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The Status of Spectroscopic Data for the EChO Mission

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ABSTRACT

The status of laboratory spectroscopic data for the EChO mission is reviewed. For many molecules (eg H_2O, CO, CO_2, H_3^+, O_2, O_3) the data are already available. For the other species work is actively in progress constructing this data. Much of the is work is being undertaken by ExoMol project (`www.exomol.com`). This information will be used to construct and EChO-specific spectroscopic database.

1 INTRODUCTION

The EChO (Exoplanet Characterisaton Observatory) mission (Tinetti et al. 2012) aims to use spectroscopy to probe the atmospheres of a range of transiting exoplanets. To ensure the success of the EChO mission it is necessary to have access to the necessary spectroscopic data which will provide inputs to radiative transport models required to interpret the observational data. For our solar system, the spectroscopic data for modelling radiative transport in planetary atmospheres is provided by specialist data bases, such as HITRAN (Rothman et al. 2009, 2013) and GEISA (Jacquinet-Husson et al. 2011), which have been compiled and refined over many years using the data recorded at or about room temperature, defined by HITRAN as 296 K. However exoplanets that will be observed by EChO are likely to be considerably hotter than the atmospheres of solar systems planets. Elevated temperatures lead to both a huge increase in the number of molecular transitions that need to be considered and, possibly, changes in the atmospheric composition. It is therefore necessary to ensure that all data required for modelling such atmospheres will be in place.

There are spectroscopic databases available for hot molecules. Kurucz has compiled data sets for models of (cool) stellar atmospheres for many years (Kurucz 2011). However data are lacking for many species in these compilations and are approximate for others. More recently the high temperature version of HITRAN, known has HITEMP, has been updated (Rothman et al. 2010). The HITEMP data can be considered as comprehensive and reliable, but is only available for five species: water, CO_2, CO, OH and NO. The ExoMol project (Tennyson & Yurchenko 2012) is currently in progress and has the specific aim of providing spectroscopic data applicable for a large range for temperatures for studying exoplanet atmospheres.

Hot molecules require significantly more data to simulate spectra at high temperatures. Fig. 1 illustrates the importance of the hot transitions of CH_4 missing in HITRAN for modelling the hot ($T = 1000$K) absorbance. This figure shows the absorption spectra simulated using the HITRAN and theoretical (ExoMol) line lists. The HITRAN spectra, being based on the room temperature data, suffers from lacking the hot transitions leading to significant underestimation of the opacity at elevated temperatures, by about 50 % at 1000 K for example.

Table 1 is taken from the initial EChO proposal as submitted in the autumn of 2010. It summarises the main spectral features that EChO planned to probe. The status of the data for each of these species is discussed in the next section. Given the rapid progress in exoplanetary research and, in particular, the discovery of new, unanticipated classes of exoplanets, it is possible that data on further species, not anticipated in the initial proposal will also be required. The status of these data are discussed in section 3.

2 STATUS

The spectroscopic properties of the atomic species listed in Table 1, namely Na, K, H Hα, H Hβ, He, Ca, are all well known and can be found in standard data sources such as NIST (see `http://www.nist.gov/pml/data/asd.cfm`).

Below we consider in turn each molecular species listed in Table 1, starting with the four species that have already been observed in exoplanets.

H_2O: The BT2 line list (Barber et al. 2006) was used to make the original identification of water in HD189733b by

[ht]

