PRESTALINE: A package for analysis and simulation of star forming regions

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Abstract. PRESTALINE is a package allowing a user to simulate and analyse spectra of various astrophysical objects. The package is based on the numerical models PRESTA (Kochina & Wiebe (2017)) and RADEX (van der Tak et al. (2007)). PRESTALINE provides the direct comparison of theoretical models with observations and allows estimating physical conditions in a studied object, such as kinetic temperature and chemical composition. Here we present the results of applying PRESTALINE to the test object DR21(OH) and discuss possible applications and future extensions of the project.

Keywords. astrochemistry, line: profiles, ISM: molecules

1. Introduction

Astrochemical modelling is a standard approach for the investigation of star-forming regions. The problem in its application is in the need of making a proper comparison of theoretical (molecular abundances calculated with a chemical model) and observational (molecular spectra) results. Usually it are the observers who make the step towards the theory: observed spectral lines are identified, and their intensities are converted into column densities of corresponding species. These observationally inferred column densities can then be compared to the column densities obtained as an output from astrochemical numerical models. But this approach is not free of complications. Generally, as all solutions of the inverse problem, it suffers from degeneracy problems. Also, to make the problem of minimisation tractable, we need many simplifying assumptions on the physical structure of the object. Conversion of line intensities into column densities is often made under the LTE assumption, which is not always adequate for realistic physical conditions. Theoreticians on the other side blindly rely on the values provided by observers, which may lead to confusion instead of discovery.

A more correct approach can be found in solving the direct problem: converting column densities obtained in numerical astrochemical models into line intensities and creating a synthetic spectrum, suitable for direct comparison with the observed spectrum. In this work we present the package PRESTALINE (Van Looveren, Kochina & Wiebe 2021) designed for that purpose. PRESTALINE simulates the chemical evolution, uses the column densities and physical properties of the object to calculate synthetic line intensities and then provides the visual comparison of the observed and calculated spectra. As a separate feature, the package allows using the observed spectrum for a rough estimation

of parameters of the studied object, such as temperature and chemical composition, in a quantitative way.

A description of the package is given in Section 2. Section 3 demonstrates capabilities of the estimation tool and its application to the spectrum of the DR21(OH) star-forming region. The conclusions and plans for further development and applications of the package are described in Section 4.

2. Synthetic spectra

PRESTA. The astrochemical module of PRESTALINE is based on PRESTA, a 1D model of the chemical evolution of prestellar and protostellar objects, which is being developed at the Institute of Astronomy of the Russian Academy of Sciences. PRESTA simulates a static or collapsing spherically symmetric protostellar core, irradiated by both diffuse external radiation and a central source (protostar) with assumed parameters. The modelled object is characterized by gas and dust temperature radial profiles (these temperatures can be different), density radial profile, and extinction for external and internal radiation. PRESTA currently uses the chemical network from the work of Albertsson et al. (2014) that includes deuterated species. The model may contain several dust populations and also may take into account evolving distributions of temperature and density (warm-up and collapse). The outputs of PRESTA are radial profiles of relative abundances as a function of time and/or column densities of each species as a function of time.

At the first step, PRESTA prepares basic files containing the information on the modelled object needed for further processing and creating the synthetic spectra. These data are kinetic temperature, density of collision partners (we consider only H_2 here), and column densities of the considered species. In order to be more consistent with the properties of the real object and allow for a more detailed study, the computational domain is divided into several zones, each with its own physical conditions. Due to limitations of RADEX on the next processing step, the number of zones cannot be too large, as the column densities of less abundant species within the zone may become smaller than the minimum that RADEX can handle. In this work we assumed that the object is divided into three zones: a hot dense inner zone, a warm dense intermediate zone, and a cold and less dense outer zone. For each of the zones separate output files are produced with average temperature, gas density, and the column densities of the species. These files are passed to the second module of the package as the input ones.

RADEX. In order to relate the chemical model of a molecular cloud to a spectrum, the column densities need to be converted into spectral intensities or similar quantities (several options for conversion are included in PRESTALINE). PRESTALINE uses RADEX to achieve this purpose. RADEX is a non-LTE, statistical equilibrium radiative transfer code developed by van der Tak et al. (2007). It provides information on each transition such as central wavelength, excitation temperature, and opacity.

