TROUBLESHOOTING WATER EMISSION OUTPUT FROM HITRAN CODES AND COMPARING SIMULATED WATER EMISSION TO DOAR 24E IRC SPECTRA

Samantha E. Thrush
Department of Physics and Astronomy, Ohio University, Honors Tutorial College, 35 Park Place, Athens, OH, 45701, USA

Abstract

Young sun-like stars are commonly thought to be surrounded by gas and dust disks as they form. An example of such a young star is DoAr 24E, a T Tauri star which has an Infrared Companion (IRC) star. Through the IRC's disk's spectra, we may glean much information about the disk's molecular content, as well as its temperature, rotational velocity, relative abundances of the molecules in comparison with molecular hydrogen. As water is of interest for planetary formation, it became desirable to have a code to simulate water emission spectra so as to identify water peaks in the spectra. So, a simple thermo-equilibrium modelling code for predicting molecular states and the subsequent emission and absorption spectra helps to better characterize the properties in the disk. The task assigned to me was to implement and use one such code that was new to UC Davis. Unfortunately, the code was initially not functioning properly with a water input file. Once the code issues were resolved, the resultant output spectra of the emission code at various disk temperatures were compared to observational data of DoAr 24E's IRC at the same infrared wavelength range. From the comparison of observation data to the simulated water emission spectra at the three separate simulation temperatures (300K, 650K, and 1000K), it was found that the disk temperature of 1000K most closely matched with the observational data. However, it was found that at smaller wavelengths, the observed peaks were shifted to lower wavelengths that what was simulated. These mismatched peaks might point to incorrect data reduction of the observed spectra of DOAR 24E's IRC, a different temperature of the disk, or a presence of different molecular species that might absorb some peaks found in water and emit different wavelengths.

1. INTRODUCTION

As planet formation and composition is of continuing interest in the astrophysical society, it has become increasingly important to observe, as well as understand, the conditions of the host disk that these planets formed under. In this way, the composition, as well as the internal conditions, of the molecular gas and dust disks around young stars has become important in ascertaining the initial conditions of a solar system prior to planet formation [1]. In order to ascertain the possible molecular composition of the planets that might form around these stars, it has become useful to employ spectral observations of these young stars and disks as such information is easiest to glean from spectra rather than from images of the objects. In addition, simulations of emission and absorption spectra of the molecules in the surrounding disk of the star allow scientists to identify characteristic peaks in the observed spectrum, identifying some of its molecular contents, as well as other characteristics of the disk, such as its temperature or radius.

This paper contains four separate sections, excluding the introduction and acknowledgements. In section two, a bit of background will be given, allowing the reader to gain pertinent background knowledge about T. Tauri stars, molecular spectroscopy, as well as DoAr 24E, our binary star system of interest. Section three will discuss the code used, what parameters are most important to the code, and the line list configuration and its relationship to HITRAN. The resulting emission spectra will then be compared to the observed spectra previously collected on DoAr 24E's Infrared Companion (IRC), and such results will be discussed in section four. The conclusion, contained within section five, will elaborate on the project as a whole, what was accomplished, what is hoped to be accomplished in the future to further this project.

2. BACKGROUND

A young star and the surrounding circumstellar disk of dust and molecular gas have much information to offer about conditions of star systems during planetary formation. As stated in Klaus M. Pontoppidan's 2010 Letter, "the molecular gas…

plays a key role in the process of planet formation, not only as a necessary reservoir for the formation of gas giants, but also in the generation and eventual delivery of volatile molecular species to terrestrial planets"[6]. For this reason, it can be of interest to gather further information the contents and conditions pertaining to the circumstellar disk.

The type of star that is utilized when studying young solar systems are T. Tauri stars as they are not yet in the main sequence; instead this type of star is held up against gravity by convection, as opposed to main sequence stars which counteracts gravity through fusion. As these stars are young, only having ages between 10^6-10^7 years old [9], they still possess a dust and molecular gas disk surrounding the parent star as the disk has not yet dispersed. In the most widely accepted model, the configuration of the disk is not flat, but instead, flared at the edges so that only the outer layer of the disk receives direct radiation while an inner core is mostly shielded and is thus colder in comparison [4].

