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High Accuracy Molecular Line Lists for Studies of Exoplanets and Other Hot Atmospheres

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The desire to characterize and model the atmospheres of the many extrasolar planets that have been discovered over the last three decades is a major driver of current astronomy. However, this goal is impacted by the lack of spectroscopic data on the molecules in question. As most atmospheres that can be studied are hot, some surprisingly so, this activity requires spectroscopic information not readily available from laboratory studies. This article will review the current status of available molecular spectroscopic data, usually presented as line lists, for studies of exoplanet atmospheres and, indeed, the atmospheres of other astronomical objects hotter than the Earth such as brown dwarfs, cool stars and even sunspots. Analysis of exoplanet transit spectra and the calculation of the relevant opacities often require huge datasets comprising billions of individual spectroscopic transitions. Conversely, the newly-developed high-resolution Doppler-shift spectroscopy technique has proved to be a powerful tool for detecting molecular species in exoplanet atmospheres, but relies on the use of smaller, highly accurate line lists. Methods of resolving issues arising from the competing demands of completeness versus accuracy for line lists are discussed.

Keywords: opacity, databases, exoplanets, brown dwarfs, cool stars, Doppler shift spectroscopy, transit spectroscopy, ExoMol

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1 INTRODUCTION

Almost 5,000 exoplanets have now been positively identified with many more candidate planets awaiting confirmation, and with both ground-based and space-borne missions regularly detecting new planets. These discoveries have sparked significant activity on characterizing these planets through their spectra. Broadly speaking there are three methods of observing the spectrum of an exoplanet: directly imaging the planet, transit spectroscopy which involves observing light from the host star as a planet passes in front (and behind) it, and high resolution Doppler shift spectroscopy.

These techniques all have different characteriztics in terms of which planets are amenable to being observed, how the observational data are obtained, what information can be obtained and, of importance for this article, the requirements in terms of laboratory data needed to interpret observations. We run the ExoMol project (Tennyson and Yurchenko, 2012) which aims to provide molecular line lists, and increasingly other data, for studies of exoplanets and other astronomical atmospheres. In this paper we review the provision of available spectroscopic data for characterization of exoplanet atmospheres. There are already a number of reviews which discuss this situation for studies involving transit spectroscopy (Tinetti et al., 2013; Tennyson and Yurchenko, 2017; Tennyson and Yurchenko, 2018; Madhusudhan, 2019) so here while we summarize the current situation regarding transit spectroscopy and direct imaging, we

concentrate particularly on the laboratory data required for the newer method of high-resolution Doppler-shift spectroscopy (HRDSS), also known as high-resolution cross-correlation spectroscopy.

2 DETECTING MOLECULES ON EXOPLANETS

The original detection of molecules on exoplanets were based on transit spectroscopy at infrared wavelengths for hot Jupiter exoplanets (Tinetti et al., 2007; Swain et al., 2008). These detections of respectively water and methane in hot objects (temperatures were generally assumed to be over 1000 K) using relatively low-resolution space telescopes relied on the detection of broad spectral features. Modeling these features requires significant quantities of laboratory data (Yurchenko et al., 2014) since the spectra of hot molecules in the infrared consists of many (10^6–10^9) individual absorption lines. Stimulated by these observations a number of groups started providing comprehensive lists of molecular transitions (line lists) appropriate for modeling molecular spectra at elevated temperatures. Besides ExoMol, the TheoRets project (Rey et al., 2016) and NASA Ames (eg., Huang et al., 2017) provide comprehensive, computed line lists for a variety of molecules while the MoLLIST project of Bernath (2020) attempts to address this problem from a more experimental standpoint. These line lists, which can be very large, are often pre-processed into cross sections representing opacities for ease of use in forward models and spectroscopic retrievals (Freedman et al., 2014; Min, 2017; Allard et al., 2000; Goyal et al., 2018; Yurchenko et al., 2018a; Tennyson and Yurchenko, 2018; Chubb et al., 2021; Gharib-Nezhad et al., 2021; Grimm et al., 2021).

