

Review

Molecular Data Needs for Modelling AGB Stellar Winds and Other Molecular Environments

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Abstract: The modern era of highly sensitive telescopes is enabling the detection of more and more molecular species in various astronomical environments. Many of these are now being carefully examined for the first time. However, to move beyond detection to more detailed analysis such as radiative transfer modelling, certain molecular properties need to be properly measured and calculated. The importance of contributions from vibrationally excited states or collisional (de-)excitations can vary greatly, depending on the specific molecule and the environment being studied. Here, we discuss the present molecular data needs for detailed radiative transfer modelling of observations of molecular rotational transitions, primarily in the (sub-)millimetre and adjacent regimes, and with a focus on the stellar winds of AGB stars.

Keywords: molecular data; stellar spectra; evolved stars; AGB stars

1. Introduction

Thanks to advances in telescope technology, more than 200 molecules have been detected in the interstellar medium (ISM) or in circumstellar environments, according to the Cologne Database for Molecular Spectroscopy (CDMS, [1–3]). Some of the richest circumstellar environments are the stellar winds of asymptotic giant branch (AGB) stars, with over 90 molecules (excluding isotopologues) detected in these outflows [4]. AGB stars are an evolved form of low- and intermediate-mass stars (with main sequence masses ~ 1 to $8 M_{\odot}$), which undergo considerable mass loss and end their lives as white dwarfs surrounded by planetary nebulae. They eject a lot of matter which goes on to form molecules and condense into dust in an outwardly expanding stellar wind, also referred to as a circumstellar envelope [5]. These stellar winds are dynamically relatively straightforward systems, typified by smooth acceleration and mainly complicated by pulsation-induced shocks in the regions very close to the stellar surface, and with temperatures ranging from ~ 2000 K close to the star to ~ 10 K in the outer parts of the circumstellar envelope. Hence, they make ideal laboratories to study molecular emission and chemistry, leading to insights which can be extrapolated to more complex environments such as, for example, protoplanetary discs, high-mass star-forming regions and exoplanet atmospheres.

A common method for understanding the behaviour of AGB stellar winds is using observations of molecular rotational transition lines (commonly found at radio frequencies) to constrain the molecular abundance stratifications via radiative transfer models (e.g., [6–9]). Such radiative transfer models solve rate equations of the molecule under study. Some molecules, such as CO, are well-known as being good tracers for the temperature and density structure and hence are used to constrain the mass-loss rate of the stellar wind. However, to properly consider radiative excitation effects, these models must take non-local thermodynamic equilibrium (non-LTE) effects into account [10]. This is done by solving (numerically) the statistical equilibrium equations to find the level populations of the molecule being

modelled [11]. To do this properly, both radiative and collisional (de-)excitation rates need to be included. Hence, accurate molecular data are required to properly understand the chemistry and dynamics of AGB stellar winds.

Here, we will discuss some of the challenges currently being faced when it comes to radiative transfer modelling of molecular lines. We hope to illustrate the importance of accurate molecular data and highlight some of the gaps that presently exist in molecular measurements and calculations. We also note that our focus is on neutral molecules and their rotational, vibrational, and rovibrational transitions and hence we do not discuss atomic or ionic data here.

While we focus on applications to AGB stellar wind modelling, the molecular data we discuss can be used to study a wide range of environments—any environments where molecules have been detected. This includes protoplanetary discs (e.g., [12]), high-mass star-forming regions, other photon-dominated regions (PDRs) (e.g., [13]), and exoplanet atmospheres (e.g., [14]). Fortney et al. [15] and Tennyson and Yurchenko [16] discuss the similar need for laboratory data (molecular and otherwise) to advance the study of exoplanet atmospheres and Roueff and Lique [17] provide an overview of such data as it relates to the interstellar medium.

2. Required Molecular Data

Detailed radiative transfer modelling of molecular lines involves solving the statistical equations in some way (see [11,18–21], for example of different methods of solving these equations). The statistical equilibrium system of equations for a transition with upper level u and lower level l is

$$\sum_{l < u} [n_u A_{ul} - (n_l B_{lu} - n_u B_{ul}) \bar{J}_{ul}] - \sum_{l > u} [n_l A_{lu} - (n_u B_{ul} - n_l B_{lu}) \bar{J}_{ul}] + \sum_{u,l} (n_u C_{ul} - n_l C_{lu}) = 0, \quad (1)$$