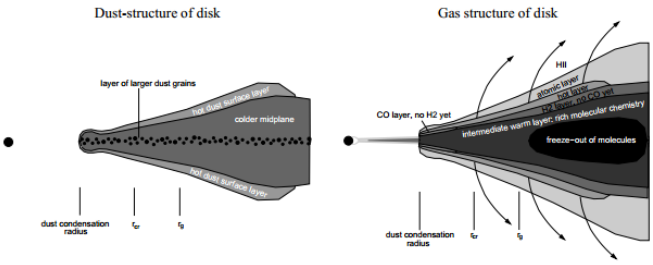

Figure 1 – The basic disk structure of a T. Tauri star with a flaring disk [4].

A T. Tauri system of particular concern to this project is DoAr 24E. This particular system is a binary star system with a separation of 2.03" inside of a star formation region that resides approximately 150 Mpc away. DoAr 24Ea is a classical T. Tauri (a young star that is still accreting material and has a circumstellar disk and is still accreting material)star with a dust and molecular gas disk while DoAr 24Eb, is the classical Infrared Companion (IRC) to the T. Tauri star [5]. From this information, it is safe to assume that both stars are approximately the same age, thus putting the IRC at such an age where it still has a thick molecular gas and dust disk, much like its companion DoAr 24Ea. Although it is common for IRC's to be dim at optical wavelengths and bright in the Infrared (thus granting it the title of and "Infrared Companion"), it is of particular interest that the IRC has high extinction that is not yet explained, although some have hypothesized that such light extinction could be due to the IRC's disk being directly in the line of sight, thus dimming the light the star gives off [5]. Also, the DoAr 24E system has been shown to have water emission, making its IRC disk an ideal subject to study and compare to synthetic water emission spectra.

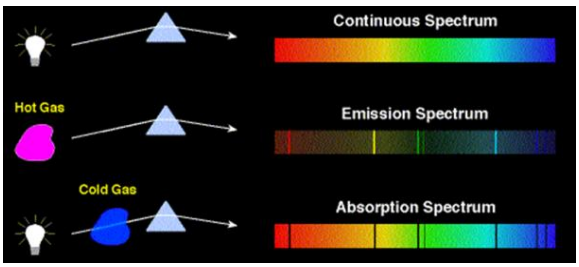

Figure 2: Emission vs. Absorption spectra. As is the case with atoms, molecules also absorb certain wavelengths in order to shift into higher excitation levels or emit certain wavelengths spontaneously in order to de-excite the molecule to a lower energy level. [1]

Since most astronomers are concerned with planet formation within 15 AU of its host star, direct observations of planet formation in the disk would not be resolvable in DoAr 24Eb's case as it is approximately 150 pc away from Earth, and, furthermore, optical observations would not provide information about the molecular content of the disk as the optical range of light does not hold any molecular spectral lines. Instead, molecular spectroscopy is used to gather information about the disk by observing the spectra of the light given off from the system.

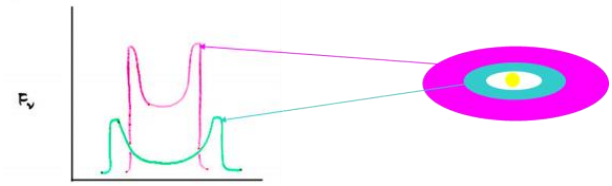

Figure 3: Velocity spreading can be easily explained of Doppler shifting of the light being emitted from the disk. From Kepler's laws, we know that the closer an orbiting body is to its main gravity well (either a star, a black hole, etc.), the greater its rotational velocity. As the object goes away or toward earth, its relative velocity (to earth) changes, which then affects the frequency of the light, thus giving rise to two Doppler shifts. From this relation, a relationship can be made between the amount of velocity spreading and emitting disk section's distance from its parent star.