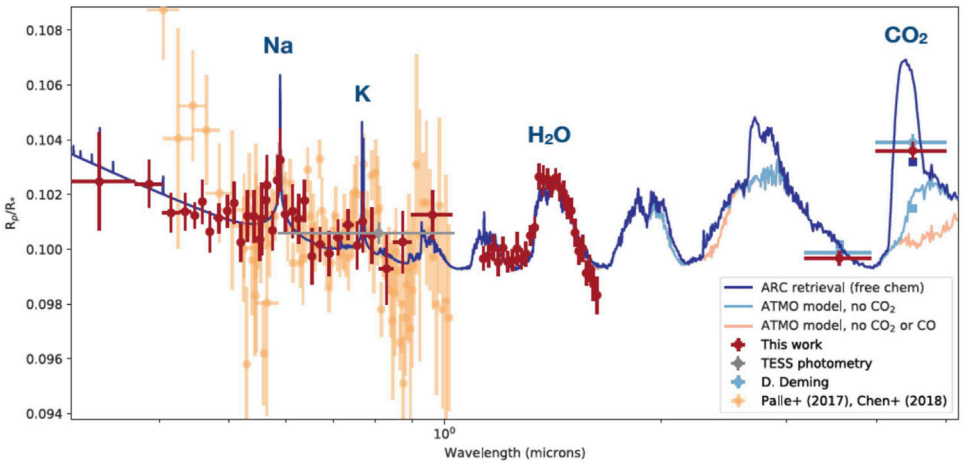
The importance of these activities can be gauged from attempts to determine C/O ratios in exoplanetary atmospheres. At the time of the initial detections of methane in short-period hot Jupiter exoplanets with temperatures typically in the 1,000–2000 K range, spectral modeling of methane relied on the existing laboratory measurements of methane spectra which were almost entirely performed at room temperature. A consequence of this was that atmospheric retrievals tended to indicate high C/O ratios due to overestimated amounts of methane detected as at room temperature higher-lying rotation-vibrations levels are not populated, leading to the opacity being underestimated. The need for a reliable methane line list or opacity has sparked a range of studies (Yurchenko and Tennyson, 2014; Rey et al., 2014; Yurchenko et al., 2014; Rey et al., 2017; Yurchenko et al., 2017; Wong et al., 2019; Hargreaves et al., 2020). The status of comprehensive line lists for methane and other molecules important in exoplanets has been discussed elsewhere (Tennyson et al., 2020). The careful use of observational data and modern, comprehensive line lists is leading to reliable abundance determinations and C/O ratios, see Line et al., 2021.

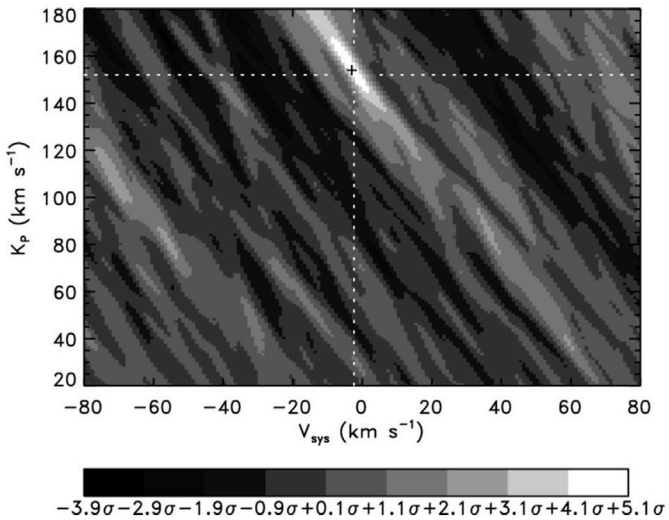
The transit spectroscopy technique is only applicable to planets whose orbit leads to them passing in front of (and behind) their host star as viewed from the Solar System. Obviously this criterion is not satisfied by most exoplanets but in fact missions have concentrated on finding transiting exoplanets which as a result make up well over half of those exoplanets detected up to now. **Figure 1** (Top) shows an example of the detection of water in the gas giant exoplanet Wasp-127b by Spake et al. (2020). Water is relatively easy to detect by this methodology (Tinetti et al., 2012; Tsiaras et al., 2018; Fraine et al., 2014; Tsiaras et al., 2019). It is also much easier to see a large exoplanet in a nearby orbit transiting so the sample of transiting exoplanets has a strong observational bias towards short period and hot planets.

