

Review Article

Laboratory spectra of hot molecules: Data needs for hot super-Earth exoplanets



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ARTICLE INFO

Article history:

Received 5 March 2017

Revised 17 May 2017

Accepted 19 May 2017

Available online 19 May 2017

Keywords:

Super-Earth

Lava-planets

Absorption Intensities

FTIR spectroscopy

Line lists

Transit spectroscopy

Exoplanets

ABSTRACT

The majority of stars are now thought to support exoplanets. Many of those exoplanets discovered thus far are categorized as rocky objects with an atmosphere. Most of these objects are however hot due to their short orbital period. Models suggest that water is the dominant species in their atmospheres. The hot temperatures are expected to turn these atmospheres into a (high pressure) steam bath containing remains of melted rock. The spectroscopy of these hot rocky objects will be very different from that of cooler objects or hot gas giants. Molecules suggested to be important for the spectroscopy of these objects are reviewed together with the current status of the corresponding spectroscopic data. Perspectives of building a comprehensive database of linelist/cross sections applicable for atmospheric models of rocky super-Earths as part of the ExoMol project are discussed. The quantum-mechanical approaches used in linelist productions and their challenges are summarized.

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1. Introduction

There are vast areas of the Universe thinly populated by molecules which are cold. However, there are also huge numbers of important astronomical bodies which support hot or highly-excited molecules. It is the spectroscopic demands of studying these hot regimes we focus on in this review. We will pay particular attention to the demands on laboratory spectroscopy of a recently identified class of exoplanets known as hot rocky super-Earths or, more colourfully, lava and magma planets. These planets orbit so close to their host stars that they have apparent temperatures such that their rocky surface should melt or even vaporise. Little is known about these planets at present: much of the information discussed below is derived from models rather than observation.

Of course hot and cold are relative terms; here we will take room temperature ($T \sim 300$ K) as the norm which means, for example, that so-called cool stars which typically have temperatures in the 2000–4000 K range are definitely hot. Much of the cold interstellar medium is not thermalised and excitation, for example by energetic photons, can lead to highly excited molecules. This can be seen, for example, from maser emissions involving transitions between highly excited states, which is observed from

a range of molecules from a variety of interstellar environments (Gray, 2012). Similarly the coma of comets are inherently cold but when bathed in sunlight can be observed to emit from very high-lying energy levels (Barber et al., 2009; Dello Russo et al., 2005, 2004).

Turning to the consideration of exoplanets. At the present it even remains unclear how to conclusively identify which planets of a few to ten Earth masses are actually rocky (Tasker et al., 2017). From density observations some of them appear to be rocky (silicate-rich), or with a fraction of ice/iron in the interior. Others suggest a structure and composition more similar to gas giants like Neptune. Density alone is not a reliable parameter to distinguish among the various cases. In addition to there is a class of ultra-short period (USP) exoplanets which are thought to be undergoing extreme evaporation of their atmospheres due to their close proximity to their host star (Gillon et al., 2014, 2012; Oberst et al., 2017; Sanchis-Ojeda et al., 2014). These objects are undoubtedly hot but as yet there are no mass measurements for USP planets. Spectroscopic investigations of atmospheres of super-Earths and related exoplanets holds out the best prospect of learning about these alien worlds. The prospects of observing the atmospheric composition for the transiting planets around bright stars make us confident we will be in a much better position in a few years time with the launch of the James Webb space telescope (JWST) and future dedicated exoplanet-characterization missions.

From the laboratory perspective, the observation of hot or highly excited molecules places immense demands on the spec-

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troscopic data required to model or interpret these species. As discussed below, a comprehensive list of spectroscopic transitions, a line list, for a single molecule can contain significantly more than 10^{10} lines. This volume of data points to theory as the main source of these line lists (Tennyson, 2012).

A line list consists of an extensive list of transition frequencies and transition probabilities, usually augmented by other properties such as lower state energies, degeneracy factors and partition functions to give the temperature dependence of the line and, ideally, pressure-broadening parameters to give the line shape. For radiative transport models of the atmospheres of hot bodies, completeness of the line list to give the opacity of the species is more important than high (“spectroscopic”) accuracy for individual line positions. This is also true for retrievals of molecular abundances in exoplanets based on the use of transit spectroscopy which, thus far, has largely been performed using observations with fairly low resolving power ($R < 3000$) (Tinetti et al., 2013). However, the situation is rather different with the high-dispersion spectroscopy developed by Snellen and co-workers (Birkby et al., 2013, 2017; Brogi et al., 2014; de Kok et al., 2013; Snellen, 2014), which is complementary to transit spectroscopy. This technique tracks the Doppler shifts of a large number of spectroscopic lines of a given species, by cross-correlating them to the reference lab data on the line positions. This exciting but challenging technique requires precise frequencies with $R \geq 100,000$, as well as a good spectroscopic coverage (hot transitions), available laboratory data is not always precise enough for this technique to work (Hoeijmakers et al., 2015a).

This review is organised as follows. First we summarise what is known about hot rocky super-Earth exoplanets. We then consider the laboratory techniques being used to provide spectroscopic data to probe the atmospheres of these bodies and others with similar temperatures. In the following section we summarise the spectroscopic data available making recommendations for the best line list to use for studies of hot bodies. Molecules for which little data appears to be available are identified. Finally we consider other issues associated with spectroscopic characterization of lava planets and prospects for the future.

2. Hot rocky super-Earths

As of the end of 2016 there are well over 100 detected exoplanets which are classified as hot super-Earths. These planets are ones which are considered to be rocky, that is with terrestrial-like masses and/or radii, see e.g. Seager et al. (2007), and which are hot enough for, at least on their dayside, their rock to melt (Kite et al., 2016). Only a handful of these planets are amenable to spectroscopic characterization with current techniques (Madhusudhan et al., 2016), which makes these few objects the ones suitable for atmospheric follow-up observations. All these rocky planets have very short orbits, meaning that they are close to their star and hence have hot atmospheres ($T \gg 300$ K). Some of these planets are evaporating with water vapour as a major constituent of the atmosphere (Barclay et al., 2013a; Batalha et al., 2011; Borucki et al., 2013; David et al., 2016; Leger et al., 2009; Madhusudhan and Redfield, 2015). The atmospheres of these planets are thought to have a lot in common with the young Earth (Alfvén and Arrhenius, 1974) and the atmosphere of a rocky planet immediately after a major impact planet is expected to be similar (Lupu et al., 2014). However, we note that as they are generally tidally-locked to their host star, hot rocky super-Earths will generally have significant day-night temperature gradients (Demory et al., 2016).

According to the NASA Exoplanets Archive (exoplanetarchive.ipac.caltech.edu), key hot exoplanets with masses and radii in the rocky-planet range include CoRoT-7b, Kepler-10b, Kepler-78b, Kepler-97b, Kepler-99b, Kepler-102b, Kepler-131c, Kepler-406b, Kepler-406c, and WASP-47e, with Kepler-36b and Kepler-93b be-

ing slightly cooler than 1673 K (Batalha et al., 2011; Carter et al., 2012; Dai et al., 2015; Hatzes et al., 2011; Howard et al., 2013; Leger et al., 2009; Moutou et al., 2013; Pepe et al., 2013; Weiss and Marcy, 2014). Most of the rocky exoplanets that have so far been studied are characterized by the high temperature of their atmospheres, e.g., about 1500 K in Kepler-36b and Kepler-93b, 2474 ± 71 K in CoRoT-7b Leger et al. (2011), 2360 ± 300 K in 55 Cnc e (Demory et al., 2012; Tsiaras et al., 2016), and around 3000 K in Kepler-10b (Kite et al., 2016). Somewhat cooler but still hot rocky planets include temperatures of 700 K in Kepler-37b (Barclay et al., 2013b), 750 K in Kepler-62b (Borucki et al., 2013), 580 K in Kepler-62c (Borucki et al., 2013), and 400–500 K in GJ 1214b (Bean et al., 2010; Charbonneau et al., 2009; Howe and Burrows, 2012).

If the main constituent of these atmospheres is steam, it will heat the surface of a planet to (and above) the melting point of rock (Zahnle et al., 1988). For example, the continental crust of a rocky super-Earth should melt at about 1200 K (Sawyer et al., 2011), while a bulk silicate Earth at roughly 2000 K (Schaefer et al., 2012). The gases are released from the rock as it heats up and melts, including silica and other rock-forming elements, and is then dissolved in steam (Fegley et al., 2016). The main greenhouse gases in the atmospheres of hot rocky super-Earths are steam (from vaporising water and hydrated minerals) and carbon dioxide (from vaporising carbonate rocks), which lead to development of a massive steam atmosphere closely linked to magma ocean at the planetary surface (Abe and Matsui, 1988; Elkins-Tanton and Seager, 2008; Fegley et al., 2016; Kasting, 1988; Lebrun et al., 2013; Matsui and Abe, 1986; Zahnle et al., 1988).

At temperatures up to 3000 K, and prior to significant volatile loss, the atmospheres of rocky super-Earth are thought to be dominated by H_2O and CO_2 ¹ for pressures above 1 bar, see Schaefer et al. (2012). These objects will necessarily have spectroscopic signatures which differ from those of cooler planets. At present interpretation of such signature is severely impacted by the lack of the corresponding spectroscopic data. For example, recent analysis of the transit spectrum of 55 Cnc e by Tsiaras et al. (2016) between 1.125 and 1.65 μm made a tentative detection of hydrogen cyanide (HCN) in the atmosphere but could not rule out the possibility that this signature is actually in part or fully due to acetylene (HCCH) because of the lack of suitable laboratory data on the hot spectrum of HCCH. The massive number of potential absorbers in the atmosphere of these hot objects also have a direct effect on the planetary albedo (Kasting, 1988) as well as the cooling and hence evolution of the young hot objects; comprehensive data is also crucial to model these processes.

