et al. [256]. The temperature and wavelength coverage is illustrated in Table 4.

The cross sections are given in the common two-column ASCII format separated by spaces, where the first column contains the wavelength in nm and the second column contains the absorption cross sections in cm^2/molecule using Fortran format: `(F10.3,1x,E13.6)`. The VUV cross section file names have the following structure

`'<ISOTOPOLOGUE>__<DATASET>__<RANGE>__T<TEMP>K__P<PRESSURE>bar__<STEP>.nm'`,

where `ISOTOPOLOGUE` is the isotopologue name, `DATASET` is the name of the line list, `RANGE` is the wavelength range in nm, `TEMP` is the temperature in K, `PRESSURE` is the pressure in bar, `STEP` is the wavelength step in nm. For example, the States file of the VUV line list for CO_2 the filename:

`12C-12O2__Venot-2018__116.90-230.00__T0800K__P0bar__0.03.nm`.

Table 4: VUV absorption cross sections on ExoMol, grid spacing 0.01–0.015 nm, presented in natural abundance.

Molecule	Temperature (K)	Range (nm)
DTU data		
H_2O	423	110–230
H_2O	573	110–230
H_2O	1630	182–237
H_2O	1773	182–237
CO_2	1160	109–324
SO_2	423	110–230
NH_3	289	113–201
NH_3	296	113–201
H_2CO	303	110–230
H_2CO	353	110–230
H_2CO	423	110–230
H_2CO	573	110–230
C_2H_4	562	113–201
Venot et al. [256]		
CO_2	170–800 K	115-220

4. Data Provided

Table 5 provides a summary of different types of data provided. The website provides two routes to accessing these data. Users can search by molecule which will show all the types of data available for each isotopologues. Alternatively it is possible to search by data type in which case a list of molecules for which data of the specified type is available. The following section lists the data types and their file name extensions for the various data and metadata provided by ExoMol. A

more technical specification of the data structures and how to access data using the application program interface (API) is provided in Section 5.

Table 5: Summary of data provided by the ExoMol Database

Data type
Line lists
Absorption cross sections
VUV absorption cross sections
Pressure broadening coefficients
Temperature dependent super-lines (histograms)
Partition functions
Cooling functions
Specific heat - heat capacity
Examples of ExoCross input files
Temperature and pressure dependent opacities
Spectroscopic Models

Table 6: Specification of the ExoMol file types. (Contents in brackets are optional.)

File extension	$N_{\rm files}$	File DSname	Contents
`.all`	1	Master	Single file defining contents of the ExoMol database..
`.def`	$N_{\rm tot}$	Definition	Defines contents of other files for each isotopologue.
`.states`	$N_{\rm tot}$	States	Energy levels, quantum numbers, lifetimes, (Landé g-factors, Uncertainties).
`.trans`	[a]	Transitions	Einstein A coefficients, (wavenumber).
`.broad`	$N_{\rm mol}$	Broadening	Parameters for pressure-dependent line profiles.
`.cross`	[b]	Cross sections	Temperature or temperature and pressure-dependent cross sections.
`.kcoef`	[c]	k-coefficients	Temperature and pressure-dependent k-coefficients.
`.pf`	$N_{\rm tot}$	Partition function	Temperature-dependent partition function, (cooling function).
`.dipoles`	$N_{\rm tot}$	Dipoles	Transition dipoles including phases.
`.super`	[d]	Super-lines	Temperature dependent super-lines (hisograms) on a wavenumber grid.
`.nm`	[e]	VUV cross sections	Temperature and pressure dependent VUV cross-sections (wavelength, nm).
`.fits`, `.h5`, `.kta`	[f]	Opacities	Temperature and pressure dependent opacitities for radiative-transfer applications.
`.overview`	$N_{\rm mol}$	Overview	Overview of datasets available.
`.readme`	$N_{\rm iso}$	Readme	Specifies data formats.
`.model`	$N_{\rm iso}$	Model	Model specification.