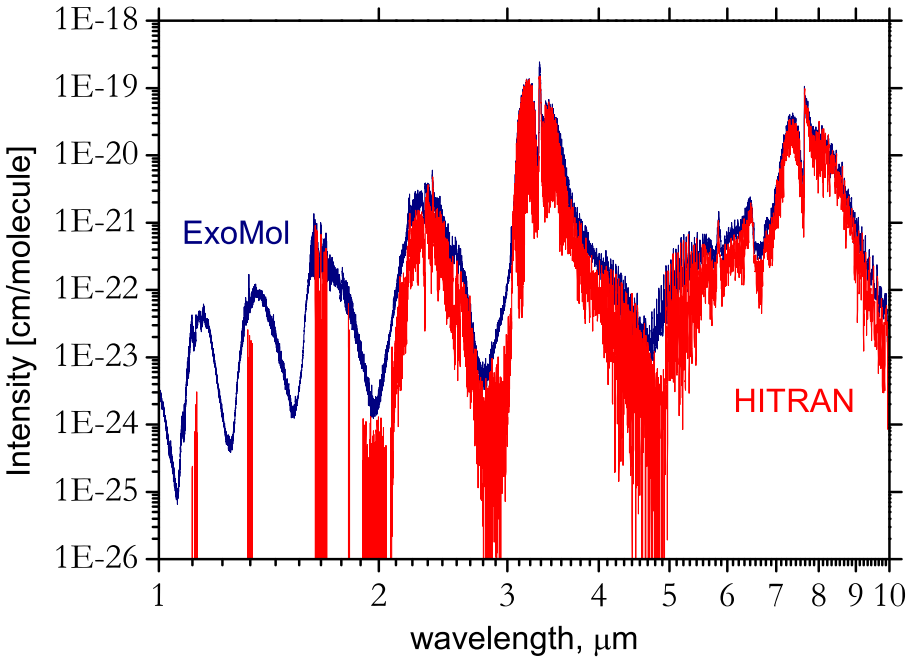

Figure 1. Absorption spectra of CH_4 simulated using the HITRAN and ExoMol line lists at $T = 1000$ K: individual lines are convolved with a Gaussian function of width 0.5 cm^{-1}.

Tinetti et al. (2007). Subsequently the BT2 line list was used as the basis for water in the HITEMP, which also made use of the available laboratory data. Although work is continuing on improving the representation of water (Lodi et al. 2011; Tennyson et al. 2013; Polyansky et al. 2013), the data in HITEMP is both comprehensive and accurate, and should prove the spectroscopic data needed for EChO.

HDO: The VTT line list (Voronin et al. 2010) provides a line list for deuterated water of a quality similar to that of BT2. The accuracy of VTT could be further improved using experimental data (Tennyson et al. 2010) but is probably already sufficient for EChO.

CO_2: HITEMP contains a comprehensive line list for carbon dioxide. However this line list has been subsequently improved and extended by Tashkun & Perevalov (2011). This new line list should be sufficient for EChO.

CO: HITEMP contains an extensive CO line list constructed using laboratory and sunspot spectra. These should be sufficient for EChO although the ExoMol project is planning new line lists which should provide data for all CO isotopologues and increase the range of the line list to all bound-bound rotation-vibration transitions.

CH_4: Despite the detection of methane in HD18733b by Swain et al. (2008) and elsewhere, the present sources of spectroscopic data for methane are insufficient for fully characterising the problem at the temperatures found in hot Jupiters. Groups in the UK, France and Canada are actively working on producing line lists for methane. Preliminary releases are already available (Waldmann et al. 2013). Good, validated line lists for hot methane will be available from the ExoMol project, and probably elsewhere, prior to any EChO launch.

CH_3D: There are no good current line lists for singly deuterated methane and the problem is harder than methane itself. Work is planned on this in France but will probably only follow after solution of the methane problem. The ExoMol project is planning to extend their CH_4 line list for the deuterated methane. A hot line list for this molecule should be available prior to any EChO launch.

C_2H_2: Extensive experimental work on acetylene has been performed in Brussels, see Moudens et al. (2011) for example,

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Table 1. Main spectral features between 0.4 and 16 μm. The asterisk indicates the molecular/atomic species already detected in the atmospheres of exoplanets. At wavelengths shorter than 2 μm spectroscopic data are often not complete, so that the use of this region is much more difficult for band identification and analysis. The main bands are illustrated in bold.