Atmospheric retrievals for hot Jupiter exoplanets such as HD 209458b, GJ 1214b and HD 189733b (Sing et al., 2016) show that transit observations can help to establish the bulk composition of a planet. However, it is only with good predictions of likely atmospheric composition allied to a comprehensive database of spectral signatures and proper radiative transfer treatment that the observed spectra can be deciphered. The completeness of the opacities plays a special role in such retrievals: missing or incomplete lab data when analysing transit data will lead to overestimates of the corresponding absorbing components.

The typical compositions of steam atmospheres have been considered by Schaefer et al. (2012), with an example for low atmospheric pressure shown in Fig. 1. The chemical processes on these objects are very similar to the young Earth (Mars or Venus) and have been studied in great detail. The major gases in steam atmospheres (equilibrated chemistry) with pressures above 1 bar and surface temperatures above 2000 K are predicted to be H_2O , CO_2 ,

¹ Molecules thought to be important for the spectroscopy of hot super-Earths are given in bold when first mentioned.

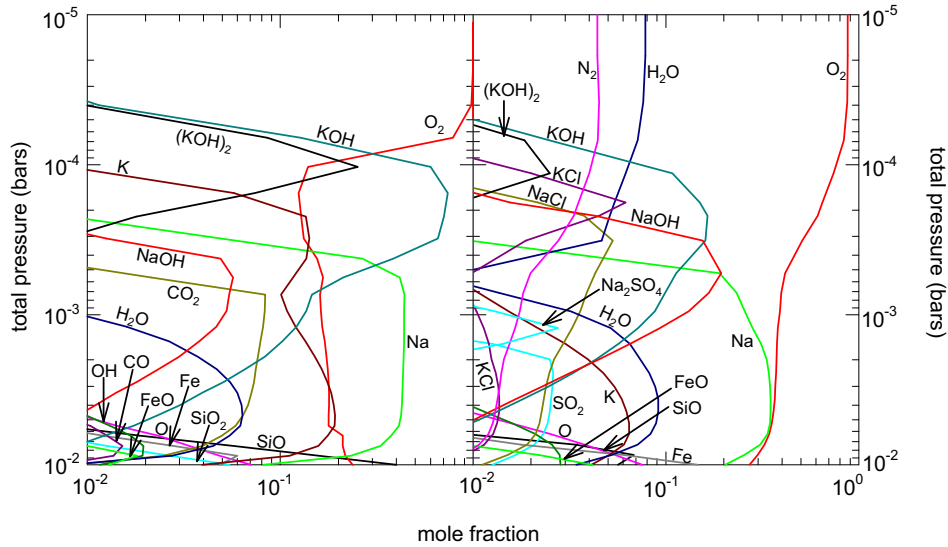


Fig. 1. Atmospheric composition for a planet similar to CoRoT-7b. Starting compositions were taken for the continental crust (left) and the bulk silicate Earth (right) at 2500 K and 10^{-2} bars. Reproduced with permission from Schaefer et al. (2012).

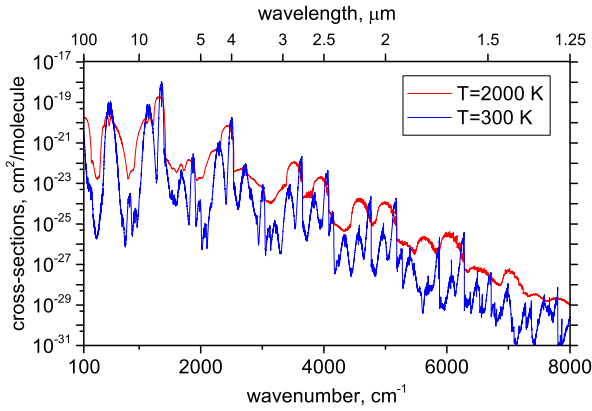


Fig. 2. Absorption spectrum of SO_2 at $T = 300$ K and 2000 K simulated using the ExoAmes line list (Underwood et al., 2016b).

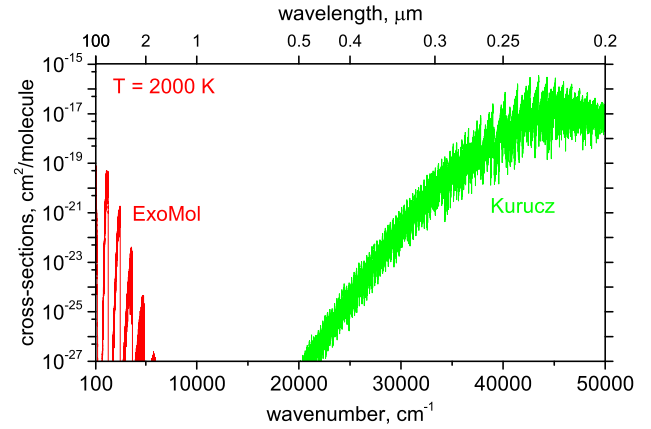


Fig. 3. SiO absorption at 2000 K: infrared data are taken from ExoMol by Barton et al. (2013) and ultraviolet data from Kurucz (2011).

O_2 , HF , SO_2 , HCl , OH , CO with continental crust (CC) magmas (in order of decreasing abundance (mole fractions $0.8 - 0.01$)) and H_2O , CO_2 , SO_2 , H_2 , CO , HF , H_2S , HCl , SO , for bulk silicate Earth (BSE) magmas. Other gases thought to be present but with smaller mole fractions ($0.01 - 0.001$) include NaCl , NO , N_2 , SO_3 , and $\text{Mg}(\text{OH})_2$ (Fegley et al., 2016).

At temperatures above about 1000 K, sulfur dioxide would enter the atmosphere, which leads the exoplanet’s atmosphere to be like Venus’s, but with steam. SO_2 is a spectroscopically important molecule that is generally not included in models of terrestrial exoplanet atmospheric models (Schaefer et al., 2012). In high concentrations (greater than a few ppm), more than one spectral feature of SO_2 are detectable even in low resolution between 4 and 40 μm (Kaltenegger and Sasselov, 2010), see also Fig. 2. This suggests that SO_2 should be included when generating models of atmospheric spectra for terrestrial exoplanets (Schaefer et al., 2012). At high temperatures and low pressures SO_2 dissociates to SO (Schaefer et al., 2012). Other atmospheric constituents of Venus-like exoplanets include CO_2 , CO , SO_2 , OCS , HCl , HF , H_2O , H_2S (Schaefer and Fegley, 2011).

Kaltenegger et al. (2010) studied vulcanism of rocky planets and estimated the observation time needed for the detection of volcanic activity. The main sources of emission were suggested to be

H_2O , H_2 , CO_2 , SO_2 , and H_2S . Again SO_2 should be detectable at abundances of a few ppm for wavelengths between 4 and 40 μm .

Apart from SO_2 , significant amounts of CH_4 and NH_3 are expected, especially in BSE atmospheres at low temperatures. Although photochemically unstable, these gases are spectroscopically important and should be considered in spectroscopic models of atmospheres. When sparked by lightning, they combine to form amino acids, as in the classic Miller-Urey experiment on the origin of life (Miller and Urey, 1959). Models of exoplanets suggest that NO and NO_2 , as well as a number of other species, are likely to be key products of lightning in a standard exoplanet atmosphere (Ardaseva et al.). Further thermochemical and photochemical processing of the quenched CH_4 and NH_3 can lead to significant production of HCN (and in some cases C_2H_2). It has been suggested that HCN and NH_3 will be important disequilibrium constituents of exoplanets with a broad range of temperatures which should not be ignored in observational analyses (Moses, 2014).

Ito et al. (2015) suggested that SiO absorption dominates the UV and IR wavelength regions with the prominent absorption features at around 0.2, 4, 10 and 100 μm , see Fig. 3. In particular, in the cases of Kepler-10b and 55 Cnc e, those features are potentially detectable by the space-based observations that should be

possible in the near future (Ito et al., 2015). Models suggest that a photon-limited, JWST-class telescope should be able to detect SiO in the atmosphere of 55 Cnc e with 10 hours of observations (Kite et al., 2016) using secondary-eclipse spectroscopy. Such observations have the potential to study lava planets even with clouds and lower-atmospheres (Samuel et al., 2014).

Other abundant species that may contribute to the transmission spectrum include CO, OH, and NO at high temperatures. These molecules should be present in a planet with an O₂-rich atmosphere and magma oceans, such as were recently suggested as the composition of the super-Earth GJ 1132b by Schaefer et al. (2016).

It is suggested that for atmospheres of hot rocky super-Earths with high temperature (> 1800 K) and low pressure almost all rock is vaporised, while at high pressure (> 100 bar) much of this material is in the condensed phase (Schaefer et al., 2012). Most elements found in rocks are expected to be soluble in steam (Fegley et al., 2016), including Mg, Si, and Fe from SiO₂-rich (i.e., felsic) silicates (like Earth's continental crust) and MgO-, FeO-rich (i.e., mafic) silicates (Schaefer et al., 2012). This can lead to gases such as Si(OH)₄, Mg(OH)₂, Fe(OH)₂, Ni(OH)₂, Al(OH)₃, Ca(OH)₂, **NaOH**, and **KOH** (Schaefer et al., 2012). Silica (SiO₂) dissolves in steam primarily via formation of Si(OH)₄ (Plyasunov, 2012), while MgO in steam leads to production of gaseous Mg(OH)₂, see, for example, Alexander et al. (1963). However it seems likely that at the temperatures under consideration many of these more complex species would fragment into diatomic or triatomic species, and water.

The predicted vaporised constituents of the steam atmosphere at higher temperatures (4000 K) include (Schaefer et al., 2012) Fe and **FeO** (products of Fe(OH)₂ fragmentation), **MgO**, Titanium dioxide TiO₂ (the major Ti-bearing gas with abundance of 1.1%), PO₂ and then **PO** (with increasing temperature), MnF₂ and MnO (from vaporised bulk Mn), CrO₂F, CrO₂, and CrO (from vaporised bulk CrO), Ca(OH)₂ and AlO (although calcium and aluminum are less abundant). TiO₂ can lead to **TiO** (Balducci et al., 1972), which is well-known to be a source of major absorption from near-infrared to the optical spectral regions of M dwarfs (Allard et al., 1997). There have been attempts to detect (Desert et al., 2008) and a recent reported detection of TiO in exoplanet atmospheres (Tsiaras et al., 2017). Whether complex polyatomic molecules like Fe(OH)₂, Ca(OH)₂, CrO₂F and P₂O₅ will survive at $T > 1000$ K is questionable. It should be noted that it is the lower pressure regimes that hold out the best prospects for analysis using transit spectroscopy, as the high pressures will tend to result in opaque atmospheres.