$N_{\rm files}$ total number of possible files;
$N_{\rm mol}$ Number of molecules in the database;
$N_{\rm tot}$ is the sum of $N_{\rm iso}$ for the $N_{\rm mol}$ molecules in the database;
$N_{\rm iso}$ Number of isotopologues considered for the given molecule.
[a] There are $N_{\rm tot}$ sets of `.trans` files but for molecules with large numbers of transitions the `.trans` files are subdivided into wavenumber regions.
[b] There are $N_{\rm cross}$ sets of `.cross` files for isotopologue.
[c] There are $N_{\rm kcoef}$ sets of `.kcoef` files for each isotopoplogue.
[d] There are N_T sets of T-dependent super-lines. [e] There are N_{VUV} sets of VUV cross sections. [f] Set of opacity files in in the format native to specific radiative-transfer programs.

The general ExoMol approach is molecule-by-molecule: a comprehensive line list is created for a particular molecule and made available in the database. The line list for each isotopologue is stored as a separate data structure which can be accessed directly or via the application program interface (API) described in the following sections. Table 6 specifies the file types that can be available for each isotopologue. The `.states` and `.trans` files are the heart of the ExoMol data structure [257] and define what has become known as the "ExoMol format". These files are available for all isotopologues; other files may not be. ExoMol format files can be used and provided by the effective Hamiltonian code PGOPHER [258].

A manual providing technical specifications of the database is included as

supplementary data to this article and is included on the website where it will be updated as the data base evolves. Only the relatively few changes that have been implemented since the 2016 release are discussed below.

4.2. Super-lines

Super-lines [80, 98] represent a novel, compact way of storing the opacity data. Super-lines are constructed as temperature-dependent intensity histograms by summing all absorption coefficients within a wavenumber bin centred around a grid point $\tilde{\nu}_k$. For each $\tilde{\nu}_k$ the total absorption intensity $I_k(T)$ is computed as a sum of absorption line intensities I_{if} from all $i \to f$ transitions falling into the wavenumber bin $[\tilde{\nu}_k - \Delta\tilde{\nu}_k/2 \ldots \tilde{\nu}_k + \Delta\tilde{\nu}_k/2]$ at the given temperature T. Each grid point $\tilde{\nu}_k$ is then treated as a line position of an artificial transition (super-line) with an effective absorption intensity $I_k(T)$. The number of data points in the super-lines can be drastically reduced without significant loss of accuracy when computing pressure-dependent cross sections and can be combined with standard, pressure, temperature and frequency dependent line profiles. The super-lines cannot be associated with any specific upper/lower states and therefore the line broadening parameters used cannot depend on quantum numbers.

The super-line list files have the format of cross sections represented by two columns, wavenumbers (cm^{-1}) and super-line absorption intensity (cm/molecule). The Fortran format is `(F12.6,1x,ES14.8)`. The super-lines are computed on a grid of temperatures from 100 K to T_{max}. For the resolution an adaptive grid of $R = 1\,000\,000$ is used. For the technical details of super-line construction and numerical tests see Yurchenko et al. [98].

Super-lines are currently available for H_2O, NH_3, CH_3Cl, C_2H_2 and C_2H_4.

4.3. Specific heat

The specific heat at constant pressure C_p is computed on a grid of temperatures of 1 K from the molecule partition function as given by [259]

$$C_p(T) = R\left[\frac{Q''}{Q} - \left(\frac{Q'}{Q}\right)^2\right] + \frac{5R}{2}, \tag{2}$$

where the second term is the translational contribution,

$$Q'(T) = T\frac{dQ}{dT},$$

$$Q''(T) = T^2\frac{d^2Q}{dT^2} + 2Q' \tag{3}$$

and R is the gas constant. The specific heat values are given in units of J mol^{-1} K^{-1} and are currently provided for H_2O (taken from Furtenbacher et al. [259]) and CH_4 (computed using the YT10to10 ro-vibrational energies [97]) only (see Fig. 3).

4.4. Line shifts using the diet format

For high resolution applications it will be important to take into account the pressure dependent line shifts. To this end a line shift diet has been introduced using the same data structure used for pressure dependent line broadening diet [260]. An example for H_2O is given in Table 7.