Taken with permission from a talk from John S. Carr

From the emission spectra output from the system, it is possible to ascertain how large the disk is through velocity spreading of spectral peaks of the emission peaks, as is seen in Figure 3. The temperature of the disk, as well as the relative abundances of molecules to hydrogen can also be found from the emission spectra output by observing how many emission lines are present. In addition, any absorption features found in observational data can reveal if there are any cooler molecules that might be absorbing some of the wavelengths from the emission spectra, possibly causing extinction.

3. EMISSION CODE

During this project, the main objective was to ensure that a provided infrared emission code, created by John S. Carr, would be able to work with input that contained water information. Initially, these water trials, as they were later called, only gave output that gave fluxes assigned to each wavelength either a value of infinity, or a value of a number divided by zero, pointing to either a fault in the code itself, or possibly in the parameter file which acted as input to the larger code. During this section, the synthetic emission code will be discussed, as well as the parameter file. In the latter section, some of the inner components, such as the line list, the temperature, and the relative molecular abundances will be further discussed.

The synthetic emission code is one of two codes, with the other being synthetic absorption code, that simulate the spectra from circumstellar disks of various temperatures, radii, as well as molecular content, and abundances of the types of molecules in comparison with the amount of hydrogen in the disk. Both codes work on an assumption that the disks in question are in local thermal equilibrium.

The emission code is composed of thirty-one separate sections. In a short overview, the code works by reading in information from a parameters file denoted by the user. This information, including the line list of important emission and absorption wavelengths of the associated molecule that is being studied, is then stored in arrays and variables. This information is then sent to various functions where wavelengths are sorted into arrays, the model disk is set up, optical depths are calculated, which then allows for the calculation of the dispersion of the given wavelengths (which contributed to flux). The flux of each wavelength is then calculated. This information is then re-binned so that the output data is more compact, and then the code is finished.

One function of particular concern when leafing through the code for problems and bugs, was the *partfnc*, which is the molecular partition function. The molecular partition function describes the sum over all molecular energy states which is can be written in this form and equals a unitless number denoting all possible excited states a molecule may reside in:

$$q = \sum e^{-\frac{E_{el} + E_{vib} + E_{rot} + E_{trans}}{kT}} \quad \dots Eq\ 1$$

Where E_{el}, E_{vib}, E_{rot}, and E_{trans} indicates the number of possible electronic, vibrational, rotational, and translational states, respectively, k is the Boltzmann constant and T is the temperature of the system. A molecular partition function is unique for each different molecular species, and thus a possible point of problem since the code worked with other molecules such as carbon monoxide but the code would not function correctly with water input [1]. After thoroughly reviewing this section, all of the equations worked as expected. As this seemed to be the only point in the code where there was a possibility of error and no errors were found, it was decided that the parameter file must then be at fault.

The parameter file for the emission code is composed of 25 different sections, each of which either controls a section of the code or sets variable values. Although some parameters are important to the code as a whole (such is the case for the output file names), others allow the user to change what is actually being simulated; as a result, if these parameters are not correctly set, many problems can occur, culminating in nonsensical fluxes (such as infinity and “not a number”) for each wavelength. These parameters are the relative abundances of molecules to hydrogen, the line list chosen, the disk temperature, the scale (which scales the fluxes), and *synlimits* (which controls the interval of wavelengths that the code will create).