Post-impact rocky planets are shown to have very similar atmospheric and therefore spectroscopic properties. According to estimated luminosities, the hottest post-giant-impact planets will be detectable with near-infrared coronagraphs on the planned 30 m class telescopes (Lupu et al., 2014). The 1–4 μm region will be most favourable for such observations, offering bright features and better contrast between the planet and a potential debris disk. The greenhouse absorbers in a rocky exoplanet atmosphere strongly influence its cooling properties. The very large cooling timescales (on the order of 10⁵ – 10⁶ yr) lead to the possibility of discovering tens of such planets in future surveys (Lupu et al., 2014). It has recently been suggested (Barr and Syal, 2017) that even gas giant planets may form visible massive, rocky exomoons as a result of giant impacts.

55 Cnc e is currently the most attractive candidate magma planet for observations (Demory et al., 2016; Tsiaras et al., 2016); its atmosphere is amenable to study using secondary-eclipse spectroscopy and high-dispersion spectroscopy observations.

It is thought that during its formation of the atmosphere of the early Earth was dominated by steam which contained water-bearing minerals (Abe and Matsui, 1988; Alfvén and Arrhenius, 1974; Elkins-Tanton and Seager, 2008; Fegley et al., 2016; Kasting, 1988; Lebrun et al., 2013; Matsui and Abe, 1986; Zahnle et al.,

Table 1

Molecules thought to be important for spectroscopy of the atmospheres of hot rocky super-Earths.

CH ₄ , C ₂ H ₂ , CO, CO ₂ , H ₂ , HCl, HCN, HF, H ₂ O, H ₂ S, KCl, KOH, MgO, Mg(OH) ₂ , NaCl, NaOH, NH ₃ , NO, OH, PO ₂ , SiO, SiO ₂ , SO, SO ₂ , SO ₃ , ZnS

1988). As Lupu et al. (2014) pointed out, modern state-of-the-art radiative transfer in runaway and near-runaway greenhouse atmospheres (Abe and Matsui, 1988; Kasting, 1988) are mainly based on the absorption of H₂O and CO₂, with rather crude description of hot bands and neglecting other opacity sources. It is important, however, that the line-by-line radiative transfer calculations of outgoing longwave radiation include greenhouse absorbers of a rocky exoplanet atmosphere affecting its cooling. Discussion of such data is given below.

It should be noted that clouds and hazes can lead to flat, featureless spectra of a super-Earth planet (Morley et al., 2015), preventing detection of some or all of the spectral features discussed above. As Morley et al. (2015) argued, it is however possible to distinguish between cloudy and hazy planets in emission: NaCl and sulphide clouds cause brighter albedos with ZnS known to have a distinct feature at 0.53 μm.

A summary of the molecules important for the spectroscopy of hot melting planets is given in Table 1. The following sections in turn discuss how suitable spectroscopic data can be assembled and the present availability of such data required for retrievals from the atmospheres of rocky super-Earths which are essential for analysis of the exoplanetary observations. Exactly these types of hot rocky objects will be the likely targets of NASA's JWST (due for launch in 2018) and other exoplanet transit observations. Models suggest that magma-planet clouds and lower-atmospheres can be observed using secondary-eclipse spectroscopy (Kite et al., 2016) and that a photon-limited JWST-class telescope should be able to detect SiO, Na and K in the atmosphere of 55 Cnc e with 10 hours of observations (Ito et al., 2015). Furthermore, albedo measurements are possible at lower signal to noise; they may correspond to the albedo of clouds, or the albedo of the surface (Demory, 2014; Rouan et al., 2011).

High quality is also needed for complementary high-dispersion spectroscopic (Hoeijmakers et al., 2015a, 2015b; Snellen, 2014) (see Fig. 4, where the technique is illustrated using Doppler shifted TiO lines). For example TiO could not be detected in the optical transmission spectrum of HD 209458b due to (arguably) poor quality of the TiO spectral data (Hoeijmakers et al., 2015b).

The above discussion concentrates on molecular species and infrared spectra. However, transit observation of atomic spectra at visible wavelengths, particularly due atomic hydrogen (Vidal-Madjar et al., 2003) and sodium (Charbonneau et al., 2002), were actually the earliest spectroscopic studies of exoplanets. More recently, the Hubble Space Telescope has been used to perform transit spectroscopy of exoplanets in the ultraviolet revealing the presence of both neutral Mg (Bourrier et al., 2015) and its ion Mg⁺ (Fossati et al., 2010), as well as the possible detection a variety of other possible atoms and atomic ions.

3. Methodology

The spectroscopic data required to perform atmospheric models and retrievals comprise line positions, partition functions, intensities, line profiles and the lower state energies E'' , which are usually referenced to as 'line lists'. Given the volume of data required for construction of such line lists is far from straightforward. When

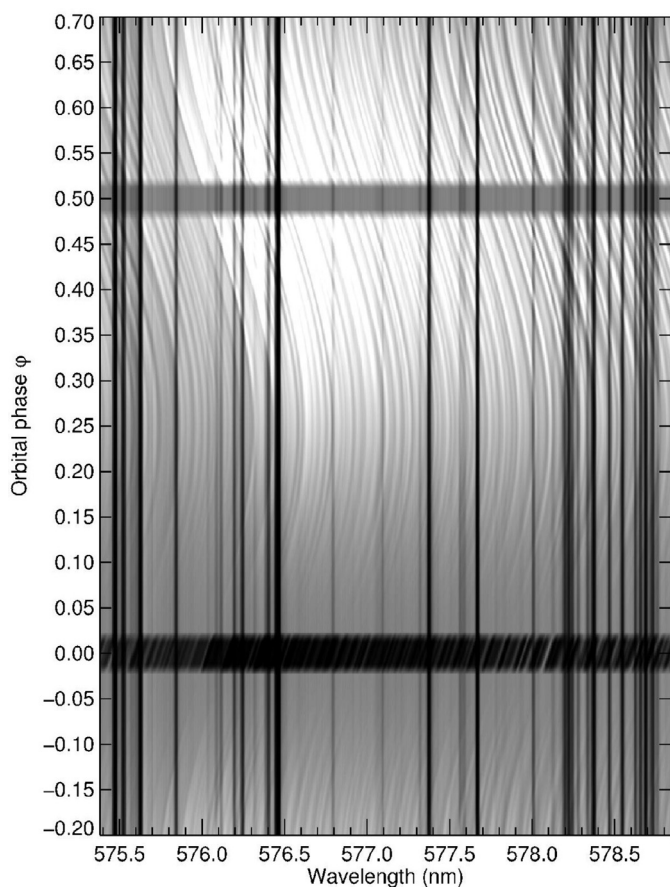


Fig. 4. Toy model of the phase-dependent Doppler shift of TiO lines along the orbit of HD 209458b. The white curves represent TiO-emission features owing to the inversion layer. The black vertical lines are stellar absorption lines, which are stable in time. This difference in the behaviour of stellar and planetary features provides a means of contrast between star and planet. Credit: Hoeijmakers et al. (2015b), reproduced with permission ©ESO.

considering how this is best done it is worth dividing the systems into three classes:

1. Diatomic molecules which do not contain a transition metal atom which we will class as simple diatomics;
2. Transition metal containing diatomics such as TiO;
3. Polyatomic molecules.

For simple diatomics it is possible to construct experimental line lists which cover the appropriate ranges in both lower state energies and wavelength. There are line lists available which are based entirely on direct use of experimental data (Yu et al., 2014) or use of empirical energy levels and calculated, *ab initio*, dipole moments and hence transition intensities (Brooke et al., 2016). It is also possible to generate such line lists by direct solution of the nuclear motion Schrödinger equation (Le Roy, 2017; Yurchenko et al., 2016b) for a given potential energy curve and dipole moment function (Yadin et al., 2012). This means that while there are still simple diatomics for which line lists are needed, it should be possible to generate them in a reasonably straightforward fashion.

When the diatomic contains a transition metal, things are much less straightforward (McKemmish et al., 2016a; Tennyson et al., 2016b). These systems have low-lying electronic states and it is necessary to consider vibronic transitions between several states plus couplings and transition dipole moments between the states. The curves required to give a full spectroscopic model of systems for which vibronic transitions are important are summarized in Fig. 5 for aluminium monoxide, AlO. AlO is a relatively sim-

ple system which only requires consideration of three electronic states. This should be contrasted with the yet unsolved case of iron monoxide, FeO, where there are more than fifty low-lying electronic states (Sakellaris et al., 2011) which means that a full spectroscopic model will require consideration of several hundred coupling curves and a similar number of transition dipoles.

Experimentally, open shell transition metal systems are challenging to prepare and the resulting samples are usually not thermal which makes it hard to obtain absolute line intensities. Under these circumstances it is still possible to measure decay lifetimes which are very useful for validating theoretical models. Lifetime measurements are currently rather rare and we would encourage experimentalists to make more of these for transition metal systems. Furthermore, the many low-lying electronic states are often strongly coupled and interact, which makes it difficult to construct robust models of the experimental data. From a theoretical perspective, the construction of reliable potential energy curves and dipole moment functions remains difficult with currently available *ab initio* electronic structure methods (McKemmish et al., 2016a; Tennyson et al., 2016b). The result is that even for important systems such as TiO (Allard et al., 2000), well-used line lists (Plez, 1998; Schwenke, 1998) are known to be inadequate (Hoeijmakers et al., 2015a).