where n_u and n_l are the populations of levels u and l , respectively, A_{ul} are the rates of spontaneous de-excitation, B_{ul} are the rates of induced de-excitation, B_{lu} are the rates of radiative excitation, C_{ul} are the collisional transition rates (discussed more in Section 2.2), and \bar{J} is the integrated mean intensity averaged over all directions [22]. The A and B parameters are the Einstein coefficients and are related and defined as follows:

$$A_{ul} = \frac{8\pi^2 \nu^3}{3\epsilon_0 \hbar c^3} |\mu_{ul}|^2 \quad (2)$$

$$= \frac{8\pi \hbar \nu^3}{c^3} B_{ul} \quad (3)$$

and

$$B_{lu} g_l = B_{ul} g_u, \quad (4)$$

where ν is the frequency of the radiation emitted due to the transition, μ_{ul} is the transition dipole moment, ϵ_0 is the permittivity of free space, $\hbar = h/2\pi$, where h is Planck's constant, c is the speed of light in a vacuum, and g_u is the statistical weight of the u energy level. The collisional excitation and de-excitation rates for upper level u and lower level l are related by

$$C_{lu} = C_{ul} \frac{g_u}{g_l} e^{-h\nu/kT_{\text{kin}}}, \quad (5)$$

where k is Boltzmann's constant and T_{kin} is the kinetic temperature.

Radiative transfer modelling of rotational lines from a given molecular species requires energy levels, statistical weights, transition frequencies, Einstein A coefficients (from which the Einstein B coefficients can easily be derived—see Equation (3)), and collisional rate coefficients. Of course, these should cover the full range of energies and temperatures of interest, which often means that vibrationally excited levels also need to be included. For example, stellar winds can reach temperatures of ~ 2000 K or higher. When modelling CO in such an environment, at least 40 rotational levels in

each of the ground and first excited vibrational state are often included (e.g., as calculated by [23]). Modelling H₂O in a similar environment and taking rotational energy levels from the $\nu_2 = 0, 1$ and $\nu_3 = 0, 1, 2$ vibrational levels into account up to energies of 5000 cm⁻¹ (as calculated by Faure et al. [24]) quickly brings the number of levels considered to more than 800.

2.1. Radiative Rates

There are presently a few useful databases collecting radiative transition data. The previously mentioned CDMS¹ [1–3] and the JPL spectroscopic database² [25] provide transition data for a vast number of atomic, molecular, ionic, and isotopic species with 924 listed in CDMS and 401 in JPL. Geared towards the preparation of observations, Splatalogue³ collates and extends data from CDMS, JPL, NIST Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions⁴, and other databases, boasting over 5.8 million lines in 1038 individual entries. There are also databases such as HITRAN⁵ and ExoMol⁶ which have a focus on cool (planetary) atmospheres and go into greater detail for a smaller number of molecules, including listing data for many rarer isotopologues. The molecular data necessary for radiative transfer modelling can be easily obtained or calculated from these databases. However, these databases are not exhaustive and gaps remain that we shall now discuss.

The inclusion of vibrationally excited states is potentially very important to the radiative transfer modelling of some molecules. This is because the star's light, which for AGB stars peaks around $\sim 2 \mu\text{m}$, can excite some molecules to vibrationally excited levels. The de-excitation follows specific quantum selection rules, yielding level populations that can be quite different to the level population distribution obtained when vibrationally excited states are neglected. This effect is called radiative pumping. For example, Schöier et al. [10] modelled NH₃ with the inclusion of the $\nu_2 = 1$ vibrationally excited state and found a derived fractional abundance about an order of magnitude lower than that found when modelling with only the ground vibrational state. With further study, Schmidt et al. [26] found that the improvement to modelling was negligible for the other vibrationally excited states of NH₃ that they tested their models with. Thus, while not all vibrationally excited states may be significant when modelling low-energy transitions, some are, and ought not to be neglected.

There is also the potential for rotational lines in vibrationally excited states to be detected, especially as telescope sensitivities improve. Historically, vibrationally excited rotational transitions of SiO [27,28] and HCN [29–31] have been frequently detected, often thanks to maser activity. These are now joined by a plethora of other molecules in vibrationally excited states such as CO [32], H₂O [33,34], SiS, SO, SO₂ [35], and others. Of course, the identification of these vibrationally excited lines requires their presence in line lists, which is true of the molecules listed above. It is difficult to gauge to what extent unidentified lines seen in various observations [35–37] are due to not yet calculated vibrationally excited rotational transitions of “known” molecules rather than transitions of molecules or isotopologues for which no line lists have been calculated yet.