As previously stated, each of these parameters must be precisely set to receive real fluxes in the output. For example, the scale parameter must be set to a wavelength range inside of the *synlimit* in order to properly scale fluxes with the equation

$$dscale = \frac{bandflux}{bsum} \quad \dots Eq\ 2$$

where *dscale* is the scale factor, *bandflux* is previously set in the parameter file and is an expression of how much flux is expected from a range of wavelengths, and *bsum* is set as the sum of the actual fluxes from the number of wavelengths inside of the line list that fall within the range set by the scale parameter. In observational quantities, the *bandflux* constant would correspond to the magnitude that is expected from a target at certain wavelengths, whereas the *bsum* constant would correspond to the magnitudes actually observed at the wavelengths in question. The quantity *dscale* is then multiplied to each flux, thus normalizing the flux. Unfortunately, if the scale parameter is incorrectly set with a range that is not included in *synlimits*, *bsum*'s value remains at zero, creating the problem with infinite and "not a number" fluxes.

While the previous parameters were specifically for the simulation's ranges, others correspond to the conditions of the disk and have a direct tie with what peaks we see. For instance, the temperature of the disk allows for higher excitation levels, which allows for more possible transitions and wavelength peaks. A parameter directly tied to the peaks that we see is the *abundance* parameter. The *abundance* parameter increases the number of peaks by increasing the number of possible molecules to be in a higher excitation level and de-excited, thus increasing the number as well as the flux of the peaks.

Unlike the other parameters discussed, the *line list* is a file that contains information converted from HITRAN (HIgh-resolution TRANsmission) files and only gives information regarding what wavelength peaks are permissible. HITRAN is a molecular database which provides information of molecular transitions used for many modeling codes. In order to have useable information for the synthetic emission code, the HITRAN information must be converted into a format that can be read by the code. This was accomplished through a simple python code, which extracted the needed *wavenumber*, isotopologue, low state energy, upper statistical weight, and the Einstein A coefficient from the desired HITRAN file. This information was then sent through a set of equations and operations, which then printed out the molecule label, the wavelength in Angstroms, the molecule ID number, the energy level of the lower level in eV, and the *gf*-value to an output file. The code does this recursively until the end of the HITRAN file is found; the code then closes the input and output files. The molecule label is the only information not read into the code and consists of five characters that accurately describe what molecule HITRAN file the output file information was attained from. To calculate the wavelength, the input wavenumber (which is in units of cm^{-1}) was input into the following equation:

$$\lambda(\text{Å}) = \frac{10^8}{wavenumber} \qquad \dots Eq\ 3$$

This wavelength was then printed with three decimal places and was forced to be contained within ten characters. Next to be calculated and printed was the molecule ID which describes not only the molecular species that is being read in, but also how abundant that isotopologue of the species is; an isotopologue is a set of molecules that are made of the same elements, but the atoms contained are different isotopes, thus making some isotopologues rarer than others. To create the molecule ID, the user must input the base molecular ID, which for water is 10108.0. The isotopologue number is then divided by ten and added to the base molecular ID. This quantity is then printed to the line. The energy level of the lower state (which was to be of the format of ten spaces and three decimal places present) is then calculated:

$$E(eV) = h * c * lower\ state\ energy * 2\pi \qquad \dots Eq\ 4$$

Where h is the Planck constant (4.136 * 10^{-15} eV*s), c is the speed of light in cm/s (2.998 * 10^{10} cm/s). The additional 2π was used to convert between h-bar and h. Ten additional spaces were then printed; these spaces are ignored by the code. Finally, the *gf*-value, which is the product of the oscillator strength of a molecular transition and the statistical weigh of the lower level (also known as the weighted oscillator strength), was calculated from an equation described in the code manual from John Carr:

$$g"f = 1.499\ cm^{-2} * Einstein\ A * upper\ stat\ weight / wavenumber^2 \qquad \dots Eq\ 5$$

Where the Einstein A coefficient is unit-less and is a number between one and zero describing the probability of the molecule to spontaneously emit a photon thus lowering the molecule into a lower state, the upper statistical weight is also unit-less and describes the probability for having a molecule in a higher excited state, and the wavenumber has units of inverse centimeters. The additional 1.499

cm^{-2} is a conversion factor so that the gf-value can be unit-less.