For polyatomic molecules there have been some attempts to construct line lists directly from experiment, for example for ammonia (Hargreaves et al., 2012b, 2012c) and methane (Hargreaves et al., 2012a, 2015). However, this process is difficult and can suffer from problems with both completeness (Hill et al., 2013) and the correct inclusion of temperature dependence. The main means of constructing line lists for these systems has therefore been variational nuclear motion calculations.

There are three groups who are systematically producing extensive theoretical line lists of key astronomical molecules. These are the NASA Ames group of Huang et al. (2014a, 2016), the Reims group of Tyuterev, Nikitin and Rey who are running the TheoReTS project (Rey et al., 2016) and our own ExoMol project (Tennyson and Yurchenko, 2012; Tennyson et al., 2016c). While there are differences in detail, the methodologies used by these three groups are broadly similar. Intercomparison for molecules such as SO₂, CO₂ and CH₄, discussed below, are generally characterized by good overall agreement between the line lists presented by different groups with completeness and coverage being the main features to distinguish them. Thus, for example, both the TheoReTS and ExoMol groups pointed out that the 2012 edition of the HITRAN database (Rothman et al., 2013) contained a spurious feature due to methane near 11 μm (Rey et al., 2014; Yurchenko and Tennyson, 2014), which led to its removal in the 2016 release of HITRAN (Gordon et al., 2017).

Fig. 6 illustrates the procedure whereby line lists of both rotation-vibration and rotation-vibration-electronic transitions are computed using variational nuclear motion calculations. These calculations are based on the direct use of a potential energy surface (PES) to give energy levels and associated wavefunctions, and dipole moment surfaces (DMS) to give transition intensities (Lodi and Tennyson, 2010). For vibronic spectra such as those encountered with the open-shell diatomics the spin-orbit (SO), electronic angular momentum (EAM) and transition dipole moments (TDM) curves are also required. The procedure is well established (Tennyson, 2012) in that for all but a small number of systems with very few electrons (Engel et al., 2005; Mizus et al., 2017; Sochi and Tennyson, 2010), the PES used is spectroscopically determined. That is, an initial high-accuracy *ab initio* PES is systematically adjusted until it reproduces observed spectra as accurately as possible. Conversely, all the evidence suggests that the use of a purely *ab initio* DMS gives better results than attempts to fit this empiri-

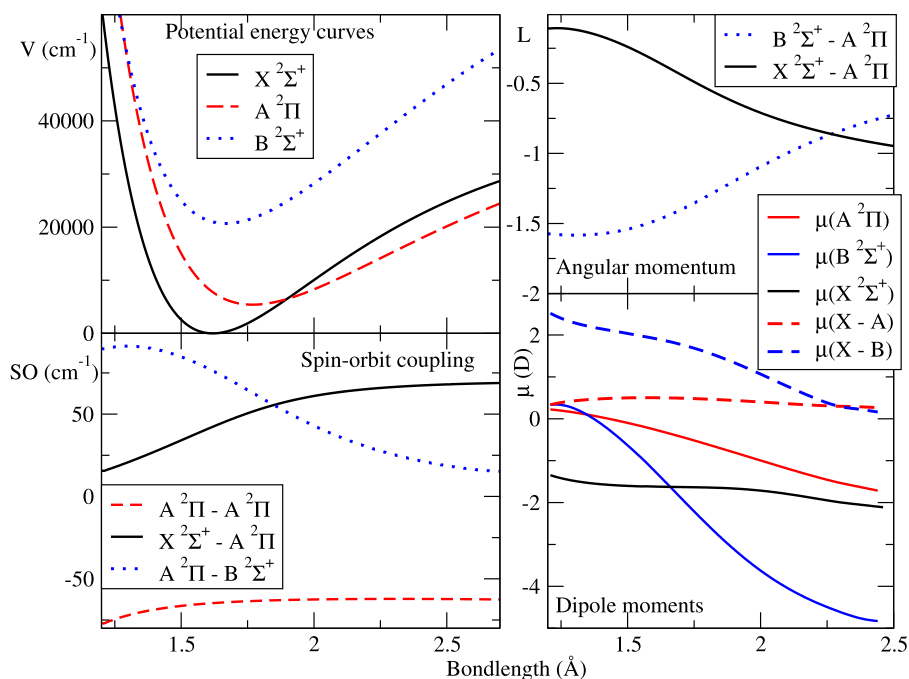


Fig. 5. Curves representing the spectroscopic model of AlO (Patrascu et al., 2014, 2015); in this model the potential energy curves are coupled by both spin-orbit and electronic angular momentum effects.

ically (Lodi et al., 2011; Lynas-Gray et al., 1995; Polyansky et al., 2015).

The PE, SO, EAM and (T)DM surfaces are usually interpolated by appropriate analytical representations to be used as an input for the nuclear motion program. The quality of the PES (as well as of the coupling curves) is improved *a priori* by refining the corresponding expansion parameters by comparison with laboratory high resolution spectroscopic data. This refinement, particularly of PESs, using spectroscopic data is now a well-developed procedure pursued by many groups. For example, the Ames group have provided a number highly accurate PES for small molecules based on very extensive refinement of the PES (Huang et al., 2011, 2012, 2014b) starting from initial, high accuracy, *ab initio* electronic structure calculations. Our own preference is to constrain such fits to remain close to the original *ab initio* PES (Yurchenko et al., 2011b); this has the benefit of forcing the surface to remain physically correct in regions not well-characterized experimentally. Such regions are often important for calculations of extensive, hot line lists. Further discussion of the methods used to refine PESs can be found in Tennyson (2012).

Our computational tools include the variational nuclear-motion programs Duo (Yurchenko et al., 2016b), DVR3D (Tennyson et al., 2004), and TROVE (Yachmenev and Yurchenko, 2015; Yurchenko et al., 2007) which calculate the rovibrational energies, eigenfunctions, and transition dipoles for diatomic, triatomic and larger polyatomic molecules, respectively. These programs have proved capable of producing accurate spectra for high rotational excitations and thus for high-temperature applications. All these codes have been adapted to face the heavy demands of computing very large line lists (Tennyson and Yurchenko, 2017) and are available as freeware.

Duo was recently developed especially for treating open-shell system of astrophysical importance (Lodi et al., 2015; McKemmish et al., 2016b; Patrascu et al., 2015; Yurchenko et al., 2016a). To our knowledge Duo is currently the only code capable of generating spectra for general diatomic molecules of arbitrary number and complexity of couplings.

DVR3D (Tennyson et al., 2004) was used to produce line lists for several key triatomics, including H₂S, SO₂, H₂O, CO₂, HCN (Azzam et al., 2016; Harris et al., 2002b; Polyansky et al., 2016a, 2017; Underwood et al., 2016b; Zak et al., 2016, 2017a, 2017b). DVR3D is capable of treating ro-vibrational states up to dissociation and above (Silva et al., 2008). A new version appropriate for the calculation of fully-rotationally resolved electronic spectra of triatomic species has just been developed and tested for the X – C band in SO₂ (Zak and Tennyson, 2017).

TROVE is a general polyatomic code that has been used to generate line lists for hot NH₃, PH₃, H₂CO, HOOH, SO₃, CH₄ (Al-Refaie et al., 2015a, 2015b; Sousa-Silva et al., 2015, 2014; Underwood et al., 2016a; Yurchenko et al., 2011a, 2017). Intensities in TROVE are computed using the new code GAIN (Al-Refaie et al., 2017) which was written and adapted for graphical processing units (GPUs) to compute Einstein coefficients (or oscillator strengths) and integrated absorption coefficients for all individual rotation-vibration transitions at different temperatures. Given the huge number of transitions anticipated to be important at elevated temperatures, the usage of GPUs provides a huge advantage. However TROVE requires special adaptation (Chubb et al., 2017) to treat linear molecules such as the astronomically important acetylene (HCCH).

An alternative theoretical procedure has been used by Tashkun and Perevalov from Tomsk. Their methodology uses effective Hamiltonian fits to experimental data for both energy levels and transition dipoles. This group has provided high-temperature line lists for the linear CO₂ (Tashkun and Perevalov, 2011) molecule and the NO₂ (Lukashevskaya et al., 2016) system. This methodology reproduces the positions of observed lines to much higher accuracy than the variational procedure but generally extrapolates less well for transitions involving states which are outside the range of those that have been observed in the laboratory. In particular, comparisons with high-resolution transmission measurements of CO₂ at high temperatures for industrial applications suggest that indeed the CDSD-4000 CO₂ line list loses accuracy at higher temperatures. We note that the Ames group have produced variational line lists

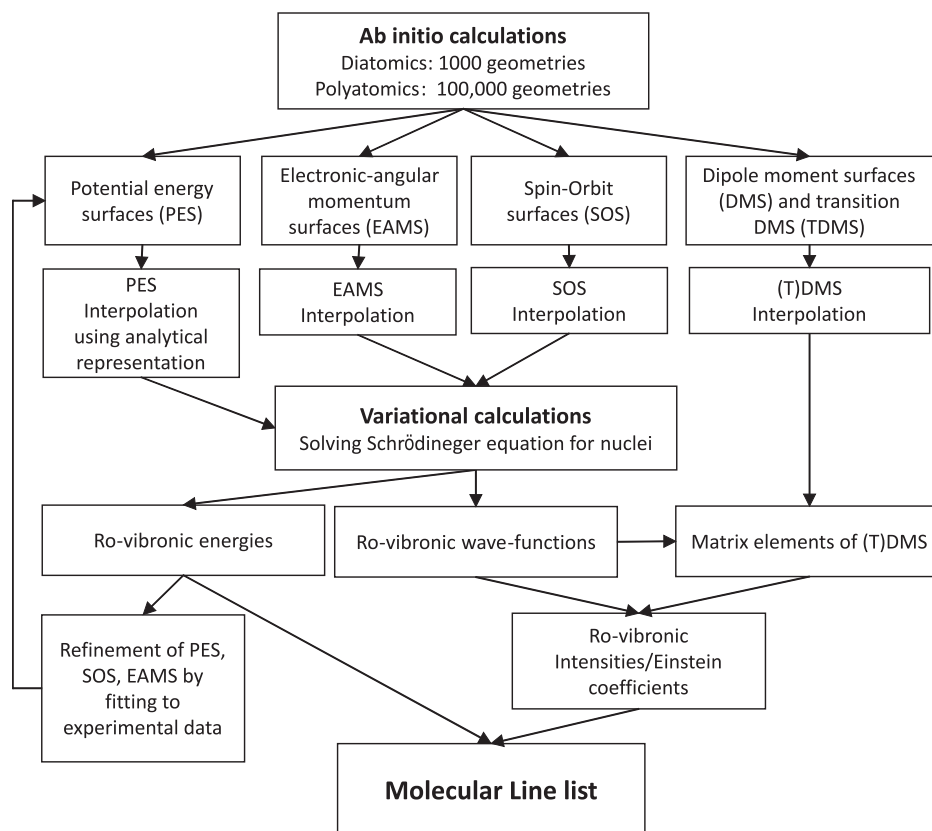


Fig. 6. The computational recipe used to produce a line list of rotation-vibration-electric (rovibronic) transitions using a mixture of *ab initio* and variational nuclear motion calculations.

for CO₂ designed to be valid up to 1500 K (Huang et al., 2013) and 4000 K (Huang et al., 2017).