A final note on vibrationally excited states: while the inclusion of vibrationally excited rotational transitions allows us to identify such lines, to be able to run models—and to include infrared pumping when the model otherwise focuses on the ground vibrational state—the (ro-)vibrational transitions linking the vibrational levels must also be included. Without these, it is not possible to run models that take vibrational levels into account in any way; the level populations cannot converge on a solution if there is no interaction between vibrational levels. While many line lists of vibrationally excited rotational transitions exist, those for (ro-)vibrational transitions are less prevalent.

¹ <http://www.astro.uni-koeln.de/cdms>.

² <https://spec.jpl.nasa.gov>.

³ The NRAO Spectral Line Catalog: www.splatalogue.net.

⁴ Lovas/National Institute of Standards and Technology: <http://physics.nist.gov/restfreq>.

⁵ The high-resolution transmission molecular absorption database: <http://hitran.org>.

⁶ High temperature molecular line lists for modelling exoplanet atmospheres: <http://exomol.com>.

2.2. Collisional Rates

The most difficult data to obtain for the purposes of radiative transfer modelling are the collisional de-excitation rates (from which the collisional excitation rates can be derived as per Equation (5)). Schöier et al. [38] provides a good overview of the situation and presents the Leiden Atomic and Molecular Database (LAMDA⁷), which hosts molecular data files with all the required information for radiative transfer modelling. Unlike radiative transitions, which connect levels according to quantum selection rules, collisional transitions result in the transfer of kinetic energy between a collider and the molecule of interest and hence can link any two levels, even those for which radiative transitions are disallowed. This leads to significantly more collisional transitions than radiative transitions linking the same set of energy levels (and can cause modelling efforts to run up against computational limitations).

BASECOL⁸ [39] is a database focussing on just the collisional rates of various species. It contains collisional rates for 59 species (including deuterated and ionic species) with four possible colliders (electron, H, He, and H₂), although collisions are generally not listed for all colliders with all species. While collisions with electrons are particularly important in regions with significant electron fractions ($\gtrsim 10^{-5}$ [40]), for example in PDRs, collisions with H₂ are most important for modelling AGB circumstellar emission. Generally, it is best to consider collisions with both ortho- and para-H₂ but when these are not available, a first order approximation can be made by scaling the rates for collisions with He, which tend to be more readily available. Similar approximations can be made when dealing with a species without collisional rates but which is structurally similar to another species for which collisional rates have been measured or calculated. From Schöier et al. [38] we have

$$\gamma_{A-B} = \gamma_{A-C} \sqrt{\frac{\mu_{A-C}}{\mu_{A-B}}}, \quad (6)$$

where γ is the collisional rate before taking the number density of the collider into account (such that the collisional rates used in Equation (1) are given by $C_{ul} = \gamma_{ul} n_{\text{H}_2}$), and the reduced mass, μ , is given by

$$\mu_{A-B} = \frac{m_A m_B}{m_A + m_B}, \quad (7)$$

where m_X the mass of component X . This of course results in very approximate collisional rates for the new species and should only be used when better-calculated rates are not available. For example, Daniel et al. [41] shows that there is no simple relationship between H₂O collisions with He, H₂, and H and that therefore each system needs to be computed separately. In the case of isotopologues, substituting the collisional rates from the more abundant isotopologue when modelling the less abundant isotopologue may seem like a reasonable assumption. However, in some cases, there can be significant differences in the collisional rates, particularly when dealing with deuterated species such as D₂O [42] and ND [43].

In choosing which collisional rates to use, the matter is further complicated by differences arising from different methods of computation. Take, for example, the case of H₂O, one of the most important and abundant molecules found in circumstellar (and many other) environments. Separate sets of recently-calculated collisional rates for H₂O with H₂ as the collider exist. The work of [44–47] calculated the rates using the close coupling method while the work of [48] used quasi-classical trajectory calculations and [24] extended this using an information theory approach. The review of [49] recommends using the rates of [44] at low temperatures (≤ 20 K), the rates of [48] at intermediate temperatures (~ 300 K), and the rates of [24] at high temperatures (≥ 300 K) since these also include vibrational excitation. Dubernet et al. [45] recommends their own rates up to ~ 400 K and those of [48] for higher temperatures. However, it is difficult to gauge which of these rates would be best used for

⁷ <http://www.strw.leidenuniv.nl/~moldata>

⁸ <http://basecol.obspm.fr>.

modelling an AGB outflow which can include a wide range of temperatures from ~ 2000 K down to ~ 10 K.