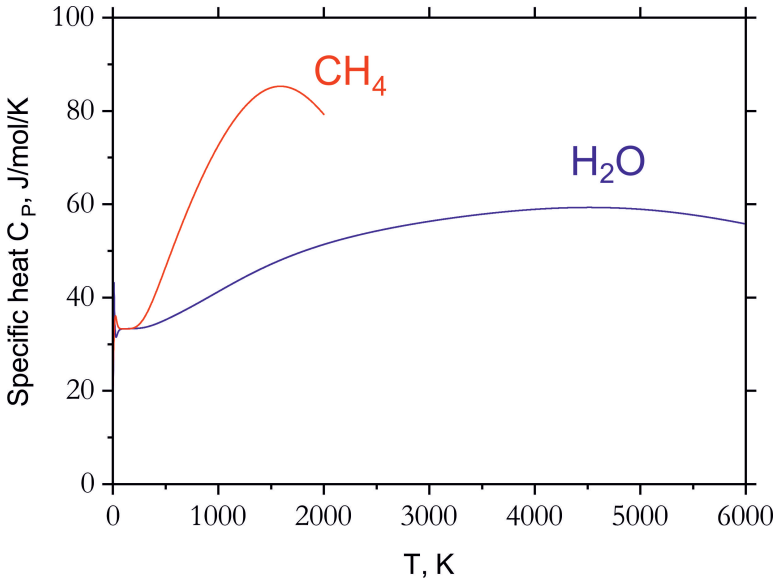

Figure 3: Specific heat at constant pressure of H_2O as computed by Furtenbacher et al. [259] and CH_4 generated the YT10to10 ro-vibrational energies [97].

Table 7: File `1H-16O2__a0.shift` A pressure line `.shift` file for H_2O: portion of the file (upper part); field specification (lower part).

Code	Shift	J
a0	0.0001	0
a0	0.0001	1
a0	0.0001	2
a0	0.0001	3
a0	0.0001	4
...	...	...

Field	Fortran Format	C Format	Description
code	A2	%2s	Code identifying quantum number set following J''*
γ_{ref}	F15.6	%15.6f	Line shift at reference temperature and pressure in cm^{-1}
J''	I7/F7.1	%7d	Lower J-quantum number

*Code definition: a0 = none

4.5. New broadening parameters

The pressure broadening parameters are provided for 15 molecules and are listed in Table 8 using the pressure-broadening diet [260].

The `.broad` file has a hierarchical structure; each record starts with four compulsory columns: a label defining the broadening scheme ('a0', 'a1', ...), values of $\gamma_{\rm ref}$, n and J''. The compulsory fields are followed by additional quantum numbers when a more detailed specification of the quantum assignments is available. The most basic scheme 'a0' represents broadening with J'' dependence only. The additional basic scheme 'a1' is used for the case with the (J', J'') dependence. Any other schemes (e.g. 'a2', 'a3', 'a4', 'b1', 'b2', 'c1', 'c2') are the molecule specific and should be described as part of the line list specifications. The broadening data format is illustrated in Table 9.

The requirement for enhanced line broadening parameters was identified by Fortney et al. [261] is their study on the need for laboratory data requirements for studies of exoplanetary atmospheres. Recognising this, our plan is significantly enhance the treatment pressure effects in future releases of the ExoMol database.

Table 8: Pressure broadening parameters in ExoMol

Molecule	Broadener	Scheme
CS	air, self	a0
HCl	H_2, He, self, air, CO_2	a0
HF	H_2, He	a0
CO	H_2, He	a0
NO	air	a0
H_2O	H_2, He, self, air	a0,a1
CO_2	air, self	a0
SO_2	H_2, He	a0, a5
HCN	He, He	a0
OCS	He, He	a0
PH_3	He, He	a0, c1
NH_3	He, He	a0
H_2CO	He, He	a0
C_2H_2	He, He	a0
CH_4	He, He, CO_2	a0, a1

Table 9: Example of the three basic broadening schemes in the ExoMol diet, 'a0', 'a1', 'a2'.

Label	γ	n	J''	J'	K
a0	0.0860	0.096	0		
a0	0.0850	0.093	1		
...					
a1	0.0860	0.096	0	1	
a1	0.0850	0.093	1	2	
...					