As mentioned above, a disadvantage of the use of variational nuclear motion calculations is that the transition frequencies are rarely predicted with spectroscopic accuracy. One method of rectifying this problem is by use of the MARVEL (measured active rotational-vibrational energy levels) procedure (Furtenbacher et al. 2007; Furtenbacher and Császár, 2012). The MARVEL procedure inverts the measured transition frequencies to provide energy levels from which not only can the original transition frequencies be regenerated but all other transitions linking these states can also be obtained with experimental accuracy. However, the MARVEL procedure does not provide any information on levels which have yet to be observed experimentally. MARVEL datasets of energy levels are available for a range of astronomically important molecules including water (Furtenbacher et al., 2017; Tennyson et al., 2014a), H₃⁺ (Furtenbacher et al., 2013a, 2013b), NH₃ (Derzi et al., 2015; Furtenbacher et al., 2017), C₂ (Furtenbacher et al., 2016), TiO (McKemmish et al., 2017) and HCCH (Chubb et al., 2017). In particular, the energy levels and transition frequencies from the analysis of TiO spectra should provide the high-resolution transition frequencies need to allow the detection of TiO in exoplanets using high-dispersion spectroscopy for which previously available laboratory data was not precise enough (Hoeijmakers et al., 2015a). Indeed this analysis pointed to a number of issues with previous analysis of observed TiO spectra and significant shifts in transition frequencies compared to those provided by the currently available line lists (Plez, 1998; Schwenke, 1998).

The MARVEL energy levels can also be used to replace computed ones in line lists. This has already been done for several line lists (Mizus et al., 2017; Paulose et al., 2015; Wong et al., 2017). This process is facilitated by the ExoMol data structure (Tennyson

et al., 2013, 2016c) which does not store transition frequencies but instead computes them from a states file containing all the energy levels. This allows changes of the energy levels at the end of the calculation or even some time later (Barber et al., 2014; Harris et al., 2006) should improved energy levels become available.

The polyatomic molecules discussed above are all closed shell species. However the open shell species PO₂ and CaOH are thought to be important for hot atmospheres (Bernath, 2009). There have been a number of variational nuclear motion calculations on the spectra of open shell triatomic systems (Bunker et al., 2007; Hirano et al., 2008; Jensen et al., 2002; Mascaritolo et al., 2013; Odaka et al., 2007; Ostojic et al., 2016), largely based on the use of Jensen's MORBID approach (Jensen et al., 1995). However, we are unaware of any extensive line lists being produced for such systems. The extended version of DVR3D (Zak and Tennyson, 2017) mentioned above should, in due course, be applicable to these problems.

For closed-shell polyatomic molecules, such as NaOH, KOH, SiO₂, for which spectra involve rotation-vibration transitions on the ground electronic state, one would use a standard level of *ab initio* theory such as CCSD(T)-f12/aug-cc-pVTZ on a large grid of geometries ($\approx 10,000$) to compute both the PES and DMS. For diatomic molecules (NaH, KCl, SiO, MgO, ZnS, SO) characterized by multiple interacted curves the multi-reference configuration interaction (MRCI) method in conjunction with the aug-cc-pVQZ or higher basis sets is a reasonable choice, with relativistic and core-correlation effects included where feasible. The potential energy and coupling curves should then be optimized by fitting to the experimental energies or transitional wavenumbers. Indeed where there is a large amount of experimental data available, then the choice of initial potential energy curves becomes almost unimportant (Barton et al., 2013). However, the *ab initio* calculation of good dipole curves is

always essential since these are not in general tuned to observation.

The ExoMol line lists are prepared so that they can easily be incorporated in radiative transfer codes (Tennyson et al., 2016c). For example, these data are directly incorporated into the UCL Tau-REx retrieval code (Waldmann et al., 2013, 2015a, 2015b), a radiative transfer model for transmission, emission and reflection spectroscopy from the ultra-violet to infrared wavelengths, able to simulate gaseous and terrestrial exoplanets at any temperature and composition. Tau-REx uses the line lists from ExoMol, as well as HITEMP (Rothman et al., 2010) and HITRAN (Rothman et al., 2013) with clouds of different particle sizes and distribution, to model transmission, emission and reflection of the radiation from a parent star through the atmosphere of an orbiting planet. This allows estimates of abundances of absorbing molecules in the atmosphere, by running the code for a variety of hypothesised compositions and comparing to any available observations. Tau-REx is mostly based on the opacities produced by ExoMol with the ultimate goal to build a library of sophisticated atmospheres of exoplanets which will be made available to the open community together with the codes. These models will enable the interpretation of exoplanet spectra obtained with future new facilities from space (Tinetti et al., 2015, Tinetti et al., 2016) and the ground (VLT-SPHERE, E-ELT), as well as JWST.

Of course there are a number of other models for exoplanets and similar objects which rely on spectroscopic data as part of their inputs. These include modelling codes such as NEMESIS (Irwin et al., 2008), BART (Blecic et al., 2016), CHIMERA (Line et al., 2013) and a recent adaption of the UK Met Office global circulation model (GCM) called ENDGame (Amundsen et al., 2016; Mayne et al., 2014). More general models such as VSTAR (Bailey and Kedziora-Chudczer, 2012) are designed to be applied to spectra of planets, brown dwarfs and cool stars. The well-used BT-Settl brown-dwarf model (Allard, 2014; Allard et al., 2012) can also be used for exoplanets. There are variety of other brown dwarfs (Burrows et al., 2006) and cool star models (Gustafsson et al., 2008; Kurucz, 2014; Tsuji, 2008). These are largely concerned with the atmospheres of the hydrogen rich atmospheres which are, of course, characteristic of hot Jupiter and hot Neptune exoplanets, brown dwarfs and stars.

Besides direct input to models, line lists are used to provide opacity functions (Bernath, 2014; Freedman et al., 2014; 2008; Kurucz, 2011; Sharp and Burrows, 2007) whose reliability are well-known to be limited by the availability of good underlying spectroscopic data (Cushing et al., 2008). Cooling functions for key molecules are also important for the description of atmospheric processes in hot rocky objects. These functions are straightforward to compute from a comprehensive line lists (Tennyson et al., 2016a); this involve computation of integrated emissivities from all lines on a grid of temperatures typically ranging between 0 to 5000 K.

4. Available spectroscopic data

Spectroscopic studies of the Earth's atmosphere are supported by extensive and constantly updated databases largely comprising experimental laboratory data (Jacquinet-Husson et al., 2016; Rothman et al., 2013). Thus for earth-like planets, by which we mean rocky exoplanets with an atmospheric temperature below 350 K, the HITRAN database (Gordon et al., 2017) makes a good starting point. However, at higher temperatures datasets designed for room temperature studies rapidly become seriously incomplete (Yurchenko et al., 2014), leading to both very significant loss of opacity and incorrect band shapes. The strong temperature dependence of the various molecular absorption spectra is illustrated in

figures given throughout this review which compare simulated absorption spectra at 300 and 2000 K for key species.

HITRAN's sister database, HITEMP, was developed to address the problem of high temperature spectra. However the latest release of HITEMP (Rothman et al., 2010) only contains data on five molecules, namely CO, NO, O₂, CO₂ and H₂O. For all these species there are more recent hot line lists available which improve on the ones presented in HITEMP. These line lists are summarised in Table 2 below.

Table 1 gives a summary of species suggested by the chemistry models as being important in the atmospheres of hot super-Earths. Spectroscopic line lists are already available for many of the key species. Most of the species suggested by the chemistry models of such objects are already in the ExoMol database, which includes line list taken from sources other than the ExoMol project itself. This includes H₂O, CH₄, NH₃, CO₂, SO₂. Line lists for other important species, such as NaOH, KOH, SiO₂, PO, ZnS and SO are currently missing. Table 2 presents a summary of line lists available for atmospheric studies of hot super-Earths.

Line lists for some diatomics are only partial: for example accurate infrared (rotation-vibration) line lists exists for CO, SiO, KCl, NaCl, NO, but none of these line lists consider shorter-wavelength, vibronic transitions which lie in the near-infrared (NIR), visible (Vis) or ultraviolet (UV), depending on the species concerned. NIR will be covered by the NIRSPEC instrument on the board of JWST only at lower resolution and therefore the completeness of the opacities down to 0.6 μm will be crucial for the atmospheric retrievals. Such data, when available, will be important for the interpretation of present and future exoplanet spectroscopic observations.

Below we consider the status of spectroscopic data for key molecules in turn.