The matter is further complicated, as noted in [50], when these H_2O collisional rates are used to approximate the collisional rates of other molecules (via Equation (6)) such as H_2S . As well as some discrepancies in the energy ordering of the levels relative to the corresponding quantum numbering, there is the question of how accurate the scaled levels might be when the dipole moments of H_2O and H_2S differ by a factor of ~ 2 with 1.8546 D for H_2O [51] and 0.974 D for H_2S [52]. The two different sets of collisional rates employed by [50] produced significantly different results for their H_2S modelling, with very different resultant line intensities for the same circumstellar model depending on the choice of collisional rates. They found the difference in results between sets of collisional rates was more significant than the difference from the inclusion or not of vibrationally excited energy levels and radiative rates. The difference was significant enough that the final H_2S abundance distributions based on their observed data varied significantly depending on the choice of collisional excitation rates, an example of which can be seen in Figure 1.

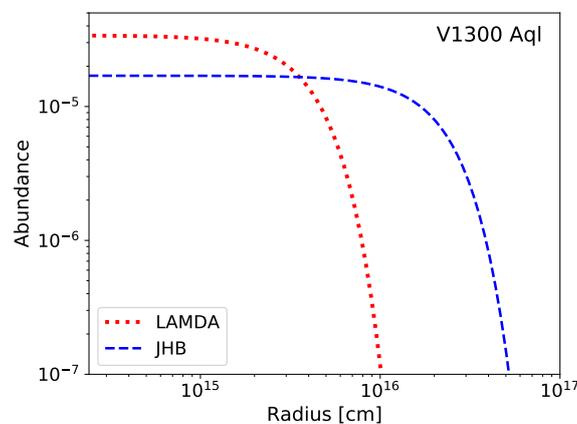


Figure 1. An example of different abundance profiles for H_2S derived from the same observations based on modelling with different collisional rates with Gaussian abundance distributions. Original modelling and data presented are from [50].

The importance of collisional rates to the H_2S results is most likely due to the fact that H_2S is significantly collisionally excited. That is to say, the collisional rates play a more significant role than the radiative rates, thanks to the relatively small dipole moment of the molecule. Other molecules with small dipole moments are also known to be collisionally excited, such as CO, the cyanopolyynes (HC_nN), and others. Good collisional rates for HC_5N and HC_7N do not exist although they are extremely important for these collisionally excited molecules. Approximate collisional rates can be computed from similar molecules such as HCN and HC_3N , as shown by Jaber Al-Edhari et al. [53], based on the proportional size of the molecules. A quick test by us indicated that scaling these approximated rates gave different line intensity results for the same circumstellar model, so the accuracy of the chosen rates remains important. Furthermore, these extrapolations can only be done where collisional rates for the smaller molecules involving levels of a given J exist. At similar frequencies, the larger molecules are more likely to be observed at higher J transitions than the smaller molecules [54], and hence observations can quickly move beyond the range for which collisional rates can be easily approximated, prohibiting the radiative transfer modelling of these transitions.

Another aspect that complicates collisional rates from the perspective of radiative transfer modelling is the inclusion of hyperfine structure. A full discussion of this issue is beyond the

scope of this paper, but a good overview is provided by Faure et al. [55]. Under an assumption of proportionality following [56], the hyperfine collisional rates can be approximated

$$\gamma(J, F \rightarrow J', F') = \frac{g(J', F')}{g(J, F)} \gamma(J \rightarrow J'), \quad (8)$$

where g is the statistical weight of the indicated level. Keto et al. [56] also compare this approximation with a set of exactly calculated hyperfine collisional rates for N_2H^+ and find minimal differences. Hence, the use of this approximation is a useful shortcut when exactly calculated hyperfine collisional rates are not available.

3. Conclusions

In summary, with growing observational capabilities, the need for molecular data is also growing rapidly. The data required for proper analysis include extensive line lists to facilitate line identification, as well as data describing radiative and collisional transitions, to facilitate radiative transfer modelling. While we have focussed primarily on the molecular stellar winds of AGB stars, most of these molecular data are useable for a range of environments. As such, a close collaboration between astronomy and chemistry will enable us to answer various science questions related to AGB research and, in general, to the field of astrochemistry.

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Abbreviations

The following abbreviations are used in this manuscript:

AGB	Asymptotic Giant Branch
CDMS	Cologne Database for Molecular Spectroscopy
HITRAN	High-Resolution Transmission Molecular Absorption Database
ISM	Interstellar Medium
JPL	Jet Propulsion Laboratory
LAMDA	Leiden Atomic and Molecular Database
LTE	Local Thermodynamic Equilibrium
NIST	National Institute of Standards and Technology
NRAO	National Radio Astronomy Observatory
PDR	Photon Dominated Region

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