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The ExoMol project: an update

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Abstract. Spectra of exoplanets, cool stars and brown dwarfs contain features due to molecular absorptions. Modelling these requires extensive line lists which are provided by the ExoMol project. Here we report on current progress and future prospects for the project.

Keywords: molecular data, stars: atmospheres, stars: low-mass, brown dwarfs, exoplanets.

1. Introduction

The ExoMol project was designed to provide comprehensive molecular line lists for use in atmospheric studies of exoplanets and other astronomical bodies (Tennyson & Yurchenko 2012). The emphasis of this work is on models of hot (say $T > 500$ K) bodies or ones outside thermodynamic equilibrium. The atmospheric studies of cooler planets, including the Earth, are well served by existing databases such as HITRAN (Gordon et al. 2017) and GEISA (Jacquinet-Husson et al. 2016). The demands of providing line lists that are complete for elevated temperatures has a number of consequences. First the resulting line lists are huge, often containing tens of billions of lines; this in turn has led to development of data compaction techniques which allow these data to be used efficiently in radiative transfer models (Rey et al. 2016; Yurchenko et al. 2017; Min 2017). Secondly, this volume of data is beyond what can reasonably be measured line-by-line in the laboratory. This makes computation using an appropriate theoretical model essential. However, pure *ab initio* procedures do not provide the accuracy required; this is particular true for molecules containing a transition metal atom (Tennyson et al. 2016a; McKemmish et al. 2016a) where current state-of-the-art quantum chemical procedures struggle to produce even qualitatively correct results for many important low-lying electronic states. This means that the approach employed by ExoMol, and indeed other similar projects (Rey et al. 2016; Huang et al. 2019), is to tune the procedure using empirical data.

The methods we use for improving on *ab initio* potential energy curves and surfaces are well documented (Tennyson 2012; Tennyson & Yurchenko 2017). However, while these methods give results which work well for modelling low-to-medium resolution spectra and overall opacities, simply tuning theoretical potentials does not in general yield spectroscopic accuracy (Canty et al. 2015). The development of high accuracy techniques for the detection of molecules in the atmospheres of exoplanets (Snellen 2004; de Kok et al. 2014) has sparked the requirement for accurate line positions. Standard line lists often do not satisfy this requirement (Birkby et al. 2017; Hoeijmakers et al. 2015). Methods for adapting ExoMol line lists for high resolution studies are discussed below.

Unlike line positions, the dipole moment surfaces, which largely determine the intensity of a given transition, are best computed *ab initio*. Detailed comparisons with experiment show that high quality *ab initio* calculations are capable of predicting measured transition intensities to within a few per cent or better in favourable cases (Polyansky et al. 2015).

The ExoMol database can be accessed at www.exomol.com and a detailed specification has been given by Tennyson et al. (2016b). The database contains line lists for some

50 molecules studied directly by the ExoMol project and about 25 other species for which data has been provided by other groups. The next section summarises the current status of ExoMol data focussing on some recent highlights. The following briefly discusses some of other line lists available on the ExoMol web pages. Section 4 discusses possible improvements to the database which is then followed by our conclusion.