H₂O: As discussed above, water is the key molecule in the atmospheres of rocky super-Earths. There are a number of published water line lists available for modelling hot objects (Allard et al., 1994; Barber et al., 2006; Jørgensen et al., 2001; Partridge and Schwenke, 1997; Rothman et al., 2010; Schwenke and Partridge, 2000; Viti et al., 1997; Wattson and Rothman, 1992). Of these the most widely used are the Ames line list of Partridge and Schwenke (1997), or variants based on it, and the BT2 line list (Barber et al., 2006), which provided the basis for water in the HITEMP database (Rothman et al., 2010) and the widely-used BT-Settl brown dwarf model (Allard et al., 2007). The Ames line list is more accurate than BT2 at infrared wavelengths but less complete meaning that it is less good at modelling hotter objects. Recently Polyansky et al. (2017) have computed the POKAZaTEL line list which is both more accurate and more complete than either of these. We recommend the use of this line list, which is illustrated in Fig. 7, in future studies.

CO₂: Again there are number of line lists available for hot CO₂. In particular Taskun and Perevalov distribute these via their carbon dioxide spectroscopic databank (CDS) (Tashkun and Perevalov, 2011; Tashkun et al., 2003), an early version of CDS formed the input for HITEMP. The Ames group produced a variational line list valid up to 1500 K (Huang et al., 2013). Recent work on CO₂ has improved computed transition intensities to point where they as accurate as the measured ones (Polyansky et al., 2015; Zak et al., 2016); this suggests that there is scope for further improvement in hot line lists for this system; some work in this direction has recently been undertaken by Huang et al. (2017). Fig. 8 illustrates the temperature-dependence of the CO₂ absorption spectrum in the infrared.

CH₄: methane is an important system in carbon-rich atmospheres and the construction of hot methane line lists has been the subject of intense recent study by a number of groups both theoretically (Ba et al., 2013; Mielke et al., 2013; Rey et al., 2013a,

Table 2
Spectroscopic line lists available for studies of the atmospheres hot super-Earth exoplanets.

Molecule	N_{iso}	T_{max}	N_{elec}	N_{lines}	DSName	Reference	Methodology
SiO	5	9000	1	254 675	EJBT	Barton et al. (2013)	ExoMol
MgH	1		3	30 896		GharibNezhad et al. (2013)	Empirical
CaH	1		2	6000		Li et al. (2012)	Empirical
NH	1		1	10 414		Brooke et al. (2014a)	Empirical
CH	2		4	54 086		Masseron et al. (2014)	Empirical
CO	9	9000	1	752 976		Li et al. (2015)	Empirical
OH	?	6000	1	$\Delta v = 13$		Brooke et al. (2016)	Empirical
CN	1		1	195 120		Brooke et al. (2014b)	Empirical
CP	1		1	28 735		Ram et al. (2014)	Empirical
HF	2		1	13 459		Li et al. (2013)	Empirical
HCl	4		1	34 250		Li et al. (2013)	Empirical
NaCl	2	3000	1	702 271	Barton	Barton et al. (2014)	ExoMol
KCl	4	3000	1	1 326 765	Barton	Barton et al. (2014)	ExoMol
PN	2	5000	1	142 512	YYLT	Yorke et al. (2014)	ExoMol
AlO	4	8000	3	4 945 580	ATP	Patrascu et al. (2015)	ExoMol
NaH	2	7000	2	79 898	Rivlin	Rivlin et al. (2015)	ExoMol
CS	8	3000	1	548 312	JnK	Paulose et al. (2015)	ExoMol
CaO	1	5000	5	21 279 299	VBATHY	Yurchenko et al. (2016a)	ExoMol
NO	6	5000	5	2 281 042	NOname	Wong et al. (2017)	ExoMol
VO	1	5000	13	277 131 624	VOMYT	McKemmish et al. (2016b)	ExoMol
H ₂ O	4 ^a	3000	1	12 000 000 000	PoKaZoTeL	Polyansky et al.	ExoMol
CO ₂	4 ^b	4000	1	628,324,454	CDS-4000	Tashkun and Perevalov (2011)	Empirical
SO ₂	1	2000	1	1 300 000 000	ExoAmes	Underwood et al. (2016b)	ExoMol
H ₂ S	1	2000	1	115 530 373	ATY2	Azzam et al. (2016)	ExoMol
HCN/HNC	2 ^c	4000	1	399 000 000	Harris	Barber et al. (2014)	ExoMol
NH ₃	2 ^d	1500	1	1 138 323 351	BYTe	Yurchenko et al. (2011a)	ExoMol
PH ₃	1	1500	1	16 803 703 395	SAITY	Sousa-Silva et al. (2015)	ExoMol
CH ₄	1	1500	1	9 819 605 160	10to10	Yurchenko and Tennyson (2014)	ExoMol

N_{iso} : Number of isotopologues considered; T_{max} : Maximum temperature for which the line list is complete; N_{elec} : Number of electronic states considered; N_{lines} : Number of lines: value is for the main isotope. DSName: Name of line list chosen by the authors, if applicable. ^a The VIT line list for HDO due to Voronin et al. (2010) and HotWat78 due to Polyansky et al. (2016a) for H₂¹⁷O and H₂¹⁸O are also available. ^b Very recently Huang et al. (2017) have computed the Ames-2016 line lists for 13 isotopologues of CO₂ which also extend to 4000 K. ^c A line list for H¹³CN/HN¹³C due to Harris et al. (2008) is also available. ^d There is a room temperature ¹⁵NH₃ line list due to Yurchenko (2015).

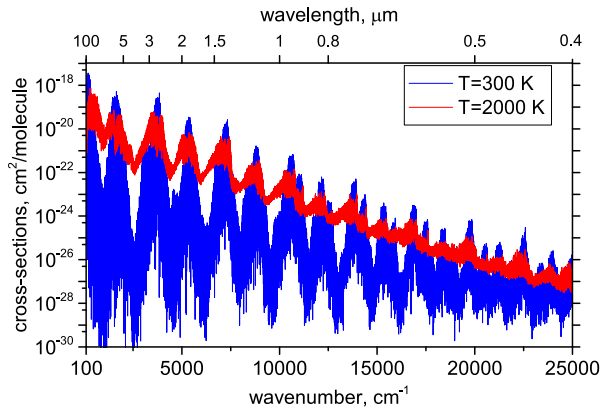


Fig. 7. Absorption spectrum of H₂O at $T = 300$ K and 2000 K simulated using the POKAZATEL line list (Polyansky et al., 2017).

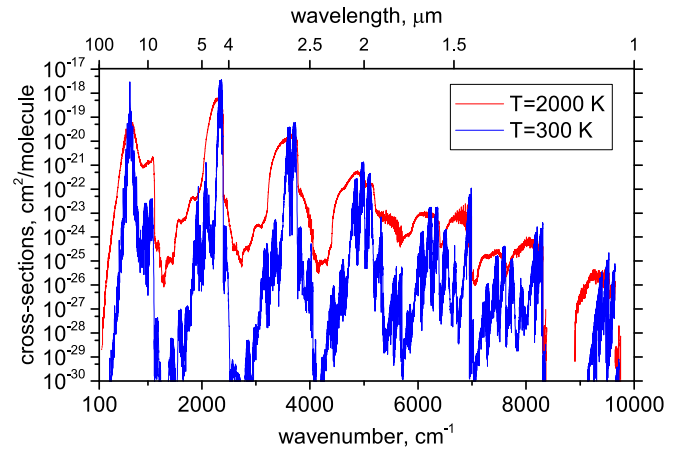


Fig. 8. Absorption spectrum of CO₂ at $T = 300$ K and 2000 K simulated using HITEMP (Rothman et al., 2010).

2013b, 2014; Schwenke, 2002; Schwenke and Partridge, 2001; Wang and Carrington, 2013; Warmbier et al., 2009; Yurchenko and Tennyson, 2014; Yurchenko et al., 2014) and experimentally (Hargreaves et al., 2012a, 2015). The most complete line lists currently available are our 10to10 line list (Yurchenko and Tennyson, 2014), which is very extensive but only valid below 1500 K, and the Reims line list (Rey et al., 2014), which spans a reduced wavelength range but is complete up to 2000 K. In fact we extended 10to10 to higher temperature some time ago but the result is a list of 34 billion lines which is unwieldy to use. We have therefore been working data compaction techniques based on the use of either background, pressure-independent cross sections (Hargreaves et al., 2015) or super-lines (Rey et al., 2016). This line list has just been released (Yurchenko et al., 2017). Fig. 9 illustrates the

temperature-dependence of the methane absorption spectrum in the infrared. The strongest bands are at 3.7 and 7.7 μm .

SO₂ and SO₃: A number of line list for SO₂ have been computed by the Ames group (Huang et al., 2014b, 2015, 2016); the most compressive is one produced in collaboration between ExoMol and Ames (Underwood et al., 2016b), see Fig. 2. This line list was validated using experimental data recorded at the Technical University of Denmark (DTU). ExoMol have also provided line lists for SO₃ (Underwood et al., 2013, 2016a). The largest of these, appropriate for temperatures up to 800 K, contains 21 billion lines. However, validation of this line list against experiments performed at DTU points to significant differences in the line intensities, suggesting that more work is required on the SO₃ dipole moment.

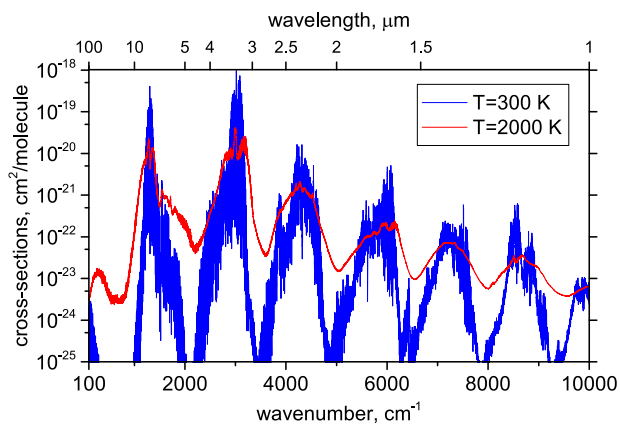


Fig. 9. Absorption spectrum of CH_4 at $T=300$ K and 2000 K simulated using the 10to10 line list (Yurchenko and Tennyson, 2014).