	0.4-1 μm	1-5 μm	5-11 μm	11-16 μm
R, baseline	300	300	$\geqslant$30	30
R, desired	300	300	300	300
Species				
*H_2O	0.51, 0.57, 0.65, 0.72, 0.82, 0.94	1.13, 1.38, 1.9, **2.69**	6.2	continuum
*CO_2	-	1.21, 1.57, 1.6, 2.03, **4.25**	-	**15.0**
C_2H_2	-	1.52, **3.0**	7.53	**13.7**
HCN	-	**3.0**	-	**14.0**
C_2H_6	-	3.4	-	**12.1**
O_3	0.45-0.75 (the Chappuis band)	4.7	9.1, **9.6**	14.3
HDO	-	2.7,3.67	7.13	-
*CO	-	1.57, 2.35, **4.7**	-	-
O_2	0.58, 0.69, 0.76, 1.27	-	-	-
NH_3	0.55, 0.65, 0.93	1.5, 2, 2.25, 2.9, **3.0**	6.1, **10.5**	-
PH_3	-	4.3	8.9, 10.1	-
*CH_4	0.48, 0.57. 0.6, 0.7, 0.79, 0.86,	1.65, 2.2, 2.31, 2.37, **3.3**	6.5, **7.7**	-
CH_3D	?	3.34, **4.5**	6.8, 7.7, **8.6**	-
C_2H_4	-	**3.22**, 3.34	6.9, **10.5**	-
H_2S	-	2.5, 3.8 ...	7	-
SO_2	-	4	**7.3**, 8.8	-
N_2O	-	2.8, 3.9, **4.5**	7.7, 8.5	-
NO_2	-	3.4	**6.2**, 7.7	13.5
H_2	-	2.12	-	-
H_3^+	-	2.0, 3-4.5	-	-
He	-	1.083	-	-
*Na	0.589	1.2	-	-
*K	0.76	-	-	-
TiO	0.4-1	1-3.5	-	-
VO	0.4-1	1-2.5	-	-
FeH	0.6-1	1-2	-	-
TiH	0.4-1	1-1.6	-	-
Rayleigh	0.4-1	-	-	-
Cloud/haze	yes	possible	silicates, etc.	-
H Hα	**0.66**			
H Hβ	0.486			
Ca	0.8498, 0.8542, 0.8662		-	-

and a line list based on this work is promised. Initial theoretical studies have been performed in London (Urru et al. 2010) and a full line list is planned as part of the ExoMol project. At least one line list should be available prior to any EChO launch.

HCN: Line lists for hydrogen cyanide were calculated by Eriksson et al. (1984) and Harris et al. (2002). However these line lists are both purely *ab initio* and do not give accurate wavelengths. Harris et al. (2006) improved their line list, which covers both HCN and HNC, using the then experimental data. Recently Mellau has performed very extensive experimental studies on both hot HCN and hot HNC, see Mellau (2011a) and Mellau (2011b) respectively. A greatly improved version of the Harris *et al* line list has been constructed using Mellau's data as part of the ExoMol project and will be released during 2013. This line list should be sufficient for EChO.

C_2H_6: there is no hot line list for ethane. One is planned as part of the ExoMol project and some preliminary calculations

have been performed. Ethane has 8 atoms and a low energy vibrational mode, so the number of lines at elevated temperatures are likely to be unmanageable. The proposal will be therefore to provide temperature-dependent cross sections for ethane (Hill et al. 2013); these should be available prior to any EChO launch.

O_3: The spectrum of ozone has been studied systematically over many years in Reims, France. This data is captured in the SMPO (Spectroscopy & Molecular Properties of Ozone) database which is accessible as part of the VAMDC project (Dubernet et al. 2010). This line list should be sufficient for EChO.

O_2: Oxygen spectra have been subject to renewed experimental studied including work at higher temperatures. This work is captured in the analysis of Yu et al. (2012), which should be sufficient for EChO.

NH_3: Extensive line lists for ammonia are available (Yurchenko et al. 2009, 2011). The BYTe line list (Yurchenko et al. 2011) was explicitly designed with the needs of exoplanet spectroscopy in mind. This line list should be sufficient for EChO.

PH_3: Phosphine is being studied as part of the ExoMol project. An initial line list has recently been released (Sousa-Silva et al. 2013). A full line list will be released in 2014. This will be sufficient for EChO.