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

Paper	Molecule	$N_{\rm iso}$	$T_{\rm max}$	$N_{\rm elec}$	$N_{\rm lines}$	DSName	Reference
I	BeH	1	2000	1	16 400	Yadin	Yadin et al. (2012)
I	MgH	3	2000	1	10 354	Yadin	Yadin et al. (2012)
I	CaH	1	2000	1	15 278	Yadin	Yadin et al. (2012)
II	SiO	5	9000	1	254 675	EJBT	Barton et al. (2013)
III	HCN/HNC	1	4000	1	399 000 000	Harris	Barber et al. (2014)
IV	CH_4	1	1500	1	9 819 605 160	YT10to10	Yurchenko & Tennyson (2014)
V	NaCl	2	3000	1	702 271	Barton	Barton et al. (2014)
V	KCl	4	3000	1	1 326 765	Barton	Barton et al. (2014)
VI	PN	2	5000	1	142 512	YYLT	Yorke et al. (2014)
VII	PH_3	1	1500	1	16 803 703 395	SAlTY	Sousa-Silva et al. (2015)
VIII	H_2CO	1	1500	1	10 000 000 000	AYTY	Al-Refaie et al. (2015)
IX	AlO	4	8000	3	4 945 580	ATP	Patrascu et al. (2015)
X	NaH	2	7000	2	79 898	Rivlin	Rivlin et al. (2015)
XI	HNO_3	1	500	1	6 722 136 109	AlJS	Pavlyuchko et al. (2015)
XII	CS	8	3000	1	548 312	JnK	Paulose et al. (2015)
XIII	CaO	1	5000	5	21 279 299	VBATHY	Yurchenko et al. (2016)
XIV	SO_2	1	2000	1	1 300 000 000	ExoAmes	Underwood et al. (2016b)
XV	H_2O_2	1	1250	1	20 000 000 000	APTY	Al-Refaie et al. (2016)
XIV	H_2S	1	2000	1	115 530 3730	AYT2	Azzam et al. (2016)
XV	SO_3	1	800	1	21 000 000 000	UYT2	Underwood et al. (2016a)
XVI	VO	1	2000	13	277 131 624	VOMYT	McKemmish et al. (2016b)
XIX	$H_2{}^{17,18}O$	2	3000	1	519 461 789	HotWat78	Polyansky et al. (2017)
XX	H_3^+	1	3000	1	11 500 000 000	MiZATeP	Mizus et al. (2017)
XXI	NO	6	5000	2	2 281 042	NOName	Wong et al. (2017)
XXII	SiH_4	1	1200	1	62 690 449 078	OY2T	Owens et al. (2017)
XXIII	PO	1	5000	1	2 096 289	POPS	Prajapat et al. (2017)
XXIII	PS	1	5000	3	30 394 544	POPS	Prajapat et al. (2017)
XXIV	SiH	4	5000	3	1 724 841	SiGHTLY	Yurchenko et al. (2018b)
XXV	SiS	12	5000	1	91 715	UCTY	Upadhyay et al. (2018)
XXVI	HS	6	5000	1	219 463	SNaSH	Yurchenko et al. (2018a)
XXVI	NS	6	5000	1	3 479 067	SNaSH	Yurchenko et al. (2018a)
XXVII	C_2H_4	1	700	1	60 000 000 000	MaYTY	Mant et al. (2018)
XXVIII	AlH	3	5000	3	40 000	AlHambra	Yurchenko et al. (2018d)
XXIX	CH_3Cl	2	1200	1	166 279 593 333	OYT	Mant et al. (2018)
XXX	$H_2{}^{16}O$	1	5000	1	1 500 000 000	Pokazatel	Polyansky et al. (2018)
XXXI	C_2	3	5000	8	6 080 920	8states	Yurchenko et al. (2018c)
XXXII	MgO	3	5000	8	72 833 173	LiTY	Li et al. (2019)
XXXIII	TiO	5	5000	13	59 000 000	ToTo	McKemmish et al. (2019)
XXXIV	PH	1	4000	2	65 055	LaTY	Langleben et al. (2019)
XXXV	NH_3	1	1500	1	xxx	CoYuTe	Coles et al. (2019a)

$N_{\rm iso}$: 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

2. Current status of the ExoMol database

Table 1 and 2 provide a summary of the line lists currently available from the ExoMol project. We (Tennyson & Yurchenko 2018) recently published an Atlas of absorption spectra for these species which is designed to illustrate the spectral coverage of each molecule as a function of wavelength and temperature. Figure 1 contain such illustrations for some molecules that have recently been added to the ExoMol database.

Recent highlights include the first comprehensive line list for the astronomically important C_2 molecule (Yurchenko et al. 2018c). Astronomical observations of C_2 are unusual as they stretch back to the middle of the nineteeth centuary and they have been made using a significant number of different electronic band systems.

A new water line list, known as POKAZATEL (Polyansky et al. 2018), has recently been published. POKAZATEL is replacement for previous, widely used water line lists as it is both higher accuracy and more complete than the Ames line list due to Partridge & Schwenke (1997) and BT2 of Barber et al. (2006) which was also used to populate HITEMP Rothman et al. (2010). It is our strong recommendation that future studies involving the spectroscopy of hot water are based on POKAZATEL rather than these earlier line lists.

The recently released ToTo line list for TiO (McKemmish et al. 2019) (see Fig. 1) also represents a significant improvement on previous lists (Schwenke 1998; Plez 1998), particularly with regards to the accuracy of individual transitions. However, as mentioned above, TiO is a challenging molecule to work on the ToTo line list does not represent the final word on this important species.