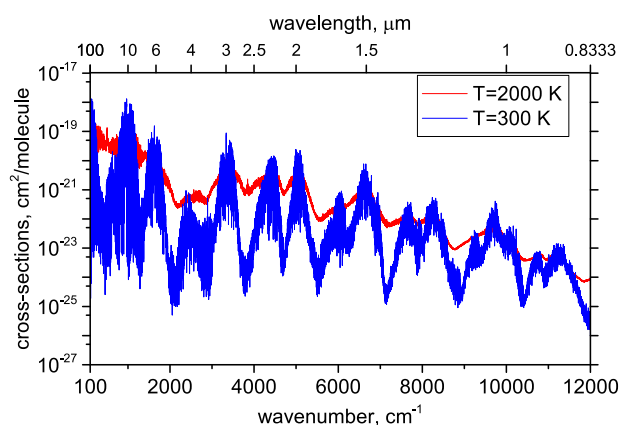


Fig. 10. Absorption spectrum of NH_3 at $T=300$ K and 2000 K simulated using the line list BYTe (Yurchenko et al., 2011a).

NH_3 : Ammonia has a very prominent absorption feature at about $10 \mu\text{m}$. Extensive line lists for ammonia are available (Yurchenko et al., 2009, 2011a). The BYTe line list (Yurchenko et al., 2011a), which was explicitly designed for needs of exoplanet spectroscopy in mind, has been used to model spectra of brown dwarfs (Bailey and Kedziora-Chudczer, 2012; Canty et al., 2015; Lucas et al., 2010). However, BYTe loses accuracy in the near infrared. Rather old laboratory measurements of room temperature for ammonia have recently been assigned (Barton et al., 2016, 2017). These data plus improved *ab initio* treatment of the problem (Polyansky et al., 2016b) and a MARVEL analysis leading to a set of accurate, empirical energy levels (Al Derzi et al., 2015; Furtenbacher et al., 2017) will form the basis of a new line list which will both extend the range and improve on the accuracy of BYTe. Fig. 10 illustrates the absorption spectra of ammonia at $T=300$ K and 2000 K. The strongest and most prominent feature is at $10 \mu\text{m}$.

H_2S : The main source of the emission of H_2S on Earth is from life (Watts, 2000). It has been, however, ruled out as a potential biosignature in atmospheres of exoplanets (Hu et al., 2013). H_2S is also generated by volcanism. Fig. 11 illustrates the absorption spectra of H_2S at $T=300$ K and 2000 K based on the AYT2 line list (Azzam et al., 2016).

HCN: Line lists for hydrogen cyanide were some of the first calculated using variational nuclear motion calculations (Eriksson et al., 1984; Harris et al., 2002b). Indeed the first of these line list was the basis of a ground-breaking study by Jørgensen et al. (1985) showed that use of a comprehensive HCN line list in a model atmosphere of a ‘cool’ carbon star made a huge difference:

extending the model of the atmosphere by a factor of 5, and lowering the gas pressure in the surface layers by one or two orders of magnitude. The line list created and used by Jørgensen and co-workers (Eriksson et al., 1984; Jørgensen et al., 1985) only considered HCN. However HCN is a classic isomerizing system and the HNC isomer should be thermally populated at temperatures above about 2000 K (Barber et al., 2002; Harris et al., 2003). More recent line lists (Barber et al., 2014; Harris et al., 2008, 2002b, 2006) consider both HCN and HNC together. All these line lists are based on the use of *ab initio* rather than spectroscopically-determined PESS, which can lead to significant errors in the predicted transition frequencies (Harris et al., 2002a). However the most recent line list, due to (Barber et al., 2014) used very extensive sets of experimental energy levels obtained by Mellau for both hot HCN and hot HNC (Mellau, 2011a, 2011b) to improve predicted frequencies to, essentially, experimental accuracy. This line list was used for the recent, tentative detection of HCN on super-Earth 55 Cancri e (Tsiaras et al., 2016). The line list of Barber et al. (2014) is illustrated in Fig. 12.

CO: is the most important diatomic species in a whole range of hot atmospheres ranging from warm exoplanets to cool stars from a spectroscopic perspective (Li et al., 2015) recently produced comprehensive line lists for the nine main isotopologues of CO. Fig. 13 illustrates the absorption spectrum of the main isotopologue, $^{16}\text{C}^{12}\text{O}$.

NO: a new comprehensive line list for nitric oxide has recently been released by Wong et al. (2017), see Fig. 14.

SiO: Fig. 3 illustrates the absorption spectrum of SiO molecule. SiO is well known in sunspots Campbell et al. (1995) and is thought likely to be an important constituent of the atmosphere of hot rocky super-Earths. An IR line list for SiO available from ExoMol (Barton et al., 2013) and a less accurate UV line list is provided by Kurucz (2011).

Line lists are available for both NaCl and KCl (Barton et al., 2014), see Fig. 15. However, these line lists do not consider electronic transitions, which are likely to be very strong; the line lists are therefore only useful for simulation of the spectra of these species at long (infrared) wavelengths. Figs. 16 and 17 illustrate line list for species whose electronic spectra give prominent features: AlO and CaO respectively. The spectra are only shown for $T=2000$ K as these species are unlikely to be found in the gas phase at 300 K.

There are a number of systems which have been identified as likely to be present in the atmospheres of hot rocky super-Earths for which there are no available line lists. Indeed for most of these species, which include NaOH, KOH, SiO_2 , MgO , PO_2 , $\text{Mg}(\text{OH})_2$, SO, ZnS (see Table 1), there is little accurate spectroscopic data of any sort. Clearly these systems will be targets of future study.

Probably the most important polyatomic molecule, at least for exoplanet and cool star research, for which there is still not a comprehensive hot line list is acetylene (HCCH). Acetylene is a linear molecule for which variational calculations are possible (Kozin et al., 2005; Urru et al., 2010) and an extensive effective Hamiltonian fit is available (Amyay et al., 2016). One would therefore expect such a line list to be provided shortly.

5. Other considerations

All the discussion above has concentrated very firmly on line spectra. However there are a number of issues which need to be considered when simulating or interpreting exoplanet spectra (Grimm and Heng, 2015). A discussion of procedures for this is given in Chapter 5 of the recent book by Heng (2017). General codes, such as HELIOS (Grimm and Heng, 2015); Malik et al., 2017) and our own ExoCross (Yurchenko et al., 2017), are available

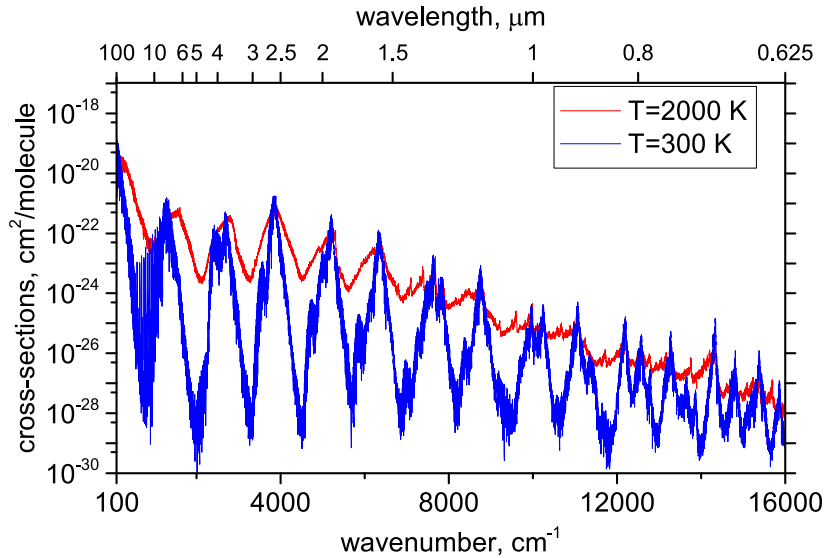


Fig. 11. Absorption spectrum of H_2S at $T=300$ K and 2000 K simulated using the ExoMol line list AY2 (Azzam et al., 2016).

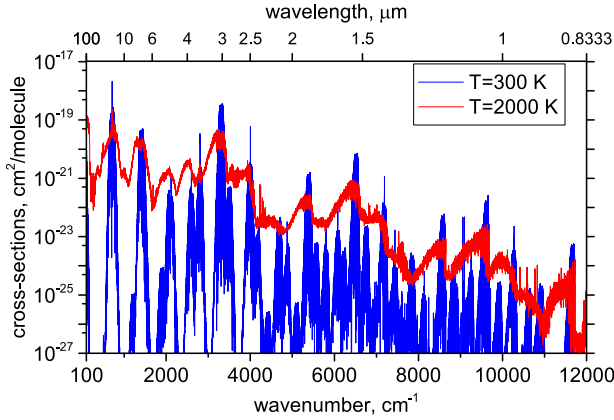


Fig. 12. Absorption spectrum of the HCN/HNC system at $T=300$ K and 2000 K simulated using the ExoMol line list (Barber et al., 2014).

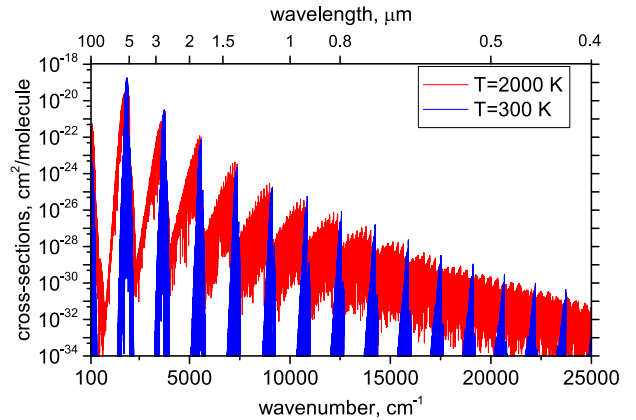


Fig. 14. Absorption spectrum of NO at $T=300$ K and 2000 K simulated using the ExoMol line list (Wong et al., 2017).

