Modeling of molecules in circumstellar media

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Resumen / Las estrellas B[e] se caracterizan por poseer líneas espectrales en emisión, tanto de transiciones prohibidas como permitidas, producidas en el disco que rodea a la estrella. Las condiciones de temperatura y densidad en estos discos permiten la formación de moléculas, cuya presencia se manifiesta en la observación de bandas moleculares en emisión. En este trabajo presentamos el código que hemos desarrollado que nos permite modelar las bandas en emisión de distintas moléculas diatómicas como CO, SiO, CS, SiS, NH, etc. El programa tiene en cuenta los distintos isótopos que componen las moléculas, ya que éstos afectan significativamente a las bandas. Con este programa podemos obtener los espectros combinados tanto de moléculas compuestas por distintos isótopos como de la superposición de distintas moléculas. Comparando con las observaciones, podemos usar estos espectros teóricos no sólo para determinar la presencia de las moléculas, sino también otros parámetros, como la temperatura y densidad de las regiones de formación de las moléculas en el disco, la velocidad de rotación, y la región del disco en donde se encuentran las moléculas. Además los podemos utilizar para determinar la relación de abundancia de los distintos isótopos de una molécula, que puede ser utilizada para determinar la etapa evolutiva de la estrella.

Abstract / B[e] stars are characterized by having spectral lines in emission, both of forbiden and allowed transitions, produced in the disk that surrounds the star. The temperature and density conditions in these disks allow the formation of molecules, whose presence is manifested in the observation of molecular bands in emission. In this work we present the code that we have developed which allows us to model the emission bands of different diatomic molecules, such as CO, SiO, CS, SiS, NH, etc. The program takes into account the different isotopes that make up the molecules, since these significantly affect the bands. With this program we can obtain the combined spectra of molecules composed of different isotopes and the superposition of different molecules. Comparing with the observations, we can use these theoretical spectra not only to determine the presence of the molecules, but also other parameters, such as the temperature and density of the regions of formation of the molecules in the disk, the velocity of rotation, and the region of the disk where the molecules are found. We can also use them to determine the abundance ratio of the different isotopes of a molecule, which can be used to determine the evolutionary stage of the star.

Keywords / stars: emission-line, Be — circumstellar matter — molecules

1. Introduction and code description

The code is programmed in FORTRAN 95 and is based on the code for modeling the CO spectrum made by Michaela Kraus (Kraus et al., 2000). It is composed of a module containing the physical, mathematical and astronomical constants. Another module contains the subroutines and functions necessary to calculate the spectra. Finally, two main programs, one for the calculation of the emission spectrum at a given point of an envelope and the other for the calculation of the emission spectrum integrated over the disk that surrounds the star. Several files are required to run the program:

- A file with the general input data containing: name of the output files, resolution, number of points in the frequency grid, spectrum range, number of molecules, name of the files with the data of the molecules, etc..
- Files for each molecule type: atomic and mass numbers, temperature, column density, abundance, file names with the data and the partition function. We consider a molecule to be different if it is composed of a different isotope.
- Files with the data of each molecule (Einstein coefficients, energy levels, quantum numbers, frequency of transitions) and files with the partition function of each molecule.
- A file with the disk parameters (inclination, number of rings, rotation velocity of the rings, number of points on the rings).

The program returns a file with the combined spectrum and a file for each molecule with the individual molecular spectrum.

2. Model fitting

The molecular emission spectra were calculated assuming local thermodynamic equilibrium. The main parameters of the model are the temperature, the column density, the abundance of the different isotopes, the inclination and the rotational velocity of the disk. It is

also possible to choose the resolution of the resulting spectrum to have the same resolution as the observed spectrum. In the following plots (Figs. 1, 2 and 3) we show how the spectrum obtained changes when certain parameters are modified. In all cases we have plotted the most important bands of each molecule.