This printed output is then read into the code and utilized for two main processes, which are the partition function, the calculation of the spectra and fluxes, which were discussed earlier.

4. RESULTS AND DISCUSSION

After many trials of attempting to achieve a linelist that works and parameters that can agree with the code (as was discussed in the previous section), synthetic emission spectras of water were finally created for the DoAr 24E IRC's disk.

Three trials were run with all of the parameters identical but the temperature. The trials were run with temperatures of 300K, 650K, and 1000K, to allow for variety of what peaks would be able to be found. It should be noted that the abundance of water was changed to be on the order of 10^7 more abundant than molecular hydrogen, as abundances below such levels gave very weak peaks, or some peaks that were permissible with the temperatures present were not observed at all.

When observing the below graph, notice that although the higher wavelength peaks seem to match fairly well, the lower peaks, such as those found within the 1000 K and 650 K trial, seem to be absent from the observed Data of the IRC's disk. Instead, the peaks that were present in the simulated data trials of 650 K and 1000K at 12.25 to 12.30 microns seemed to have matching peaks in the observation data in the interval of 12.23 to 12.27, although the strongest peak in the simulated trials at 12.28, if it indeed was shifted down to a lower wavelength, does not correspond to the strongest peak in the observational data.

This is very puzzling, as the most prominent peak in both trials seems to be either missing or shifted to a lower wavelength. This can possilby be explained by two separate hypotheses, the first of which is that the code has made wrong assumptions or used inaccurate equations to describe the disk system, but this is almost certainly not the case as this code has accurately described many other emissions and absorptions that match up well with observations.

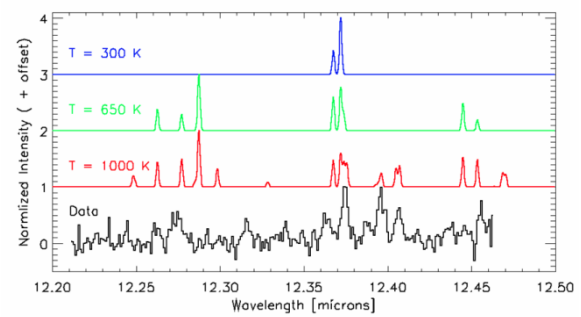

Figure 4: Above is the spectral comparison of water emission from the Syn emission code at temperatures 300K, 650K, and 1000K created with parameters modeling DOAR 24E's IRC's disk and the observed IRC's spectra. Please note that although the higher wavelengths of the simulations agree very well with the observed data, there seem to be discrepancies between the simulated emission and the observed data at wavelengths lower than 12.35μm.

A second possiblilty is that the observed data might have been incorrectly reduced, as very strong peaks are found at similar separation intervals at the wavelength range of 12.23-12.27 microns to those peak intervals found in the wavelength range of 12.25- 12.30 microns in the simulated spectra. This points to a possibility of incorrectly reducing data.

Further checking of both the observed data and the simulated spectra would be needed to discover the true reason for the missing or missplaced peaks.

5. CONCLUSION

Throughout this project, the object of quandary has been DoAr 24E's Infrared companion star. As this star was previously known to contain water, it appeared to be the perfect candidate to compare its observational data to in order to ascertain the accuracy of simulated water emission spectra at various temperatures.

Initially, the emission code created by John Carr to describe molecular emission of circumstellar disks around IRC's was unable to function with water input. In order to ameliorate the issue, it had to be ascertained if the problem was with the input given to the code or the code itself. After searching through the code and seeing its inner workings, and comparing this knowledge to what was actually set in the parameter file, it was found that one variable in the parameter file was set incorrectly, forcing the code to not function correctly.

Once the problem with the parameter file was repaired, three separate trials of simulated water

emission from DoAr 24E's IRC were run. All of the parameters were kept constant with the exception of temperature, and the temperature was set to 300 K, 650 K, and 1000 K. In addition to changing the temperatures from what was previously set in the parameter file given, the relative abundance of water to hydrogen was set to approximately $5*10^7$, meaning that there were $5*10^7$ molecules of water for every one molecule of hydrogen. This was done to increase the number of peaks seen. These resulting emission spectras were then compared to observational data obtained on the DoAr 24E IRC's disk.