4.6. ExoMolOP: Opacities

Recently Chubb et al. [262] computed opacity cross sections and k-tables for all molecules available from the ExoMol database plus some atomic data from NIST. These data are formatted for use in various retrieval codes including Tau-REx [13–15], ARCiS [24], petitRADTRANS [28], and NEMESIS [17]. Data were calculated on temperature-pressure grids suitable for characterising a variety of exoplanet and stellar atmospheres. Broadening parameters were taken from the literature where available, with broadening parameters used for a known molecule with a similar dipole moment, where they are not available. Tables of cross sections and k-coefficients are provided on ExoMol as part of the line list webpage. The format of the data and the resolution (grid spacing) is application dependent, for example the opacities for ARCiS, petitRADTRANS, and NEMESIS are given as k-tables at the resolving power of R= 1000 while Tau-REx works with cross-sections with $R = 15\,000$.

The opacity cross sections and k-tables will also be made available via the virtual atomic and molecular data centre (VAMDC) portal [263, 264]. We note that ExoMol data has also been extensively used to construct the EXOPLINES molecular absorption cross-Section database for brown dwarf and giant exoplanet atmospheres [265].

4.7. Post-processing

ExoMol provides post-processing capabilities through the program ExoCross [266]. ExoCross has many functions such as generating pressure and temperature dependent cross sections, partition functions, specific heat, state-resolved radiative lifetimes, non-LTE spectra, electric dipole, electric quadrupole and magnetic dipole spectra. ExoCross can read data in both ExoMol and HITRAN [267] formats and output it in these formats as well as SPECTRA (`http://spectra.iao.ru/`) and Phoenix formats [16]. Should data be needed in say

HITRAN format, it is strongly recommended that the data is downloaded to a local computer in the much more compact ExoMol format and then processed using ExoCross. Examples of ExoCross input files are provided on the website.

There are also a number of Python utilities available on the ExoMol website. These are now largely redundant as ExoCross provides all functionality required to work with ExoMol line lists. However, we mention them for completeness: Utility `extract__trans.py` reads the `.trans` in `.bz2` format without requiring it to be uncompressed. The `ExoMol_to_HITRAN.py` script converts ExoMol format to HITRAN format; this should be used with caution as ExoMol format is significantly more compact than HITRAN format and the line list files are large. The program `exomol2gf.py` can be use to generate oscillator strengths.

4.8. New web services

New web services include:

- A molecule and line list search.
- A graphical illustration of a line list represented by absorption spectra at two or three temperatures (e.g. 300 K, 2000 K and 5000 K) computed using a Doppler line profile on a grid of 1 cm^{-1}.
- The ExoMol bibliography in the BibTeX format is stored at and version controlled by GitHub at `https://github.com/ExoMol/bib`.

5. ExoMol data formats and API

5.1. Format of the `states` and `trans` files

The formats of the States and Transitions files are specified in Table 10 and 11. Tables 12 and 13 show typical examples of the States (.states) and Transitions (.trans) files. A significant new feature of the 2020 update is the uncertainty field

(cm^{-1}) in the States file appearing as column 5 after the J values; this currently an optional feature but will become a compulsory column for the ExoMol States file. The uncertainty values typically come from three different sources: (i) the uncertainties of the MARVEL energies (∼0.000001–0.1 cm^{-1}), (ii) uncertainties obtained as the fitting observed – calculated error of energies as part of the refinement to experimental data (energies or line positions) participated in the refinement (∼ 0.001 – 1 cm^{-1}) and (iii) roughly estimated uncertainties for all other states that cannot be verified against existing experiment (∼ 0.1 – 10 cm^{-1}). The uncertainty in the States file are given using the same format as the energy term values, i.e. with six decimal places after the decimal point, see Table 10.

To date the new standard of the States file has being applied to the only a number of key/ recent line lists namely H_2O (POKAZATEL) [61], AlH (AlHambra) [122], C_2 8states [124, 194], HCCH (aCeTY) [130], CO_2 (UCL-4000) [132], H_3O^+ (eXeL) [133] and TiO (Toto) [126]. A rolling programme is in place for updating the other files so the uncertainty is uniformly available for all sources.