In Fig. 1, we show the spectrum of CO, considering the isotopic variants of $^{12}C^{16}O$ and $^{13}C^{16}O$. The models were calculated with a column density of 1.0×10^{21} cm^{-2} and for different temperatures between 1 500 K and 2 400 K. The models are normalized to be compared, and to show how the temperature affects the molecular bands. In particular, we can see how the intensity of the second band head changes noticeably respect to the first one with the temperature.

On the other hand, in Fig. 2, we show the spectrum of SiO, at a temperature of 1 800 K, but for different column densities between 1.0×10^{19} cm^{-2} and 5.0×10^{20} cm^{-2}. In this case we have included only three of the five available isotopic variants for this molecule: $^{28}Si^{16}O$, $^{29}Si^{16}O$, $^{30}Si^{16}O$. In both cases we have considered a model without a disk.

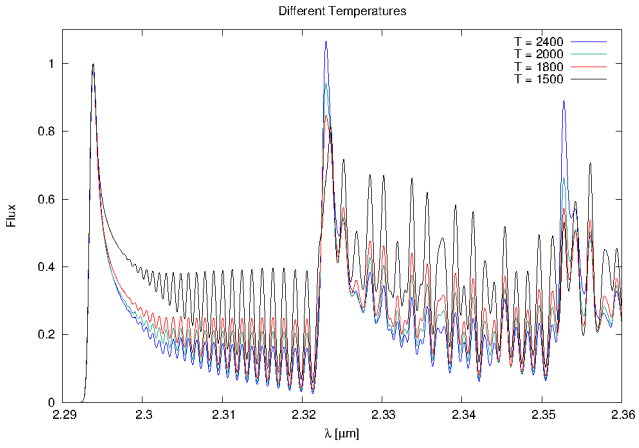

Figure 1: Normalized molecular spectra of CO for different temperatures: 1 500, 1 800, 2 000 and 2 400 K. The column density was fixed to 1.0×10^{21} cm^{-2}.

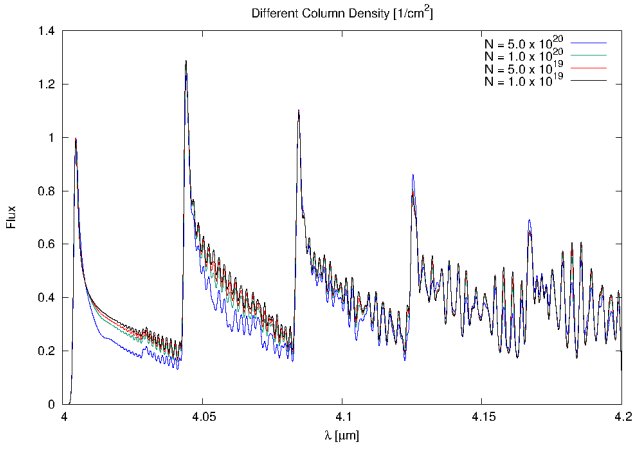

Figure 2: Normalized molecular spectra of SiO for different column densities: 1.0×10^{19} cm^{-2}, 5.0×10^{19} cm^{-2}, 1.0×10^{20} cm^{-2} and 5.0×10^{20} cm^{-2}. The temperature was fixed to 1 800 K.

In Fig. 3, we show two different models of CO with a temperature set at 1 800 K and a column density of 1.0×10^{21} cm^{-2}. In both cases the inclination of the disc is 30°. To obtain the integrated spectrum we calculate the models at 72 points distributed in a rotating ring. In the two models shown the rotational velocities are 30 and 50 km s^{-1}. The spectra show the characteristic double peaks originated in a rotating disk.

