# The ExoMol project: Molecular opacity calculations at University College London

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**Abstract.** Absorption by hot molecules, which dominates the opacities of cool stars and brown dwarfs, have taken on a new significance with the discovery of exoplanets. At high temperatures molecules can undergo many billions of transitions: too many to be determined by experiment. Progress in computing molecular line list under the auspices of the ExoMol project is described.

## 1. Introduction

The international Opacity Project ran from University College London (UCL) during the 1980s and 1990s under the guidance of Mike Seaton. Seaton (1987) set-up and outlined the parameters of the project; the results of which were published in a series of 24 papers in the Journal of Physics B and summarized in two books: The Opacity Project Team & Seaton (1995) and The Opacity Project Team & Berrington (1994). Updates to the opacity project continued well into the current century with the release of OP 2005 posthumously as Seaton (2007).

I arrive at UCL in 1985 and in the late 1980's Seaton approached me on a number of occasions suggest that I extend the opacity project to cooler stars by considering the contribution of molecules. The result was a first water line list with the initial results reported on at the opacity conference in Caracas (Miller et al. 1992) and the full line list was used by Allard et al. (1994) to study the influence of $H_2O$ line blanketing on the spectra of cool dwarf stars. This water line list was modest in size compared with the more recent equivalents such as those of Partridge & Schwenke (1997), Barber et al. (2006) and Polyansky et al. (2017b). In some senses this early work was a proof-of-principle with the first really complete line list being the one produced by Neale et al. (1996) for $H_3^+$ for which an accompanying partition function (Neale & Tennyson 1995) was also produced. The partition function gave values between one and two orders of magnitudes larger than previous studies at $T \approx 4000$ K.

Although the original impetus for computing molecular line lists came from the demands opacity models for cools stars and brown dwarfs, the project gained huge impetus from attempts to characterize exoplanet atmospheres using spectroscopy. In particular, use of the BT2 water line list (Barber et al. 2006) was instrumental in the first detection of water on exoplanet HD189733b (Tinetti et al. 2007). Initial attempts to use the smaller direct numerical diagonalization (DND) line list of Wattson & Rothman (1992), as used in the then current release of HITEMP, did not reproduce the observed shape of the low-resolution transit spectrum.

This development shifted the focus of calculations from stars to exoplanets and in direct response to this the ExoMol project was born. While ExoMol has been largely an in-house activity at UCL, the publication strategy followed directly from Seaton's described above. An initial paper (Tennyson & Yurchenko 2012) setting out the parameters for the project is being followed by a series papers which are delineated in Table 1 below.

## 2. Methodology

The underlying methodology used by ExoMol is summarized by the phrase *ab initio* quantum mechanics informed by experiment. This methodology has been extensively discussed elsewhere, see Lodi & Tennyson (2010) and Tennyson (2012) for example, and the reader is referred to these papers for further information.

Figure 1 gives an overview of this approach. Briefly, *ab initio* electronic structure calculations can give dipole moment surfaces and hence transition dipole moments which are competitive in accuracy with the best experimental determinations, see Polyansky et al. (2015) for example. Conversely, the potential energy surfaces computed using the same procedure are only capable of giving transition frequencies of acceptable accuracy for systems with very few electrons. Thus for most molecules experimental information needs to incorporated into the calculation either by tuning the *ab initio* potential energy surface to experimental data or by replacing the computed energy levels with empirically-determined ones, or both.

To aid this process Furtenbacher et al. (2007) developed the MARVEL (measured active rotational-vibrational energy levels) procedure to extract robust empirical energy levels from a the whole variety of available measurement sources. This procedure has been extensively developed (Császár et al. 2016), and has been applied to a number of astrophysically important species such as $C_2$ (Furtenbacher et al. 2016), TiO (McKemmish et al. 2017) and HCCH (Chubb et al. 2017). ExoMol line lists for these species are currently under construction.

ExoMol line lists are actually produced using variational solutions of the nuclear motion problem. These calculations become computationally challenging for polyatomic systems. As a result extensive updates of the programs used to solve these nuclear motion problem has been performed as part of the ExoMol project (Tennyson & Yurchenko 2017b). Of particular significance is the development of a completely new program Duo (Yurchenko et al. 2016b). Duo treats the fully-coupled rovibronic spectroscopy problem for diatomic molecules: all spectra (rotational, vibrational, electronic) can be computed for diatomics with mix of electronic states and including full treatment of spin-orbit and other coupling terms (Tennyson et al. 2016b).