Table 10: Updated specification of the ExoMol States file.

Field	Fortran Format	C Format	Description
i	`I12`	`%12d`	State ID
E	`F12.6`	`%12.6f`	State energy in cm^{-1}
$g_{\rm tot}$	`I6`	`%6d`	State degeneracy
J	`I7/F7.1`	`%7d/%7.1f`	J-quantum number (integer/half-integer)
(ΔE)	`F12.6`	`%12.6f`	Energy uncertainty in cm^{-1} (currently optional)
(τ)	`ES12.4`	`%12.4e`	Lifetime in s (optional)
(g)	`F10.6`	`%10.6f`	Landé g-factor (optional)
(Extra)	-	-	Extra quantum numbers, any format (optional)

Table 11: Specification of the Transitions file.

Field	Fortran Format	C Format	Description
i	`I12`	`%12d`	Upper state ID
f	`I12`	`%12d`	Lower state ID
A	`ES10.4`	`%10.4e`	Einstein A coefficient in s^{-1}
$\tilde{\nu}_{fi}$	`E15.6`	`%15.6e`	Transition wavenumber in cm^{-1} (optional).

Table 12: An example of an extract from the final States file for UCL-4000 of CO_2 [132].

i	$\tilde{E}$	$g_{\rm tot}$	J	unc.	Γ	e/f	n_1	$n_2^{\rm lin}$	l_2	n_3
1	0.000000	1	0	0.000500	A1	e	0	0	0	0
2	1285.408200	1	0	0.000500	A1	e	0	2	0	0
3	1388.184200	1	0	0.005000	A1	e	1	0	0	0
4	2548.366700	1	0	0.000500	A1	e	1	2	0	0
5	2671.142957	1	0	0.005000	A1	e	2	0	0	0
6	2797.136000	1	0	0.005000	A1	e	1	2	0	0
7	3792.681898	1	0	0.005000	A1	e	1	4	0	0
8	3942.541358	1	0	0.005000	A1	e	3	0	0	0
9	4064.274256	1	0	0.005000	A1	e	3	0	0	0
10	4225.096148	1	0	0.005000	A1	e	1	4	0	0
11	4673.325200	1	0	0.000500	A1	e	0	0	0	2
12	5022.349428	1	0	0.005000	A1	e	1	6	0	0
13	5197.252900	1	0	0.005000	A1	e	3	2	0	0
14	5329.645446	1	0	0.005000	A1	e	4	0	0	0
15	5475.553054	1	0	0.000500	A1	e	3	2	0	0
16	5667.644584	1	0	0.005000	A1	e	2	4	0	0
17	5915.212302	1	0	0.000500	A1	e	0	2	0	2

i: State counting number.

$\tilde{E}$: State energy in $\rm cm^{-1}$.

$g_{\rm tot}$: Total state degeneracy.

J: Total angular momentum.

unc.: Uncertainty in $\rm cm^{-1}$.

Γ: Total symmetry index in $\mathcal{C}_{2\rm v}$(M).

e/f: Kronig rotationless parity.

n_1: Normal mode stretching symmetry (A_1) quantum number.

$n_2^{\rm lin}$: Normal mode linear molecule bending (A_1) quantum number.

l_2: Normal mode vibrational angular momentum quantum number.

n_3: Normal mode stretching asymmetric (B_1) quantum number.

Table 13: Extract from the Transitions file for CaO.

f	i	A_{fi}	$\tilde{\nu}_{fi}$
10571	10884	9.5518E-06	120.241863
21053	21375	1.9515E-05	120.242886
8726	9672	1.8658E-04	120.243522
11655	11950	5.0065E-06	120.243733
93209	93967	5.7055E-03	120.244192
2228	3175	7.3226E-07	120.244564
46727	46432	1.0599E-04	120.244658
44436	44774	1.4626E-04	120.245583
29037	28723	1.8052E-04	120.245669
4458	4805	1.0431E-08	120.246396
69313	68434	5.0531E-06	120.248178
22640	22985	1.1281E-07	120.248891
57027	56721	7.1064E-06	120.250180

f: Upper state counting number; i: Lower state counting number; A_{fi}: Einstein-A coefficient in s^{-1}; $\tilde{\nu}_{fi}$: transition wavenumber in cm^{-1}.