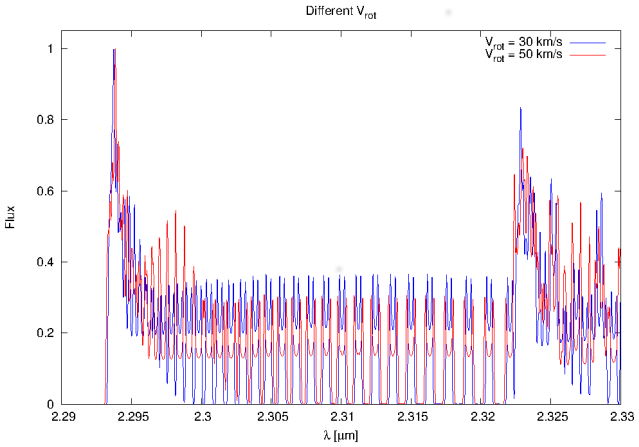

Figure 3: Molecular spectrum of CO considering a disk with an inclination $i = 30°$ for rotation velocities of 30 and 50 km s^{-1}.

In Figs. 4, 5 and 6 we show, as an example, the spectra obtain with a temperature of 1 800 K, a column density of 1×10^{20} cm^{-2}, a disk inclination of 45° and a rotational velocity of 40 km s^{-1} for different molecules. Fig. 4 corresponds to different isotopes of CS, $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$ and $^{13}C^{32}S$, while Fig. 5 corresponds to HCl and Fig. 6 to HN.

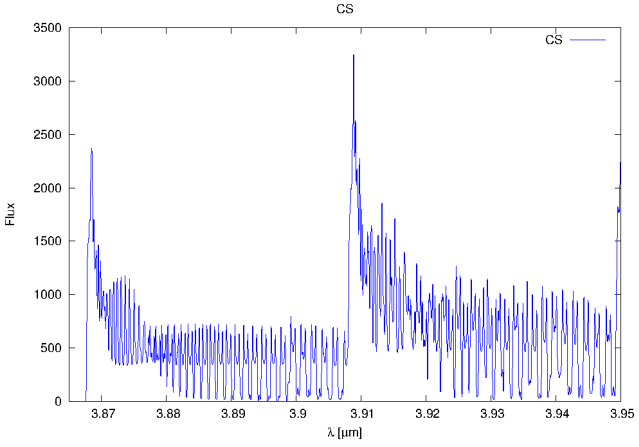

Figure 4: Molecular spectrum of CS considering $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$ and $^{13}C^{32}S$. The parameters are $T_{CS} = 1\,800$ K, $N_{CS} = 1\times10^{20}$ cm^{-2}, $i = 45°$ and $v_{rot} = 40$ km s^{-1}.

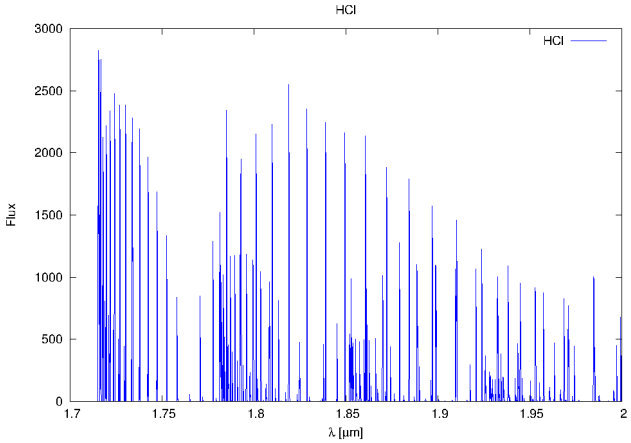

Figure 5: Molecular spectrum of HCl. $T_{HCl} = 1\,800$ K, $N_{HCl} = 1 \times 10^{20}$ cm^{-2}, $i = 45°$ and $v_{rot} = 40$ km s^{-1}.