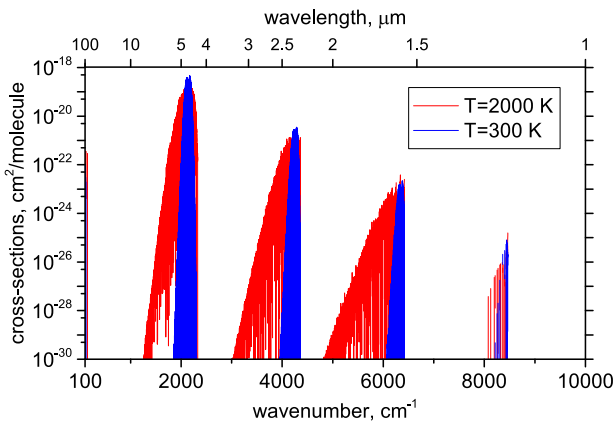


Fig. 13. Absorption spectrum of CO at $T=300$ K and 2000 K, generated using the data of Li et al. (2015).

for taking appropriate line lists and creating inputs suitable for radiative transfer codes.

The first issue to be considered is the shape of the individual spectral lines. Lines are Doppler broadened with temperature due to the thermal motion of the molecules and broadened by pressure

due to collisional effects. While the total absorption by an optically thin line is conserved as function of temperature and pressure; this is not true for optically thick lines. For these lines use of an appropriate line profile can have a dramatic effect (Amundsen, et al., 2014; Tinetti et al., 2012). The nature of primary transit spectra, where the starlight has a long pathlength through the limb of the exoplanet atmosphere, is good for maximizing sensitivity but also maximizes the likelihood of lines being saturated. This means that it is important to consider line profiles when constructing line list for exoplanet studies.

While it is straightforward to include the thermal effects via the Doppler profile; pressure effects in principle depend on the collision partners and the transition concerned. Furthermore, there has been comparatively little work on how pressure broadening behaves at high temperatures (Tennyson et al., 2014b). Studies are beginning to consider broadening appropriate to exoplanet atmospheres (Barton et al., 2017a; Faure et al., 2013; Hedges and Madhusudhan, 2016; Barton et al., 2017b). However, thus far these studies have concentrated almost exclusively on pressure effects in hot Jupiter exoplanets, which means that molecular hydrogen and helium have been the collision partners considered. The atmospheres of hot rocky super-Earths are likely to be heavy meaning that pressure broadening will be important. Clearly there is work

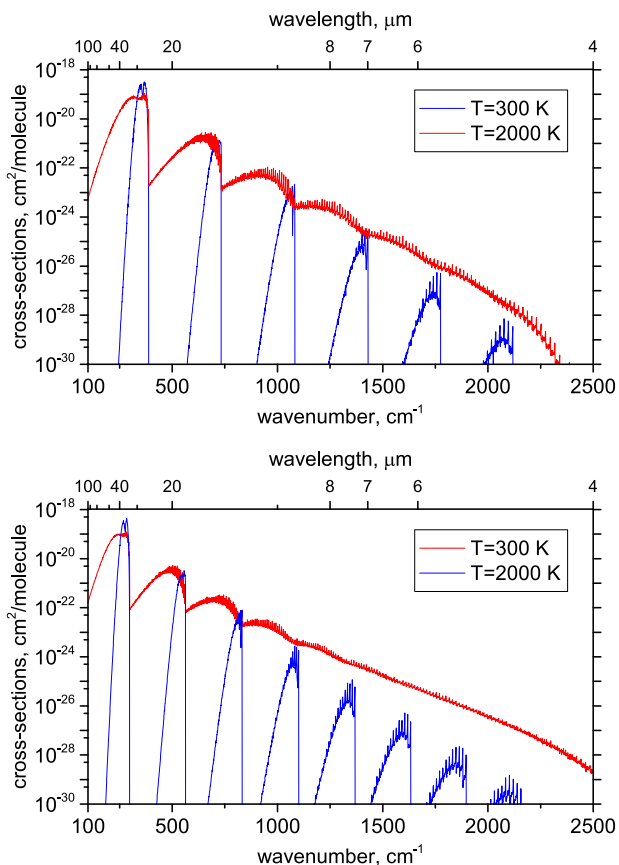


Fig. 15. Infrared absorption spectra of NaCl (upper) and KCl (lower) at $T = 300$ K and 2000 K simulated using the ExoMol line list (Barton et al., 2014).

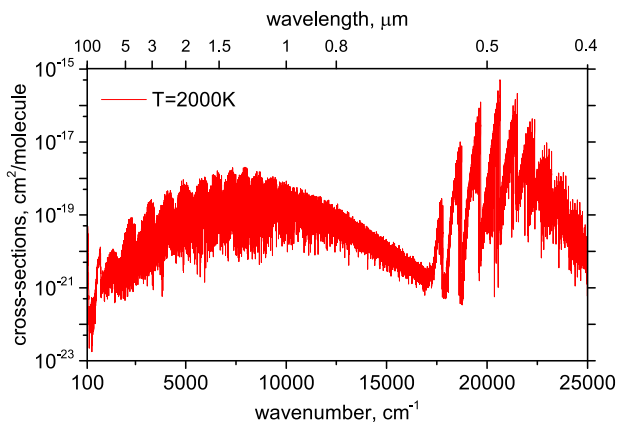


Fig. 16. Absorption spectrum of AlO at $T = 2000$ K simulated using the ExoMol line list (Patrascu et al., 2015).

to be done developing appropriate pressure-broadening parameters for the atmospheres of these planets. We note, however, that line broadening parameters appropriate for studies of the atmosphere of Venus are starting to become available, largely on the basis of theory (Gamache et al., 2016, 2011; Lavrentieva et al., 2014; Sagawa et al., 2009).

Besides broadening, it is also necessary to consider collision-induced absorption in regions where there are no spectral lines. On Earth it is known that the so-called water continuum makes an important contribution to atmospheric absorption (Shine et al., 2012). Similarly collision induced absorption (CIA) in H_2 is well known to be important in hydrogen atmospheres (Abel et al., 2011). CIA has

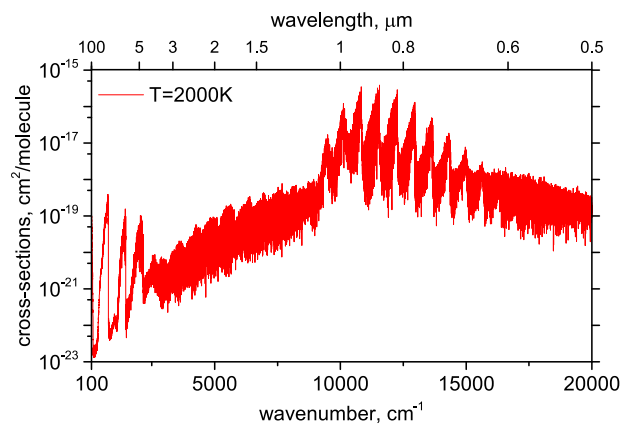


Fig. 17. Absorption spectrum of CaO at $T = 2000$ K simulated using the ExoMol line list (Yurchenko et al., 2016a).

also been detected involving K-H_2 collisions (Morley et al., 2014). What CIA processes are important in lava planets is at present uncertain.

Finally it is well-known that the spectra of many (hot Jupiter) exoplanets are devoid of significant features, at least in the NIR (Sing et al., 2016; Tsiaras et al., 2017). It is thought that this is due to some mixture of clouds and aerosols, often described as hazes. Such features are likely to also form in the atmospheres of rocky exoplanets. It remains unclear precisely what effect these will have on the resulting observable spectra of the planet.

6. Conclusions

To conclude, the atmospheres of hot super-Earths are likely to be spectroscopically very different those of other types of exoplanets such as cold super-Earth or gas giant due to both the elevated temperatures and the different atmospheric constituents. This means that a range of other species, apart from the usual H_2O , CH_4 , CO_2 and CO , must be also taken into consideration. A particularly interesting molecule that is likely to feature in atmospheric retrievals is SO_2 . Detection of SO_2 could be used to differentiate super-Venus exoplanets from the broad class of super-Earths. A comprehensive line list for SO_2 is already available (Underwood et al., 2016b). SiO , on other hand, is a signature of a rocky object with potentially detectable IR and UV spectral features. Another interesting species is ZnS , which can be used to differentiate clouds and hazes. At present there is no comprehensive line list for ZnS to inform this procedure.

Models of hot super-Earths suggest that these exoplanets appear to resemble many properties of the early Earth. An extensive literature exists on the subject of the early Earth, which can be used as a basis for accurate prediction of the properties of the hot rocky exoplanets. Super-Earths also provide a potential testbed for atmospheric models of the early Earth which, of course, are not amenable to direct observational tests. Post-impact planets may also be also very similar in chemistry and spectroscopy.

From different studies of the chemistry and spectroscopy of hot super-Earth we have identified a set of molecules suggested either as potential trace species or sources of opacities for these objects. The line list for a significant number of these species are either missing or incomplete. Our plan is systematically create line lists for these key missing molecules and include into the ExoMol database.

Acknowledgments

We thank Giovanna Tinetti, Ingo Waldmann and the members of the ExoMol team for many fruitful discussions, and Laura Schaefer for providing a figure. The ExoMol project was supported by the ERC under the Advanced Investigator Project 267219. This work was supported by the UK Science and Technology Research Council (STFC) No. ST/M001334/1. This work made extensive use of the DiRAC@Darwin and DiRAC@COSMOS HPC clusters. DiRAC is the UK HPC facility for particle physics, astrophysics and cosmology which is supported by STFC and BIS. The support of the COST action MOLIM No. CM1405. This research has made use of the NASA Exoplanet Archive, which is operated by the California Institute of Technology, under contract with the National Aeronautics and Space Administration under the Exoplanet Exploration Program.

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