5.2. Formats for other data types

Table 14 shows the format of the `.broad` files containing the line broadening parameters. Table 15 shows the format of the cross section `.cross` and superlines `.super` files. Tables 16 and 17 show the format of the partition function `.pf` and specific heat `.cp` files.

Table 14: Specification of the mandatory part of the pressure broadening parameters file.

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	F6.3	%6.3f	Temperature exponent
J''	I7/F7.1	%7d/%7.1f	Lower J-quantum number integer/half-integer

Fortran format, J integer: `(A2,1x,F6.4,1x,F6.3,1x,I7)`

or J half-integer: `(A2,1x,F6.4,1x,F6.3,1x,F7.1)`

Table 15: Specification of the `.cross` cross section and `.stick` file format

Field	Fortran Format	C Format	Description
$\tilde{\nu}_i$	`F12.6`	`%12.6f`	Central bin wavenumber, cm^{-1}
σ_i	`ES14.8`	`%14.8e`	Absorption cross section, $\mathrm{cm}^2\,\mathrm{molec}^{-1}$
α_i	`ES14.8`	`%14.8e`	Absorption coefficient, $\mathrm{cm\,molec}^{-1}$

Fortran format: `(F12.6,1x,ES14.8)`

Table 16: Specification of the `.pf` partition function file.

Field	Fortran Format	C Format	Description
T	`F8.1`	`%8.1d`	Temperature in K
$Q(T)$	`F15.4`	`%15.4d`	Partition function (dimensionless).
$W(T)$	`ES12.4`	`%12.4e`	Cooling function in ergs s^{-1} $\mathrm{molecule}^{-1}$ (if available).

Fortran format: `(F8.1,1x,F15.4,1x,ES12.4)` or `(F8.1,1x,F15.4)`

Table 17: Specification of the `.cp` specific heat file.

Field	Fortran Format	C Format	Description
T	`F8.1`	`%8.1d`	Temperature in K
$C_p(T)$	`F15.4`	`%15.4d`	Specific heat function (dimensionless).

Fortran format: `(F8.1,1x,F15.4)`

5.3. API

5.3.1. Searching for data through the API

The molecules and isotopologues available in ExoMol are listed in a master file located at: `www.exomol.com/exomol.all`. Given a molecule or list of isotopologues, ExoMol can be searched for recommended datasets using the API which can be queried using the `HTTP GET` request method described below. The structure of a JSON file is illustrated in Fig. 4.

```
{<ISOTOPOLOGUE>:
    {'<DATATYPE>':
        {'<DATASET>':
            'description': <DATASET-DESCRIPTION>,
            'files': [{'description': <FILE-DESCRIPTION>,
                       'url': <URL>,
                       'size': <SIZE>
                      },
                      ...
                     ]
        },
        {'<DATASET>':
            ...
        },
        ...
    },
    {'<DATATYPE>':
        ...
    },
    ...
},
{<ISOTOPOLOGUE>:
    {
    ...
    }
}
```

Figure 4: A JSON API structure used for search queries using the `HTTP GET` request in ExoMol.

To search for all data sets (and their files) related to a single molecule, use the query:

`http://exomol.com/api?molecule=<MOLECULE>`

For example, the URL `http://exomol.com/api?molecule=NH3` returns a JSON data structure describing all files related to the ammonia molecule. Within this, the list of files belonging to the BYTe-15 line list for $^{15}N^{1}H_3$ is accessible by traversing the JSON object with:

`json_result['(15N)(1H)3']['linelist']['BYTe-15']['files']`

and the URL for the States file belonging to this line list is at:

`jsonresult['(15N)(1H)3']['linelist']['BYTe-15']['files'][1]['url'].`

Note that molecules are identified by simple text strings (no subscript or superscript symbols) but that special characters must be URL-encoded: for example, the HeH^+ cation is identified by `molecule=HeH%2B`. Most software will provide this "percent-encoding" automatically.