C_2H_4: Work on a hot line list for ethylene has just started as part of the ExoMol project. A full line list should be available by 2016.

H_2S: Hydrogen sulphide is being studied as part of the ExoMol project. A full line list is essentially complete and will be released during 2013.

SO_2:A line list for SO_2 has recently been (yet to be published) computed at NASA Ames. This line list is for temperatures appropriate to solar system planets (notably Venus). It has been agreed that ExoMol will collaborate with NASA Ames and construct a high temperature SO_2 line list. This full line list should be available in late 2014.

NO: HITEMP contains a line list for constructed using laboratory (lower excitations) and extrapolated (high v, J) data. This line list probably sufficient but this will be checked as part of the ExoMol project and an extended line list computed if necessary.

N_2O: A theoretical, approximate hot line list in the 4.5 μm region was created by Rosenmann et al. (1997). A very comprehensive room temperature line list for N_2O is provided by the HITRAN data base constructed using laboratory covering all frequency ranges required. These data should be extended to elevated temperatures. This work will be undertaken at UCL should the EChO launch be approved.

NO_2 A room temperature line list for NO_2 is provided by the HITRAN data base and is constructed using laboratory data covering the frequency range required EChO. These data should be extended to elevated temperatures. This work will be undertaken at UCL should the EChO launch be approved.

H_2: A comprehensive hot line list for this molecule covering bound-bound quadruple transitions has been constructed very recently by Campargue et al. (2012). Continuum induced absorption (CIA) may be also required. CIA data has recentky incorporated into HITRAN for a number of homonuclear diatomic species including H_2 (Richard et al. 2012). These data should be sufficent for EChO.

H_3^+: A comprehensive and widely used line list for H_3^+ was provided by (Neale et al. 1996). Although a new, upgraded line list is likely to become available in the next few years, the list due to Neale *et al* is already sufficent for EChO.

TiO: A very extensive, hot line list for TiO was constructed by Schwenke (1998). This line list has been criticized but has so far proved sufficient for exoplanetary studies. If necessary, ExoMol will produce a new line list.

VO: Experimental, partial line lists are available from Ram et al. (2002) and Ram & Bernath (2005). Work is already underway in the ExoMol project which will use this data to make a comprehensive line list which will be sufficient for EChO.

FeH: Experimental partial line lists are available from Dulick et al. (2003), further observational data is available from high resolution studies of M-dwarf star (Hargreaves et al. 2010; Wende et al. 2010) and sunspot (Fawzy 2009) spectra. These

data will be used by ExoMol to make a comprehensive line list which will be sufficient for EChO.

TiH: A partial line list for TiH is available from Burrows et al. (2005). Some work has already been performed by the ExoMol project producing TiH cross sections for exoplanetary studies (unpublished). ExoMol will produce a comprehensive line list which will be sufficient for EChO.

3 OTHER SPECIES

Apart from the molecules listed above, ExoMol is undertaking work on line lists for molecules with the potential to become important for exoplanetary atmospheric modeling. Some of such molecules are listed below.

SiO ExoMol has just released a comprehensive line lists for all key isotopologues (Barton et al. 2013) which will be sufficient for EChO.

BeH, MgH and CaH ExoMol has recently released comprehensive hot line lists for these species (Yadin et al. 2012) which will be sufficient for EChO.

AlH, AlO, C_3 CrH, KCl, NaH, NiH, SiH, SO_3, YO Work is already underway in the ExoMol project which will use this data to make comprehensive line lists for EChO.

4 CONCLUSIONS

The EChO mission will place very significant demands on the laboratory data for spectroscopic interpretion of the observations. Assembling all the required data requires considerable effort on the part of laboratory astrophysicists. Much of this data is already available and plans for the compiling the remainder on an appropriate timescale for the EChO mission are well underway. This information will be used to construct and EChO-specific spectroscopic database prior to any launch. This data will be presented in a format suitable for use in EChO-specific software such as EChOSIM (Waldmann et al. 2013).

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