It is also worth noting that the ability to predict Einstein-A coefficients and hence transition intensities with an accuracy exceeding most experiments has led to this work having applications to radiative transport within our own atmosphere. Line lists for water (Lodi & Tennyson 2012; Birk et al. 2017; Kyuberis et al. 2017) and $CO_2$ (Zak et al. 2016, 2017b,a) constructed using MARVEL energy levels and *ab initio* intensities dominate the recommended data for these molecule in the recent release of HITRAN (Gordon et al. 2017).

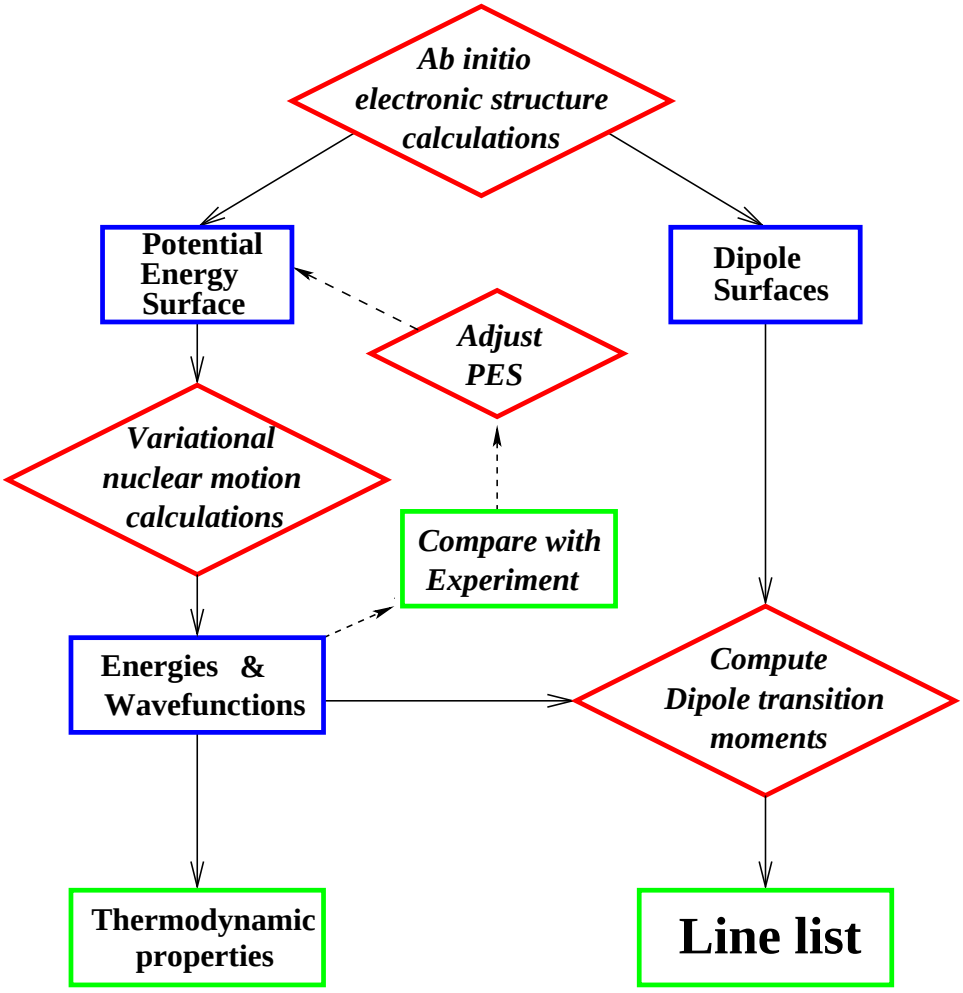


Figure 1. Summary of approach used to compute line lists by the ExoMol project.

## 3. Accuracy versus completeness

An important issue in constructing molecular line lists is the balance of accuracy against completeness. Experimentally-determined line lists are often significantly more accurate, at least for line positions, than the ones provided by direct computation. However, given that line list for polyatomic species contain many billions of lines, their complete experimental determination is not really feasible.