The most recent line list listed in Table 1 is the CoYuTe line list for ammonia ($^{14}NH_3$) due to Coles et al. (2019a); note a separate line list for $^{15}NH_3$ has been provided by Yurchenko (2015). CoYuTe represents a major improvement in both accuracy and coverage compared to the BYTe $^{14}NH_3$ line list of Yurchenko et al. (2011). In part this improvement was aided by a series newly-assigned laboratory spectra of both hot (Zobov et al. 2011; Barton et al. 2015, 2017d; Beale et al. 2017) and room-temperature (Barton et al. 2016, 2017c; Zobov et al. 2018; Coles et al. 2018) ammonia. Assignment of these spectra in turn was aided by use of the BYTe line list. This illustrates the iterative nature by which line lists can be improved. One interesting early application of the CoYuTe line list was made by Irwin et al. (2019) who used the preliminary, room temperature version (see Fig. 2) to analyse the visible absorption spectrum of gaseous ammonia in of Jupiter; a region not addressed by the earlier BYTe line list.

Another interesting recent result is the possible identification of aluminum oxide (AlO) in the atmosphere of the ultra-hot Jupiter exoplanet WASP-33 b by von Essen et al. (2019). This identification relies entirely on the ATP line list of Patrascu et al. (2015),

3. Non-ExoMol line lists

It is important to note that not all line lists we produce are get included into the ExoMol series in Table 1. For example, while developing a spectroscopic model for a given system, we tend to compute preliminary, usually smaller, lower temperature line lists and usually straight from the *ab initio*, not refined curves or surfaces. We consider this a useful exercise to test the accuracy of the model and assess the amount of time and computational resources required for the full, accurate line lists. As part of such an exercise, a number of molecular line lists have been recently produced in our group, which are listed in Table 2. Some of them (AsH_3, NH_3, P_2H_2, YO and CH_3) are also illustrated in Fig. 2.

Table 2. Datasets created by outside the ExoMol project and included in the ExoMol database.

Molecule	$N_{\rm iso}$	$T_{\rm max}$	$N_{\rm elec}$	$N_{\rm lines}$	DSName	Reference
CH_3	1	1500	1	2 058 655 166	AYYJ	Adam et al. (2019)
NH_3	1	300	1	312 273 690	C2018	Coles et al. (2018)
PF_3	1	300	1	68 000 000 000	MCYTY	Mant et al. (2019)
cis-P_2H_2	1	300	1	11 020 092 365	Cis	Owens & Yurchenko (2019)
trans-P_2H_2	1	300	1	10 667 208 951	Trans	Owens & Yurchenko (2019)
AsH_3	1	300	1	3 636 112	CYT18	Coles et al. (2019b)
ScH	1	5000	6	1 152 827	LYT	Lodi et al. (2015)
YO	1	5000	6	3 015 331	SSYJ	Yurchenko et al. (2019)
CO_2	13	300	1	161 944	Zak	Zak et al. (2016)

$N_{\rm iso}$: 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 addition to the computed line lists summarized in Tables 1 and 2, the ExoMol website all host line lists for a number of other species. These lists are substantially experimental in origin and mainly originate from Peter Bernath's group. As they are constructed directly from measurements they generally do not conform to ExoMol stan-