Searches can be further refined by isotopologue by setting the query keyword `isotopologues` to a comma-delimited sequence; for example:

`http://exomol.com/api/?isotopologues=(12C)(32S),(12C)(34S)`

Restricting the search by datatype is also supported:

`http://exomol.com/api/?molecule=H2O&datatype=linelist`

returns the details of linelists for the isotopologues of water, omitting partition functions, cooling functions, opacities, etc. Valid values for the `datatype` parameter are: `linelist`, `energylevels`, `opacity`, `super` ("Super" line lists), `Cp` (heat capacity), `broadening_coefficients`, `coolingfunction`, `partitionfunction`.

5.3.2. Accessing the data via the API

There are a number of ways of accessing the data. First, all data sets are available on the ExoMol website (`www.exomol.com`) and can be downloaded manually. Many ExoMol line lists contain in excess of 10 billion transitions. In this case the file of transitions are generally split into chunks in frequency. These files are compressed using `.bz2` format.

However, if multiple datasets are required manual downloads are inefficient. The systematic structure of the ExoMol database filesystem allows for automated downloads from within software or using utilities such as `wget` and `curl`. As described in detail in the ExoMol2016 release, the API structures the ExoMol data resource files as URLs of the form:

`http://exomol.com/db/<MOLECULE>/<ISOTOPOLOGE>/<DATASET>/<FILENAME>`

where <FILENAME> is structured '<ISOTOPOLOGUE>__<DATASET>.<DATATYPE>'. For example, the States file of the YYLT line list for $^{31}P^{15}N$ is obtainable at the URL http://exomol.com/db/PN/31P-15N/YYLT/31P-15N__YYLT.states.bz2.

Furthermore, each dataset has a *manifest* that lists the data files it is comprised of and their sizes (in bytes). The manifest is a single text file located at the above URL with the filename '<ISOTOPOLOGUE>__<DATASET>.manifest'. For example, the contents of http://exomol.com/db/PN/31P-15N/YYLT/31P-15N__YYLT.manifest are:

```
http://exomol.com/db/PN/31P-15N/YYLT/31P-15N__YYLT.states.bz2 142161
http://exomol.com/db/PN/31P-15N/YYLT/31P-15N__YYLT.trans.bz2 1803083
http://exomol.com/db/PN/31P-15N/YYLT/31P-15N__YYLT.pf 175000
http://exomol.com/db/PN/31P-15N/YYLT/31P-15N__YYLT.def 4761
http://exomol.com/db/PN/31P-15N/YYLT/31P-15N__YYLT.manifest 323
```

6. Moving to higher spectral resolution

Table 18: Molecules of importance for the ExoMol project with published MARVEL datasets.

Molecule	$N_{\rm iso}$	$N_{\rm elec}$	$N_{\rm levels}$	Reference(s)
H_2O	7	1	18 486	Tennyson et al. [217, 223, 224, 268]
update	1	1	19 200	Tóbiás et al. [269], Furtenbacher et al. [270]
H_3^+	3	1	652	Furtenbacher et al. [231, 271]
NH_3	1	1	4951	Al Derzi et al. [188]
update	1	1	4936	Furtenbacher et al. [272]
C_2	1	14	5699	Furtenbacher et al. [193]
update	1	20	7087	McKemmish et al. [194]
TiO	1	9	10 564	McKemmish et al. [126, 199]
HCCH	1	1	11 213	Chubb et al. [235]
SO_2	3	1	15 130	Tóbiás et al. [234]
H_2S	1	1	11 213	Chubb et al. [230]
ZrO	1	10	8088	McKemmish et al. [273]
O_2	1	6	4279	Furtenbacher et al. [274]
NH	1	4	1058	Chubb et al. [235]
CaOH	1	5	1954	Wang et al. [275]
H_2CO	1	1	4841	Al-Derzi et al. [236]
NO	1	1	4106	Wong et al. [115]
AlH	2	2	331	Yurchenko et al. [122]
BeH	3	2	1264	Darby-Lewis et al. [172]
CN	1	10	7779	Syme and McKemmish [276]

$N_{\rm iso}$ Number of isotopologues considered;

$N_{\rm elec}$ Number of electronic states considered;

$N_{\rm levels}$ Number of energy levels extracted: value is for the main isotopologue.