Our approach has been to ensure completeness while trying to be as accurate as possible. As an important part of this we always attempt to give an upper temperature for which the line list can be considered reliable. These temperatures can be obtained from careful analysis of partition functions using the approach originally introduced by Neale & Tennyson (1995).

Figure 2, which is adapted from the work of Yurchenko et al. (2014), gives an important illustration of this approach. The figure shows two attempts to model the observed spectrum of a methane-rich brown dwarf. The original VSTAR model of Bailey

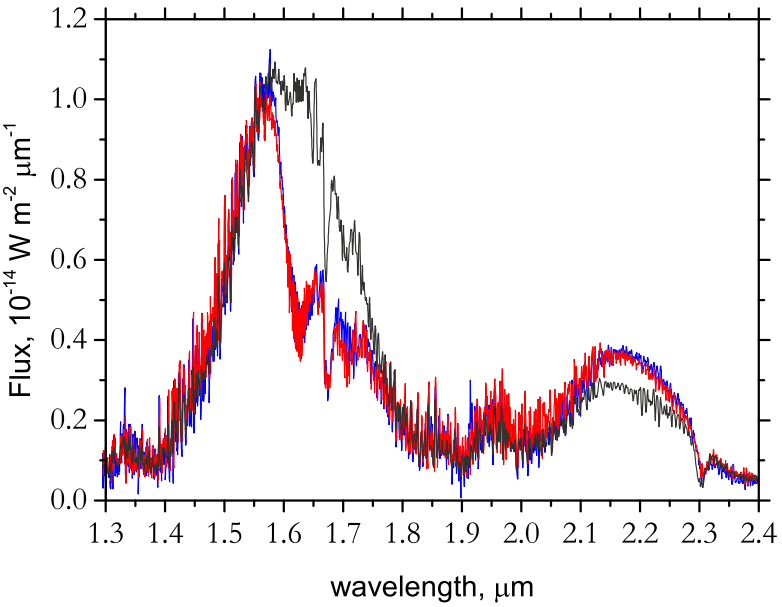


Figure 2. Spectra of the T 4.5 dwarf 2M 0559-14. The observed spectrum (blue line) was taken with the SpeX instrument on the 3-m NASA Infrared Telescope Facility (IRTF). Models were performed with VSTAR for $T$ = 1500 K using (a) the empirical STDS line list of Wenger & Champion (1998) and (b) the computed 10to10 line list of Yurchenko & Tennyson (2014). The figure is adapted from the work of Yurchenko et al. (2014).

& Kedziora-Chudczer (2012) used the best available empirical line list for methane, the STDS line list of Wenger & Champion (1998). This line list is very accurate but far from comprehensive. The more recent work used the comprehensive but less accurate 10to10 ExoMol line list (Yurchenko & Tennyson 2014). Computational experiments suggested that it was necessary to retain at least 3 billion of the 10 billion lines in the 10to10 list to get reliable results for the 1.6 $\mu$m feature. It should be noted that the study of Yurchenko et al. (2014) also used an improved treatment of the $H_2$ collision-induced absorption band at 2.2 $\mu$m. It is clear that completeness of the methane line list plays an important part in obtaining the excellent agreement between the newer model and the observations.

## 4. ExoMol line lists

The current status of the ExoMol line lists is given in Table 1. I note that this series has already exceeded that of the (atomic) opacity project and there are a number of further molecules for which line lists are actively under construction or planned.

ExoMol has always taken a fairly pragmatic approach to constructing line lists; if other high quality line lists are available then these are recommended and no attempt is made to replicated them. A number of these alternative line lists are available via the

Table 1. Datasets created by the ExoMol project and included in the ExoMol database (Tennyson et al. 2016c).