As was discussed in the results and discussion section, although simulated emission spectras for water were created, the lower peaks of the lower wavelengths did not agree with those found in the observed data, but instead seemed to either be missing from the spectra all together, or the observational peaks seemed to be shifted lower than what was simulated by the code.

To further this code, it would be advantageous to look into expanding what temperatures are simulated and seeing how that affects what peaks are present and the flux of those peaks. Also, another avenue to explore would be seeing how other molecular species would affect the emission of water, and how varying the abundances of the molecules would affect the output seen. Additionally, the observational data could be checked for data reduction errors if the problem lies with the observational data provided, or a better description of the dust in the disk could be needed if the discrepancy between the observations and the simulations is the fault of the simulations.

6. ACKNOWLEDGEMENTS

I would like to thank my Advisor, Dr. Matt Richter for allowing me to work with him on this project, as well as for his wonderful guidance throughout my time with him. In addition, I would like to thank the University of California, Davis REU selection committee and Dr. Rena Zieve for selecting me to take part in their wonderful REU program and providing a fun and informative summer. And finally, I would like to thank the NSF for funding the UC Davis REU with grant number 1263201.

7. REFERENCES

[1] "Atomic Absorption and Emission Spectra." Astronomy 162 Stars, Galaxies, and Cosmology. N.p., n.d. Web. 8 Aug. 2013. <csep10.phys.utk.edu/astr162/lect/light/absorption.html>.

[2] Carr, John S., and Joan R. Najita. "Organic Molecules and Water in the Planet Formation Region of Young Circumstellar Disks." Science 14 (2008): n. pag. NCBI. Web. 15 May 2013.

[3] Carr, John. S. , and Joan R. Najita. "Organic Molecules and Water in the Inner Disks of T. Tauri Stars." The Astrophysical Journal 733.102 (2011): n. pag. arXiv. Web. 1 June 2013.

[4] Dullemond, C. P., D. Hollenbach, I. Kamp, and P. D'Alessio. "Models of the Structure and Evolution of Protoplanetary Disks." arXiv 1 (2006): n. pag. arXiv. Web. 28 Feb. 2006.

[5] Kruger, Andrew J., Matthew J. Richter, Andreas Seifahrt, John S. Carr, Joan R. Najita, Margaret M. Moerchen, and Greg W. Doppmann. "Gas and Dust Absorption in the DOAR 24E System." Astrophys. J. 760.18 (2012): n. pag. arXiv. Web. 1 June 2013.

[6] "Molecular Partition Functions." Molecular Dynamics Lab. N.p., n.d. Web. 17 Aug. 2013. <www.chem.iitb.ac.in/~bltembe/pdfs/ch_3.

[6] Pontoppindan, Klaus M., Colette Salyk, Geoffrey A. Blake, and Hans Ulrich Kaufl. "Spectrally Resolved Pure Rotational Line of Water in Protoplanetary Disks." The Astrophysical Journal 722.L173-L177 (2010): n. pag. arXiv. Web. 1 June 2013.

[7] Rothman, L.S., and et. al.. "The HITRAN 2004 Molecular Spectroscopic Database." Journal of Quanitative Spectroscopy & Radiative Transfer 96 (2005): 139-204. Print.

[8] Shirley, Yancy L.. "A Quick & Dirty Guid to Astrophysical Molecular Rotation Spectroscopy." NRAO 12 (2003): n. pag. NRAO. Web. 1 June 2013.

[9] White, Russel J., and Lynne A. Hillenbrand. "A Long-lived Accretion Disk around a Lithium-depleted Binary T Tauri Star." The Astrophysical Journal 621 (2005): L65-L68. Print.