Conversely, direct imaging relies on being able to separate the spectral signature of a planet from that of its host star. This is most easily done for nearby stars with planets in large orbits. Planets that orbit far from their star should be cool as they receive only weak starlight. However, in this case such planets would also be faint and hard to detect. Young planets, however, are formed hot due to the heating generated by gravitational collapse. As a result observation and characterization of directly imaged planets has largely concentrated on very young (a few tens of millions years old) planets. Progress is being made on the characterization of young, self-luminous giant planets at wide orbital separations from their host stars by direct imaging; an example of a recent detection of water in directly imaged exoplanet HD 106906b by Zhou et al. (2020) is given in **Figure 1** (Bottom).

In fact, the most secure detections of molecules thus far have not been made by transit spectroscopy or direct imaging. Observations using these methods have relied on use of relatively low resolution methods resulting in spectra showing broad features rather than individual transitions. While these broad features can be associated with certain molecules, the results are open to alternative explanations, see Blain et al. (2021) for an example. The HRDSS method pioneered by Snellen and co-workers (Snellen, 2014) involves recording spectra of the combined star and exoplanetary system over the entire orbit of the exoplanet, which does not have to be transiting. Molecular signatures can then be identified using the combination of line positions and appropriate Doppler shifts. This technique has been used to make a number of molecular detections at 5σ level or better (Birkby, 2018; Brogi and Line, 2019). **Figure 1** (Middle) shows the detection of water in hot Jupiter exoplanet HD 189733b by Birkby et al. (2013). In this case the figure confirming the detection does not look like a standard spectrum but instead takes the form of a cross-correlation diagram obtained using a particular set of molecular transitions and appropriate Doppler shifts.

The HRDSS method is powerful but requires high resolution laboratory data to be successful, see Hoeijmakers et al. (2015) for example. Typically to be useful, wavelengths, λ, need to be known with a resolving power $R = \frac{\lambda}{\Delta\lambda}$ of 100,000 or better. While such accuracies are routinely obtained by laboratory high resolution spectroscopy experiments, they are only achievable by theory for a few exceptional (few electron) molecules. Therefore to satisfy the data needs of HRDSS observations a different approach is required for the construction of molecular line lists.





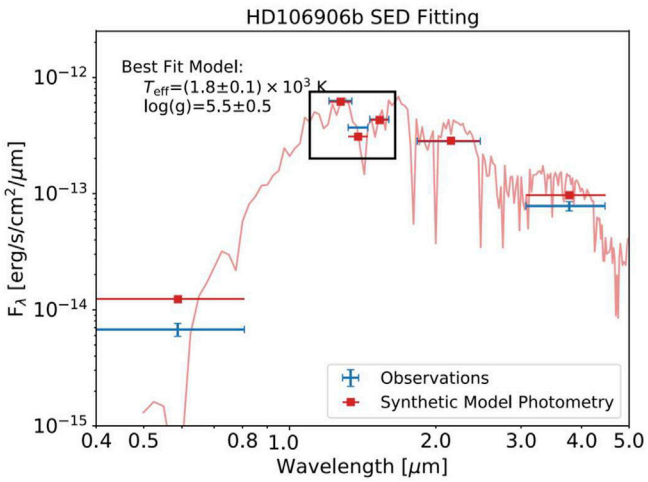


FIGURE 1 | Detection of water in exoplanets: Top, Transmission (Hubble Space Telescope and Spitzer) spectrum of transiting exoplanet Wasp-127b (reproduced from Figure 18 of Spake et al., 2020); Middle, high-resolution detection of water in with significance of 4.8σ (reproduced from Figure 3 of Birkby et al., 2013); Bottom, first 1.4 μm water band photometric measurement for HD 106906 by Zhou et al., 2020. (©AAS. Reproduced with permission.)

3 HIGH RESOLUTION MOLECULAR LINE LISTS

Given that theory alone cannot provide line positions accurate enough for HRDSS studies, it is necessary to find an alternative procedure. For temperate planets the HITRAN database (Gordon et al., 2022), which largely comprises data from laboratory measurements, provides a good starting point. However, for hotter exoplanets or ones with exotic atmospheres one has to move beyond this towards computed line lists. Using experimental data to improve the underlying potential energy surface used in a nuclear motion calculations is a standard procedure, see Tennyson (2012), but not one which yields the required accuracy for HRDSS. We have therefore adopted an alternative approach based on use of the MARVEL (measured accurate rotation vibration energy levels) procedure.