| Paper | Molecule | $N_{\rm iso}$ | $T_{\rm max}$ | $N_{elec}$ | $N_{\rm lines}$ | DSName | Reference |
|---|---|---|---|---|---|---|---|
| I | BeH | 1 | 2000 | 1 | 16 400 | Yadin | Yadin et al. (2012) |
| I | MgH | 3 | 2000 | 1 | 10 354 | Yadin | Yadin et al. (2012) |
| I | CaH | 1 | 2000 | 1 | 15 278 | Yadin | Yadin et al. (2012) |
| II | SiO | 5 | 9000 | 1 | 254 675 | EJBT | Barton et al. (2013) |
| III | HCN/HNC | 2[a] | 4000 | 1 | 399 000 000 | Harris | Barber et al. (2014) |
| IV | $CH_4$ | 1 | 1500[b] | 1 | 9 819 605 160 | YT10to10 | Yurchenko & Tennyson (2014) |
| V | NaCl | 2 | 3000 | 1 | 702 271 | Barton | Barton et al. (2014) |
| V | KCl | 4 | 3000 | 1 | 1 326 765 | Barton | Barton et al. (2014) |
| VI | PN | 2 | 5000 | 1 | 142 512 | YYLT | Yorke et al. (2014) |
| VII | $PH_3$ | 1 | 1500 | 1 | 16 803 703 395 | SAlTY | Sousa-Silva et al. (2015) |
| VIII | $H_2CO$ | 1 | 1500 | 1 | 10 000 000 000 | AYTY | Al-Refaie et al. (2015) |
| IX | AlO | 4 | 8000 | 3 | 4 945 580 | ATP | Patrascu et al. (2015) |
| X | NaH | 2 | 7000 | 2 | 79 898 | Rivlin | Rivlin et al. (2015) |
| XI | $HNO_3$ | 1 | 500 | 1 | 6 722 136 109 | AlJS | Pavlyuchko et al. (2015) |
| XII | CS | 8 | 3000 | 1 | 548 312 | JnK | Paulose et al. (2015) |
| XIII | CaO | 1 | 5000 | 5 | 21 279 299 | VBATHY | Yurchenko et al. (2016a) |
| XIV | $SO_2$ | 1 | 2000 | 1 | 1 300 000 000 | ExoAmes | Underwood et al. (2016b) |
| XV | $H_2O_2$ | 1 | 1250 | 1 | 20 000 000 000 | APTY | Al-Refaie et al. (2016) |
| XIV | $H_2S$ | 1 | 2000 | 1 | 115 530 3730 | AYT2 | Azzam et al. (2016) |
| XV | $SO_3$ | 1 | 800 | 1 | 21 000 000 000 | UYT2 | Underwood et al. (2016a) |
| XVI | VO | 1 | 2000 | 13 | 277 131 624 | VOMYT | McKemmish et al. (2016) |
| XIX | $H_2{}^{17,18}O$ | 4[c] | 3000 | 1 | 1 500 000 000 | HotWat78 | Polyansky et al. (2017a) |
| XX | $H_3^+$ | 1[d] | 3000 | 1 | 11 500 000 000 | MiZATeP | Mizus et al. (2017) |
| XXI | NO | 6 | 5000 | 2 | 2 281 042 | NOName | Wong et al. (2017) |
| XXII | $SiH_4$ | 1 | 1200 | 1 | 62 690 449 078 | OY2T | Owens et al. (2017a) |
| XXIII | PO | 1 | 3000 | 1 | 1 500 000 000 | POPS | Prajapat et al. (2017) |
| XXIII | PS | 1 | 3000 | 3 | 1 500 000 000 | POPS | Prajapat et al. (2017) |
| XXIV | SiH | 4 | 5000 | 3 | 1 724 841 | ?Name | Yurchenko et al. (2017b) |

$N_{\rm iso}$ Number of isotopologues considered;
$T_{\rm max}$ Maximum temperature for which the line list is complete;
$N_{elec}$ Number of electronic states considered;
$N_{\rm lines}$ Number of lines: value is for the main isotope.
[a] A line list for $H^{13}CN/HN^{13}C$ due to Harris et al. (2008) is also available.
[b] Yurchenko et al. (2017a) have recently extended 10to10 to 2000 K. The new line list which they present in compressed form contains 34 billion lines and is known as 34to10.
[c] Line lists for $H_2{}^{16}O$ (BT2) due to Barber et al. (2006) $HD^{16}O$ (VTT) due to Voronin et al. (2010) are also available.
[d] A line list for $H_2D^+$ due to Sochi & Tennyson (2010) is also available.

ExoMol website, see Table 2. Others, such as the recent comprehensive line lists for all isotopologues of $CO_2$ by Huang et al. (2017), have to be obtained directly from the original source.