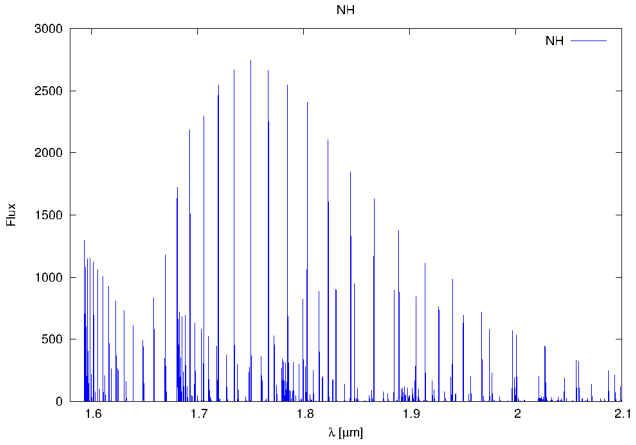

Figure 6: Molecular spectrum of HN. $T_{HN} = 1\,800$ K, $N_{HN} = 1 \times 10^{20}$ cm^{-2}, $i = 45°$ and $v_{rot} = 40$ km s^{-1}.

3. Code testing

To test the code, we compared our synthetic spectra of CO and SiO with the observations and modeling made by Cidale et al. (2012) and Kraus et al. (2015), respectively, for the star CPD-52 9243. The parameters used are the same employed by the authors cited: $T_{CO} = T_{SiO} = 2\,400$ K, $N_{CO} = 4.0 \times 10^{22}$ cm^{-2}, $N_{SiO} = 1.0 \times 10^{21}$ cm^{-2}, $V_{rot} = 33$ km s^{-1}, $i = 40°$ and resolution = 6 km s^{-1}. The fractional abundances are $[^{12}C^{16}O] = 0.95$, $[^{13}C^{16}O] = 0.05$, $[^{28}Si^{16}O] = 0.920$, $[^{29}Si^{16}O] = 0.047$, $[^{30}Si^{16}O] = 0.031$. In Fig. 7 we compare our synthetic molecular spectrum of CO with the observed spectrum of the star CPD-52 9243. It is possible to compare this figure with Fig. 1, left lower panel, of the paper of Cidale et al. (2012) (p. 325) and see that our model agrees with those results. For reasons of space, we do not show here the spectrum for SiO.

4. Conclusions

We have developed a program that so far allows us to calculate the emission spectra of several diatomic molecules individually or simultaneously, if necessary. These are: CO (2 isotopic variants), SiO (5 variants), CS (8 variants), SiS (12 variants), NH and HCl. With these models it is possible to determine the presence of a molecule, but also some parameters such as the temperature and density of the molecular gas, as well as in the case of disks, the rotation velocity and eventually the distribution of the different molecules in the disk. We have verified the right operation of the code by comparing with the fitting made by other authors. Furthermore, we have used the program to determine the CO parameters of the discs of some stars (see the article "High resolution near-infrared observations of B[e] supergiants", M.L. Arias et al. in this Bulletin).

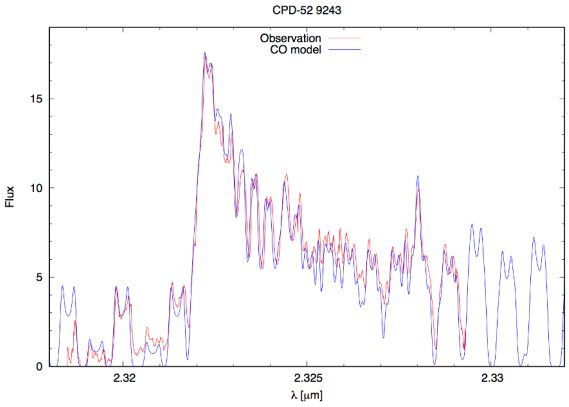

Figure 7: Synthetic spectrum of CO (blue) used to test our code with observations of the star CPD-52 9243 (red).

5. Future work

To model the spectra we require data on the transitions frequencies and rotovibrational levels of the molecules. In general, we use the data provided by the ExoMol database. Our intention is to include more molecules, mainly the most frequent ones detected in stellar discs and envelopes such as TiO, CaO, CN, NO, OH, VO, CH, NS, etc. As molecular data is released, we will be able to adapt it to our code and expand the number of molecules available.

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