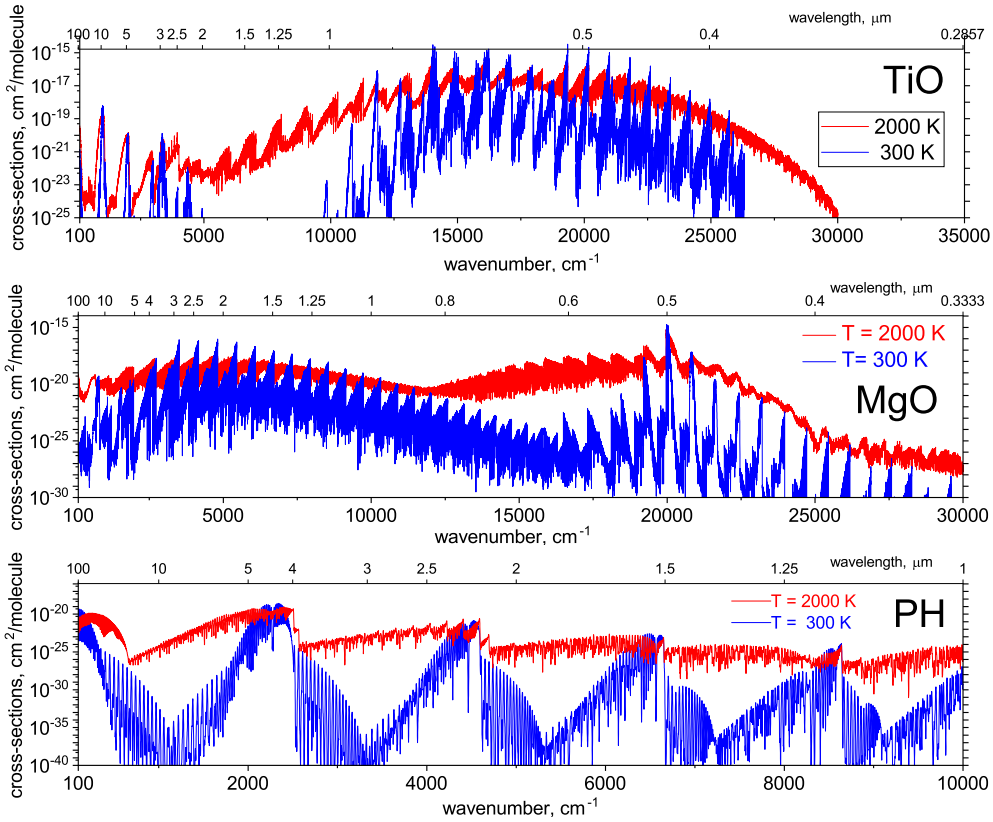

Figure 1. Cross sections for TiO (McKemmish et al. 2019), MgO (Li et al. 2019) and PH (Langleben et al. 2019).

dards of completeness. Key species include: CH (Masseron et al. 2014), NH (Brooke et al. 2014a), OH (Brooke et al. 2016), CO (Li et al. 2015), CrH Burrows et al. (2002), HCl Li et al. (2011), FeH Wende et al. (2010), CN (Brooke et al. 2014b), CP (Ram et al. 2014). TiH Burrows et al. (2005), AlCl (Yousefi & Bernath 2018), AlF (Yousefi & Bernath 2018), LiF (Bittner & Bernath 2018), LiCl (Bittner & Bernath 2018), OH^+ (Hodges & Bernath 2017), MgF (Hou & Bernath 2017), CaF (Hou & Bernath 2018), NaF (Frohman et al. 2016) and KF (Frohman et al. 2016). A paper presenting this aspect of the ExoMol database is currently in preparation (Yixin Wang & Yurchenko 2019).

4. Future improvements

Table 3. Summary of MARVEL analyses performed for astronomically important molecules.

Molecule	$N_{\rm iso}$	$N_{\rm trans}$	N_E	Reference(s)
H_2O	9	182 156	18 486	Tennyson et al. (2009, 2010, 2013a, 2014a)
H_3^+	3	1410	911	Furtenbacher et al. (2013b,a)
NH_3	1	28 530	4961	Al Derzi et al. (2015)
C_2	1	23 343	5699	Furtenbacher et al. (2016)
TiO	1	48 590	10 564	McKemmish et al. (2017)
HCCH	1	37 813	11 213	Chubb et al. (2018a)
SO_2	3	40 269	15 130	Tóbiás et al. (2018)
H_2S	1	39 267	7651	Chubb et al. (2018b)
ZrO	1	21 195	8329	McKemmish et al. (2018)
O_2	1	30 671	6295	Furtenbacher et al. (2019b)
NH	1	3002	1120	Darby-Lewis et al. (2019)

$N_{\rm iso}$: Number of isotopologues considered;
$N_{\rm trans}$: Number of transitions validated for the main isotopologue.
N_E: Number of energy levels given for the main isotopologue.

The process of improving the ExoMol database is a continuous one. In particular new species are systematically considered and included. These are prioritised according the demands, actual or perceived, of astronomers. At present a particular focus is on those molecules thought to be important in the atmospheres of hot, rocky exoplanets which are also known as lava planets, see Tennyson & Yurchenko (2017). However, there are other aspects of the database that also warrant improving.