MARVEL was originally developed by Furtenbacher et al. (2007) to address the challenge of obtaining a consistent and accurate set of empirical energy levels for the main isotopologues of water (Tennyson et al., 2014a). The MARVEL algorithm has subsequently been improved (Furtenbacher and Császár, 2012; Tóbiás et al., 2019), largely to improve the treatment of uncertainties. Put simply, the procedure involves assembling assigned transitions with uncertainties from all high resolution spectroscopy experiments which are then inverted to give empirical energy levels using the MARVEL procedure, which is available as an online tool. In practice a considerable amount of data cleaning is usually required before final answers are obtained. The empirical energy levels obtained using MARVEL are then validated against the appropriate line list allowing the reliability of those energy levels characterized by only one or two transitions to be assessed. The resulting empirical energy levels can then be used to substitute those calculated in a computed line list, which are then assigned the uncertainty obtained in the MARVEL process. This approach not only guarantees that a line list reproduces the observed transitions accurately, but results in many other, as yet unmeasured, transitions being predicted with the accuracy of high resolution spectroscopy. The replacement of energy levels in the full line list also ensures the retention of the original line list completeness.

A recent example of this appropach is provided by a MARVEL study on formaldehyde (CH_2O) by Al-Derzi et al., 2021 who compiled a list of 16,403 non-redundant observed transitions taken from 43 experimental sources. Using MARVEL gave 5,029 empirical energy levels which were validated by comparing with the predictions of the AYTY ExoMol line list (Al-Refaie et al., 2015). Substituting these empirical energy levels back into this line list yields 367,779 transition frequencies with accuracy good enough to be used for HRDSS astronomical studies. This represents a more than twenty-fold increase compared to the original experimental measurements.

Thus the basic strategy for computing a high accuracy line list is clear. Step 1 is to compute a line list using the best available potential curves or surfaces, which should be tuned to the experimental data if possible. Step 2 is to use available empirical energy levels obtained from a MARVEL study to replace computed ones where possible. This already gives a significant improvement for many predicted transitions. The NASA Ames group have also used MARVEL energy levels in this fashion (Huang et al., 2019b). However, this strategy can be further improved on (Bowesman et al., 2021; McKemmish et al., 2022). **Table 1** summarizes MARVEL studies on molecules of interest for exoplanets studies.

We note that MARVEL is an active procedure which means that when new data become available they can simply be added to an existing compilation and the process re-run. As can be seen from **Table 1** a number of updates to existing MARVEL compilations have been published. Indeed experiments are now being designed and performed to explicitly update available MARVEL compilations by, for example, performing measurements for transitions critical for improving the network (Tobias et al., 2020; Diouf et al., 2021).

The traditional method of representing the energy levels obtained from high resolution molecular spectroscopy is *via* so-called effective Hamiltonians which use rotational and other constants to represent the observed levels. Effective Hamiltonians have a proven record of providing compact and highly accurate representations of molecular energy levels. However, there are two issues with their use. Firstly, while they accurately interpolate between observed data, their extrapolation properties are known to be problematic in many cases (Polyansky et al., 1994; Furtenbacher et al., 2020a). Secondly, they often struggle to accurately represent so-called resonance states: ones which are perturbed by interactions with states of the same symmetry but belonging to another vibrational or vibronic state. Representing states in resonance using effective Hamiltonians usually requires many parameters and a significant amount of extra experimental data. While MARVEL uses (approximate) quantum number assignments for states, these are actually just a labelling scheme which makes no assumptions about the underlying physics of the state involved. MARVEL simply obtains a value for the observed energy level and its behavior is not affected by any unexpected or resonant interactions.

However, one issue with using MARVEL is that it may not give complete coverage: levels may be missing because transitions to them have yet to be observed. Effective Hamiltonians can be used to fill in these missing energy levels, see the recent study of AlO by Bowesman et al. (2021) for example. Bowesman et al. (2021) also found that the observed minus calculated energy levels can also give information allowing further improvement to be achieved for yet to be observed transitions involving to be observed states.