Visualisation. The next part of PRESTALINE is a visualisation module. As thermal broadening is usually the dominant broadening mechanism in molecular clouds, a Gaussian line shape is a good approximation, so the excitation temperatures calculated by RADEX are converted into the amplitudes of Gaussians. To ensure that the lines and only the lines are modeled in sufficient detail, a window around the central wavelength is created. If a new line overlaps with an earlier modelled line, their intensities are added. This allows for line blending and more realistic spectra. Additionally, the visualisation takes into account the optical depth of a transition to reproduce the broadening of saturated lines.
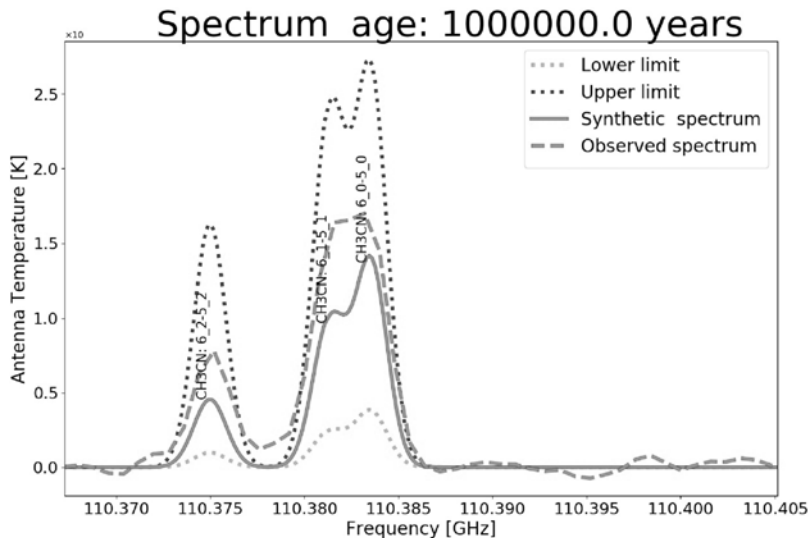
Figure 1. An example of a synthetic spectrum compared with the observed spectrum of DR(21)OH. The dotted lines represent the upper (calculated with column density times 5) and lower (calculated with column density divided by 5) limits.

All lines originating within a zone are combined into a single spectrum. This spectrum is then used as the background radiation of the next, more outward zone. The background reduced in intensity according to the opacity of the zone closer to the observer. This process is repeated for all the three zones to get the emergent spectrum. This approach allows for more complex spectra as outer zones can diminish and even extinguish the contribution of the inner ones.

In order to demonstrate the capabilities of PRESTALINE, we used the spectrum of DR21(OH), a well-known region of massive star formation belonging to the Cygnus-X complex. The spectrum was kindly provided by S. Kalenskii (Kalenskii & Johansson 2010). The region has already been studied with PRESTA (Kochina et al. (2013)), so for the test modelling we could use information on the physical properties we already have. The comparison of the synthetic spectrum created by PRESTALINE with the observed spectrum is shown in Figure 1. To provide a quick way to assess how close a synthetic spectrum is to an observed one, PRESTALINE produces error margins. This is done by dividing the column density of each considered species by a factor of 5 for the lower margin and multiplying it by 5 for an upper margin.

3. Estimation tool

The PRESTALINE package also has the capability to estimate the parameters of an object by analysing the observed spectrum. The first of these parameters is the temperature of the molecular cloud. The temperature can then be used to fit the column densities of various species.

Temperature estimation. The temperature is the first parameter which PRESTALINE fits, as further parameters depend on the temperature. The temperature is estimated through a rotation diagram, a method discussed in detail in Kalenskii & Johansson (2010). In this method the line intensity is related to the energy of the transition, which depends on the gas temperature. The energy of the transition can be calculated from molecular data. The line intensity is found by fitting a Gaussian to the observed spectrum
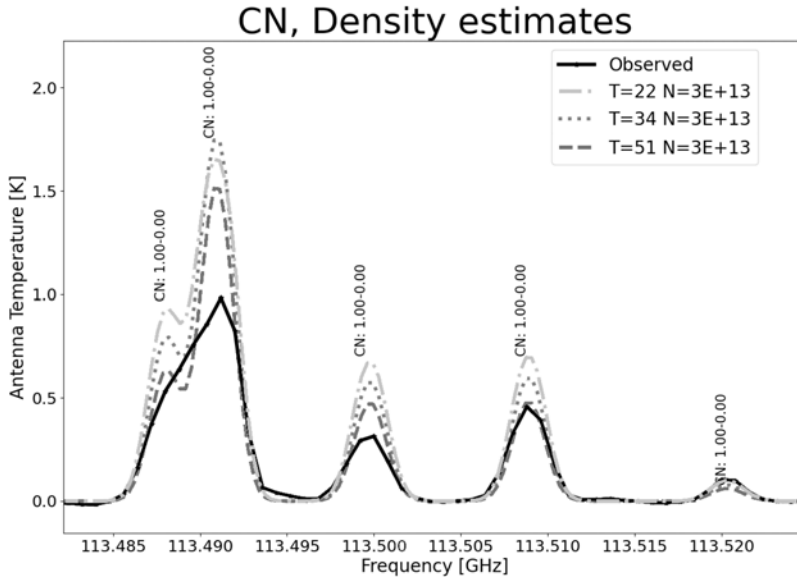
CN, Density estimates

Figure 2. Estimation of CN column density for different temperatures using a 1-zone approach. A 1-zone approach is unable to reproduce the ratios of transitions of the observed spectrum.

and calculating the area under it. In the case of two overlapping lines, two Gaussians are fitted simultaneously to get the best result. As the lines selected for this purpose are either single or a blended pair, a double Gaussian is sufficient. The slope described by these points is the inverse of the temperature. It is important to note that this method assumes optically thin lines, making the selection of lines important.