Pressure broadening can significantly alter the amount of radiation absorbed by a particular transition, particularly if it is optically thick. However, pressure broadening parameters depend on the individual transition being considered, the colliding species and the temperature. There is an urgent need for sets of good pressure broadening parameters for studies of exoplanets (Fortney et al. 2019). Compiling full sets of parameters for a database of the size of the ExoMol represents a formidable task. Initial steps were taken for constructing the ExoMol diet of line-by-line pressure-broadening parameters (Barton et al. 2017b,a). Recently Gamache & Vispoel (2018) have proposed an expression which correctly models the temperature dependence of the pressure broadening over a large temperature ranges. Further improvements in the ExoMol diet should clearly include implementation of this function. We would like to note the recent work by Gharib-Nezhad et al. (2019), who have reported the broadening parameters of CH_4 by H_2 using ExoMol's diet format.

As mentioned above, high-resolution observations of molecular spectra in exoplanets require line positions of higher accuracy than is routinely available for much of the data provided by ExoMol. We have been actively working on a method of solving this problem

based on the MARVEL (measured active rotational-vibrational energy levels) procedure. MARVEL works by inverting measured laboratory transition frequencies (and associated uncertainties) to obtain a set of empirical energy levels (and uncertainties) which can be used to regenerate not only the originally observed transitions but also yet-to-be-