Figure 2 shows the coverage of the MARVEL data in providing accurate transition frequencies for water by using the ExoMol POKAZATEL line list for $H_2^{16}O$ (Polyansky et al., 2018). At room temperature the contribution from the high accuracy MARVEL transitions is nearly complete up to 20,000 cm^{-1} ($\lambda > 0.5\,\mu$m). Even though the higher temperature spectrum ($T = 3000$ K) loses the MARVEL completeness by about 1 μm, it is important that the strongest features remain dominated by the MARVEL transitions, which should still be reasonably well covered for the HRDSS applications but care is required to ensure that the correct, accurately determined, lines are used in any such application. This point is further illustrated in **Figure 3** which shows water cross sections at $T = 3000$ K for $1.5 < \lambda < 2.4\,\mu$m and compares

TABLE 1 | Astronomically important molecules with published MARVEL datasets.

Molecule	N_{iso}	N_{elec}	N_{levels}	References
H_2O	7	1	18,486	Tennyson et al. (2009), Tennyson et al. (2010), Tennyson et al. (2013a), Tennyson et al. (2014b)
updates	3	1	19,225	Tóbiás et al. (2019), Furtenbacher et al. (2020b), Furtenbacher et al. (2020c)
H_3^+	3	1	652	Furtenbacher et al. (2013a), Furtenbacher et al. (2013b)
NH_3	1	1	4,951	Al Derzi et al. (2015)
update	1	1	4,936	Furtenbacher et al. (2020a)
C_2	1	14	5,699	Furtenbacher et al. (2016)
update	1	20	7,087	McKemmish et al. (2020)
TiO	1	9	10,564	McKemmish et al. (2017), McKemmish et al. (2019)
HCCH	1	1	11,213	Chubb et al. (2018a)
SO_2	3	1	15,130	Tóbiás et al. (2020)
H_2S	1	1	11,213	Chubb et al. (2018b)
ZrO	1	10	8,088	McKemmish et al. (2018)
O_2	1	6	4,279	Furtenbacher et al. (2019)
SO_2	3	1	15,130	Tóbiás et al. (2018)
NH	1	4	1,058	Chubb et al. (2018a)
CaOH	1	5	1954	Wang et al. (2020)
H_2CO	1	1	5,029	Al-Derzi et al. (2021)
NO	1	1	4,106	Wong et al. (2017)
update	1	4	6,306	Qu et al. (2021)
AlH	2	2	331	Yurchenko et al. (2018b)
BeH	3	2	1,264	Darby-Lewis et al. (2018)
CN	1	10	7,779	Syme and McKemmish (2020)
H_2CO	1	1	5,029	Al-Derzi et al. (2021)
AlO	1	7	6,152	Bowesman et al. (2021)

N_{iso} *Number of isotopologues considered;* N_{elec} *Number of electronic states considered* N_{levels} *Number of energy levels extracted: value is for the main isotopologue.*