Transit spectroscopy of exoplanets has thus far been performed at rather low resolution; however, very precise spectroscopic data are required for high

resolution Doppler spectroscopy [277–279]. This has proved to be an issue for important species [70]. Indeed the ExoMol datasets described above were generally constructed with greater emphasis on completeness than obtaining very precise transition frequencies [280]. In practice, however, the use of empirical energy levels in the States file means that some transition frequencies are indeed reproduced with high (experimental) accuracy; however, with the ExoMol2016 data structure it was not possible to tell how accurately a particular transition was predicted.

Although some work has been done on using ExoMol data to provide the input for high resolution studies [214], there is a clear need to adapt the database to provide the laboratory data needed for these studies. For this reason we have updated the data structure to allow the uncertainty in a particular transition frequency to be determined. This is done via uncertainties in the energy levels which are now specified (optionally) in the States file, see Table 10.

To improve the accuracy of the predicted spectra, the ExoMol States files are being systematically updated using empirically-determined energy levels. The main means of doing this is via the MARVEL (measured active rotational-vibrational energy levels) procedure [190, 269, 281]. MARVEL inverts available high resolution spectra for a given isotopologue to give a list of empirical energy levels with associated uncertainties. For levels determined by MARVEL these uncertainties are now given in the States file. Otherwise the (usually much larger) uncertainty arising from the calculation used to generate the line list is given. By combining the uncertainty of upper and lower states (ΔE_u, ΔE_l) using the standard formula

$$\Delta E_\nu = \frac{1}{\sqrt{2}} \sqrt{((\Delta E_u)^2 + (\Delta E_l)^2)} \tag{4}$$

gives the uncertainty in the transition wavenumber, ΔE_ν.

To help improve the accuracy of key line lists we have been running MAR-

VEL projects on relevant molecules. Table 18 lists the astronomically important molecules for which MARVEL studies have been completed. We note that a number of these studies [199, 230, 235, 273, 282] have been performed as part of the so-called ORBYTS schools outreach project, see Sousa-Silva et al. [283] for a discussion of this. We are in the process of working through all the molecules in the ExoMol database running MARVEL projects for those isotopologues for which there are enough high accuracy laboratory data available to justify this activity.

7. Other Future development

The ExoMol project already maintains extensive molecule by molecule bibliography files. These are stored on LaTeX's BibTex format and are freely accessible at `https://github.com/ExoMol/bib/tree/master/exomol`. Our aim is to make referencing to the original data as easy and convenient as possible, including automatic generation of the list of references to cite in the appropriate format such as BibTex, Endnote etc. Such services have been developed and offered by HITRAN [284].

We are in the process of moving the database to a more powerful platform. After the move we plan to offer the ability to compute cross sections for a given species, temperature and pressure on the fly. This will be done using super-lines which greatly reduce the computing time. We will also facilitate the computation of k-tables for a given atmospheric model.

Finally the move should allow much greater integration with the code Tau-REx [13, 14]. Tau-REx is an open source retrieval code for exoplanetary atmospheres which has just undergone a major upgrade [15]. Integration with the Tau-REx-III upgrade via a graphical interface is currently in progress.

8. Conclusions

The ExoMol database presented here is a molecule-by-molecule set of comprehensive line lists for modelling spectra and other properties of hot gases. The choice of molecules is dictated by the need to model the atmospheres of exoplanets and other hot astronomical objects, but the spectroscopic data have much wider applications than this. We are still in the process of adding molecules to the database and are receptive to suggestions of other key species to include. In addition we are working on improving the accuracy of the line positions, particularly for strong lines, enhancing the treatment of pressure broadening, and extending the range of wavelengths covered into the ultra-violet for molecules where this is considered important. In addition, we also plan to expand the database to consider temperature dependent photodissociation.

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