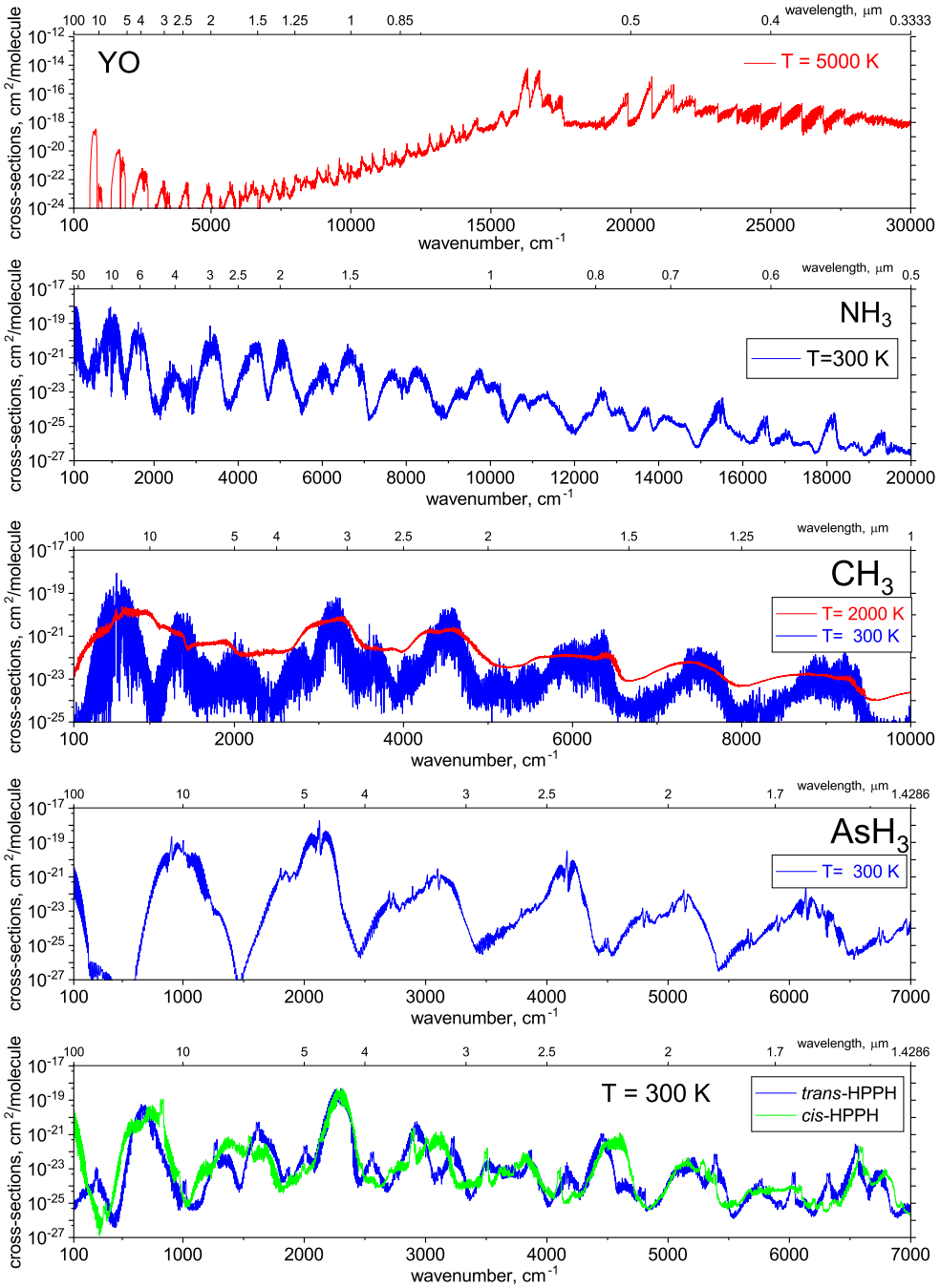

Figure 2. Cross sections for NH_3 (Coles et al. 2019a), CH_3 (Adam et al. 2019), AsH_3 (Coles et al. 2019b), P_2H_2 (Owens & Yurchenko 2019) and YO (Yurchenko et al. 2019).

seen transitions involving these energy levels. The MARVEL procedure was originally developed for an IUPAC task group studying water spectra (Furtenbacher et al. 2007; Tennyson et al. 2014b) and has subsequently been systematically improved (Furtenbacher & Császár 2012; Tóbiás et al. 2019).

The data structure used by ExoMol (Tennyson et al. 2013b) is designed to allow the energy levels, and hence the computed transition frequencies, to be improved in a straightforward manner after the construction of a line list, see Barber et al. (2014) for example. This means that a MARVEL study can be used *post hoc* to improve the ExoMol transitions frequencies.

Table 3 summarises the currently available MARVEL studies for astronomically important species. Huang et al. (2019) recently noted that use of MARVEL energy levels significantly improved the quality of their SO_2 line lists. Although several MARVEL studies have been performed in conjunction with the construction of ExoMol line lists, so far this has not been done systematically for molecules of important for exoplanet observations. We plan to do this in the future. In this context we note that the "A" in MARVEL stands for active which means that the MARVEL database itself can be updated as new data becomes available. MARVEL update projects for both water (Furtenbacher et al. 2019c) and ammonia (Furtenbacher et al. 2019a) have just been completed.

A MARVEL project typically involves assembling and digitising laboratory spectra for the molecule in question for all available sources. For a typical MARVEL project many such sources are often available and thus assembling and validating them is significant undertaking. Several of the MARVEL studies listed in Table 3 (McKemmish et al. 2017; Chubb et al. 2018a,b; McKemmish et al. 2018; Furtenbacher et al. 2019b; Darby-Lewis et al. 2019) were performed in collaboration with high school students as part of schools outreach project focused on involving school students in performing original research. A discussion of this has been given by Sousa-Silva et al. (2018).

Very recently Molliere & Snellen (2019) have suggested that the cross-correlation technique represents a potential technique for the measurement of atmospheric isotope ratios in exoplanets. Clearly successful application of this technique will require precise frequencies for the molecular isotopologues in question. Given the differences in isotope abundances between Earth and other locations in the Universe, there is no guarantee that good laboratory frequencies will be available for all isotopologues of importance. Polyansky et al. (2017) proposed a procedure, which they tested on water, for making accurate predictions of energy levels and hence transition frequencies for minor isotopologues. It is our plan to exploit this method, which may also be useful for identifying weeds in spectra recorded in the interstellar medium, in future work.

5. Conclusion

The ExoMol project has assembled very extensive line lists of molecular transitions. These line lists have been extensively used for astronomical studies on a variety of objects including exoplanets, cool stars, brown dwarfs and comets. They have also been used for a variety of terrestrial studies ranging from combustion models to molecular steering. The ExoMol project is continuing to provide new line lists for key species. At the same time the focus is changing to improve the quality of laboratory data provided by, for example, appropriate pressure broadening parameters and much more accurate line positions which are required for high resolution studies of exoplanet spectra.

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