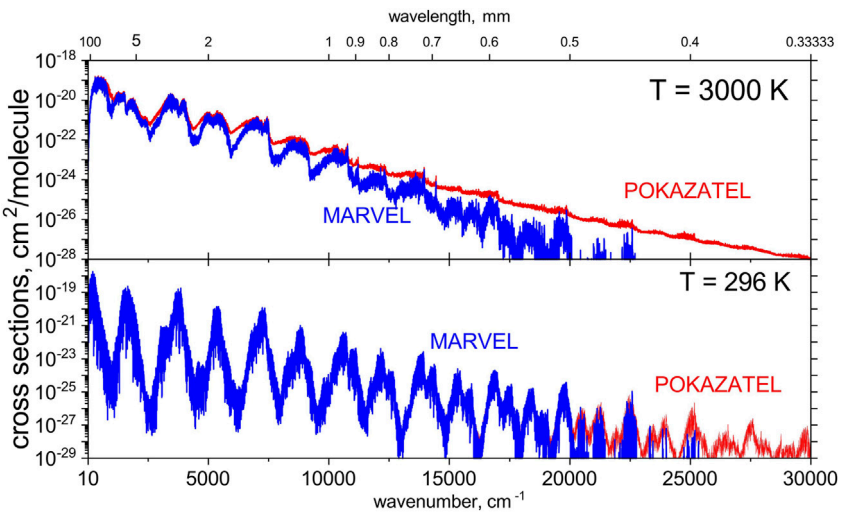


FIGURE 2 | Contribution of MARVEL states to the spectra of $H_2^{16}O$ (MARVEL) compared to the full spectra (POKAZATEL) for two temperatures, T = 296 and 3000 K. In both cases the intensities are from the POKAZATEL line list (Polyansky et al., 2018). Note that the MARVEL curve represents only that part of the overall intensity given by transitions between energy levels determined using the MARVEL procedure. Here a Gaussian line profile of half-width-half-maximum (HWHM) of 1 cm^{-1} was used.

them to cross sections contributed from MARVEL states only. This spectral window of ExoMol's POKAZATEL was recently used in HR spectral characterization of the atmosphere of WASP-77Ab (Line et al., 2021).

Very recently Zhang et al., 2021 reported the first detection in an exoplanet of an isotopically substituted molecule, an isotopologue, in this case ^{13}CO. As isotopic abundances vary across the Universe, the abundance of isotopologues will also vary and their observation has the capability of yielding significant extra information about exoplanets; an increasing number of such studies can be anticipated. Although a number of MARVEL studies have provided energy levels for isotopologues, see **Table 1**,

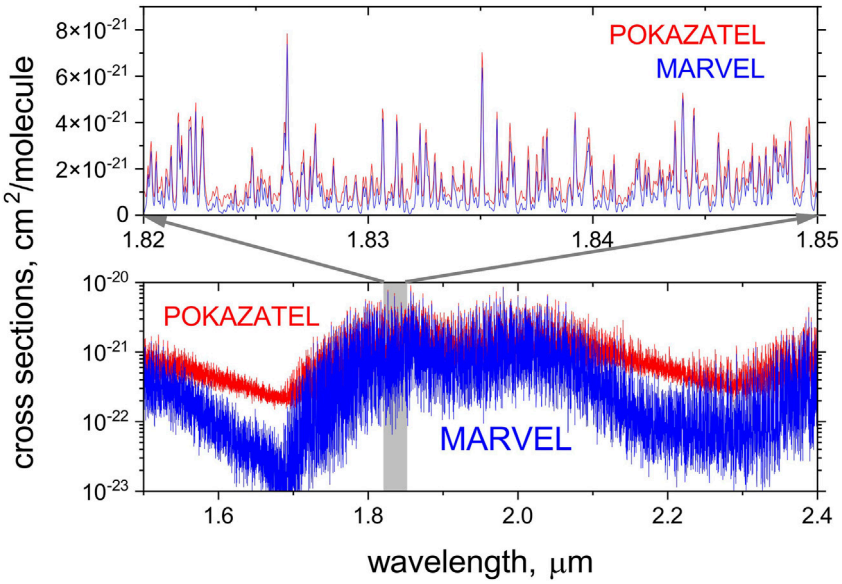


FIGURE 3 | Same as **Figure 2** but at higher resolution (R = 45,000): contribution of MARVEL states to the spectra of $H_2^{16}O$ (MARVEL) compared to the full spectra (POKAZATEL) for high temperature, T = 3000 K. In both cases the intensities are from the POKAZATEL line list (Polyansky et al., 2018). The cross sections were computed using the Voigt line profile using the broadening parameters of H_2O from the ExoMol diet (Barton et al., 2017).

it is true to say that there is always significantly less information available for these minor species than for the most abundant or parent isotopologue.

Polyansky et al. (2017) showed that it was possible to use the observed minus calculated residues in the energy levels of the main (parent) isotopologue to improve the predicted energy levels of the minor isotopologues. This procedure, which was further improved by Furtenbacher et al. (2020c), can greatly increase the number of levels and hence transitions which are known to high accuracy for the minor isotopologues. The effectiveness of this procedure for obtaining what are termed pseudo-experimental energy levels has been shown by a recent independent high resolution spectroscopy study of $H_2^{17}O$ in the visible by Sinitsa et al. (2021). This procedure is being increasingly adopted by us to improve isotoplogue predictions for ExoMol line lists. For example, predictions for isotopologues of TiO in the ExoMol Toto line list of McKemmish et al. (2019) proved accurate enough to identify several isotopologues of TiO in the visible spectrum of two M-dward stars (Pavlenko et al., 2020) and has been used to model titanium isotope ratios in exoplanet atmospheres (Serindag et al., 2021). Again we note that the NASA Ames group have used a mass-dependent fitting procedure which also improves the accuracy of predicted isotopologue spectra (Huang et al., 2019a).