Table 2. Other molecular line lists which can be obtained from the ExoMol website.

| Molecule | $N_{\rm iso}$ | $T_{\rm max}$ | $N_{elec}$ | $N_{\rm lines}$ | DSName | Reference | Methodology |
|---|---|---|---|---|---|---|---|
| $H_2O$ | 2[b] | 3000 | 1 | 505 806 202 | BT2 | Barber et al. (2006) | ExoMol |
| $NH_3$ | 2[c] | 1500 | 1 | 1 138 323 351 | BYTe | Yurchenko et al. (2011) | ExoMol |
| $HeH^+$ | 4 | 10000 | 1 | 1 431 | Engel | Engel et al. (2005) | Ab initio |
| $HD^+$ | 1 | 12000 | 1 | 10 119 | CLT | Coppola et al. (2011) | Ab initio |
| LiH | 1 | 12000 | 1 | 18 982 | CLT | Coppola et al. (2011) | Ab initio |
| $LiH^+$ | 1 | 12000 | 1 | 332 | CLT | Coppola et al. (2011) | Ab initio |
| ScH | 1 | 5000 | 6 | 1 152 827 | LYT | Lodi et al. (2015) | Ab initio |
| MgH | 1 | | 3 | 30 896 | 13GhShBe | GharibNezhad et al. (2013) | Empirical |
| CaH | 1 | | 2 | 6000 | 11LiHaRa | Li et al. (2012) | Empirical |
| NH | 1 | | 1 | 10 414 | 14BrBeWe | Brooke et al. (2014a) | Empirical |
| CH | 2 | | 4 | 54 086 | 14MaPlVa | Masseron et al. (2014) | Empirical |
| CO | 9 | 9000 | 1 | 752 976 | 15LiGoRo | Li et al. (2015) | Empirical |
| OH | 1 | 6000 | 1 | 45 000 | 16BrBeWe | Brooke et al. (2016) | Empirical |
| CN | 1 | | 1 | 195 120 | 14BrRaWe | Brooke et al. (2014b) | Empirical |
| CP | 1 | | 1 | 28 735 | 14RaBrWe | Ram et al. (2014) | Empirical |
| HCl | 1 | | 1 | 2588 | 11LiGoBe | Li et al. (2011) | Empirical |
| CrH | 1 | | 2 | 13 824 | 02BuRaBe | Burrows et al. (2002) | Empirical |
| FeH | 1 | | 2 | 93 040 | 10WEReSe | Wende et al. (2010) | Empirical |
| TiH | 1 | | 3 | 181 080 | 05BuDuBa | Burrows et al. (2005) | Empirical |

$N_{\rm iso}$ Number of isotopologues considered;
$T_{\rm max}$ Maximum temperature for which the line list is complete;
$N_{elec}$ Number of electronic states considered;
$N_{\rm lines}$ Number of lines: value is for the main isotope.
[a] There is a $H_2D^+$ line list available from Sochi & Tennyson (2010).
[b] The VTT line list for HDO due to Voronin et al. (2010) is also available.
[c] There is a room temperature $^{15}NH_3$ line list due to Yurchenko (2015).

As part of the ExoMol project the database and underlying data structures have undergone systematic development. The original data structure was to provide line lists in using two files: a states file containing energy levels and quantum numbers, and a transitions file listing Einstein-A coefficients (Tennyson et al. 2013). Given the very large number of lines found for many molecules, Hill et al. (2013) extended this approach to provide cross sections. Recently, Tennyson et al. (2016c) undertook a thorough revision of the database including features such an application program interface (API) to enable direct reading of the data in user programs. Additional functionality was also added such as the provision of state lifetimes (Tennyson et al. 2016a), Landé $g$-factors for open shell diatomic species (Semenov et al. 2017), cooling functions and transition dipoles. At present the use transition dipoles, which involves retaining the phase information for the transitions, is largely for laboratory applications (Owens et al. 2017b), but these data can provide input for future studies of polarization effects.

## 5. Conclusions

The ExoMol project, very much inspired by the (atomic) opacity project, has provided comprehensive line lists for key astronomical molecules. This process is not complete. The discovery of very hot planets with temperatures thought to be 2000 K or more and compositions which may well be rocky, has created a whole list of possible new species

for which line lists need to be provided. The data needs for these so-called lava planets have recently been reviewed by Tennyson & Yurchenko (2017a).

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