4 DATA FORMATS AND UNCERTAINTIES

The ExoMol project has a well-developed data structure (Tennyson et al., 2013b; Tennyson et al., 2020) which is designed to give a compact representation of what are very large datasets. This data structure, which can be read by post-processing programs such as ExoCross (Yurchenko et al., 2018a) and the effective Hamiltonian program PGOPHER (Western, 2017), is based about the use of two files. A states file which contains all the energy levels of the molecule (isotopologue) in question plus associated meta data such as quantum numbers, and a trans file which is simply a list of two state numbers plus an Einstein A coefficient. This structure means that it is easy to incorporate improved energy levels from a MARVEL project as it is only the states file that needs to be updated; doing this automatically updates the transition wavenumbers which are computed as energy differences (upper minus lower) from the states file. In the current way ExoMol handles its datasets, updating the states file with, for example, improved energy levels represents an update of the underlying line list rather than a new line list. The update becomes a new version with version number given by the date in YYYYMMDD format.

One important thing missing from the original ExoMol format was any consideration of uncertainties. This was done to conserve space but in an era where the data are being used to both give comprehensive opacities and to model high resolution spectra it has become important to indicate the uncertainty with which the wavenumber (or wavelength) of a given transition is predicted. Therefore in the latest release of the ExoMol database, Tennyson et al. (2020) revised the data format to allow an uncertainty to be included for each energy level. This update is still in the process of implementation but our plan is that this will become a compulsory part of the ExoMol format. At present there is no corresponding uncertainty in the intensities (or Einstein A coefficients). Our judgement is that at present the benefit of including this extra information does not justify the further increase in size of already very large datasets which would be required to implement it.

5 CONCLUSION

The provision of spectroscopic data for studies of exoplanets and other hot astronomical atmospheres is being driven by the demands of astronomers both modeling and observing various heavenly bodies. In particular, important developments in techniques have driven the demand that molecular line lists that should not only be complete, an essential requirement for producing accurate opacity functions, but at least for strong lines, they should also be accurate. In this paper we describe measures being taken to ensure that line lists meet these dual requirements. This has meant the upgrading of many ExoMol line lists, see Bowesman et al., 2021 for example, to include available high accuracy empirical energy levels obtained using the MARVEL procedure; a process we refer to as refactoring. This process is still ongoing.

With modern technological advances in astrophysical exploration allowing studies of increasingly complex phenomena in atmospheres of exoplanets, it is becoming possible to study non-local thermodynamic equilibrium (non-LTE) effects (Fisher and Heng, 2019) which are already well-known elsewhere, such as in the spectra of stars, planets, comets and interstellar medium (ISM) (López-Puertas and Taylor, 2001). Non-LTE spectroscopy is based on modeling of rotational, vibrational and electronic populations and therefore introduces special requirements both on the molecular data and spectral simulation software, such as, for example, provision of ro-vibronic assignment or non-Boltzmann populations, with non-LTE methods of different levels of complexity ranging from simplified bi-temperature models (Pannier and Laux, 2019; Clark and Yurchenko, 2021) to sophisticated non-LTE radiative transfer calculations (Funke et al., 2012). This line of research is been actively explored by ExoMol (Wright et al., 2021).

The ExoMol database contains approximately 700 billion lines. Even once refactoring is complete it can be anticipated that only a small minority of these lines, maybe several tens of millions, will be determined with spectroscopic accuracy. By and large these lines constitute the most important and strongest lines for each molecule. Separately identifying these lines can be important for purposes such as line assignment in well-resolved spectra. For this reason we have updated our spectral modeling program ExoCross (Yurchenko et al., 2018a) to allow accuracy of predicted line positions to be a selection criterion when generating model spectra. We are also in the process of creating an interactive database, ExoMolHR, which will allow astronomers and others to search for high resolution data contained in the ExoMol database.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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