For this work, CH_3CCH and CH_3CN are chosen. The first of these is associated with the warm dense intermediate region, whereas the latter is most commonly found in the hot dense core region. When this method is applied to the observed spectrum, it results in $34 \pm 12K$ and $51 \pm 9K$ for transitions of CH_3CCH and CH_3CCN, respectively. Figure 2 shows a synthetic spectrum for a 1-zone model of 22 K (the lower error bound), 34 K (the CH_3CCH temperature), 51 K (the CH_3CN temperature) and the observed spectrum. From this graph it is clear that the temperature strongly influences both the intensity of the lines and the ratio between intensities of the same molecule's lines. The 1-zone models cannot reproduce the observed spectrum satisfactorily. By combining multiple zones with different parameters (e.g. different temperatures), better agreement with the observation can be achieved. This multiple zone model is also more representative of real protostellar objects.

Density estimation. With the temperature determined, the next parameter is the column density. The column density of each species is fitted separately and can be fitted either with a 1-zone or a 3-zone model. At this step, RADEX is used again to calculate the line intensities for each transition. This requires the previously determined temperature and a column density, the parameter we wish to fit. As RADEX can handle 20 orders of magnitude in number density, it can be time consuming to fully cover all possible combinations especially when using multiple zones. For this reason PRESTALINE currently uses a random search algorithm to probe the parameter space.

Each set of column densities is turned into a synthetic spectrum as described above. The spectra are then compared to the observation to determine the uncertainty of the
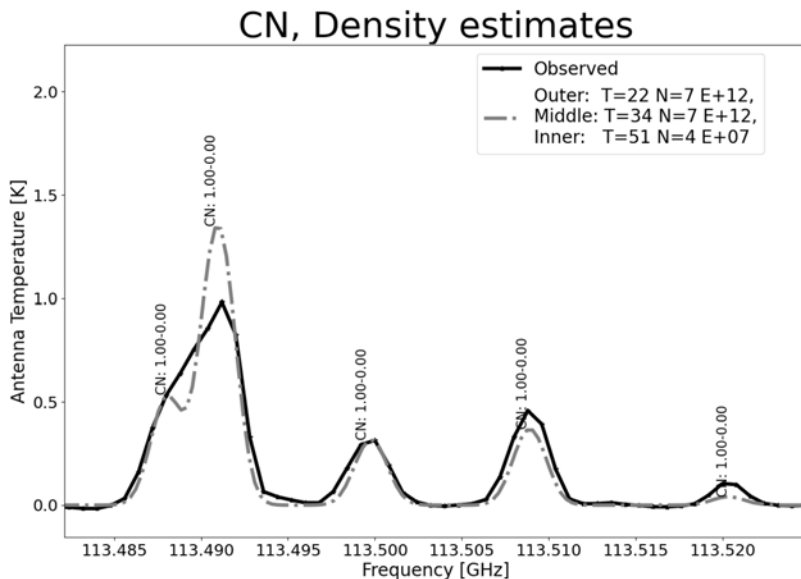
Figure 3. Estimation of CN column density using a 3-zone approach. A 3-zone approach allows much better agreement with the observations.

fit. Using the 3-zone model allows the fitting procedure to find better fits for some complex lines as shown in figure 3, but it also adds uncertainty to the results. When an outer zone is very dense and opaque, different parameters for the inner zone result in the same spectrum and uncertainty. Additionally, an error calculation cannot see the difference between overestimation or a comparable underestimation, though this can have significant physical meaning. For this reason PRESTALINE will then store the three best fits for the user to compare.

4. Conclusion

At the symposium we presented PRESTALINE, a package for the numerical analysis of molecular spectra. The tool intends to bridge a gap between theoretical and observational astrochemistry, both by deriving synthetic spectra from astrochemical models and by deriving parameters from observed spectra. The synthetic spectra allow a chemical model to be compared directly to observations through statistical equilibrium, which avoids the assumption of LTE. On the other hand, the estimation tool allows the user to quickly assess some of the object parameters.

In the section on temperature estimation, we alluded to the importance of temperature tracers for different regions. Adding molecules to the temperature estimation and grouping them according to their formation region will further improve the derived temperature profile and consequently the density profiles. To further improve the ease of use, the estimation part will be expanded with a tool for the analysis of the radial velocity.

One of the future applications of PRESTALINE is to build an atlas of spectra for a grid of objects with the given parameters and facilitate estimating specifics of studied objects.

PRESTALINE can be used for studies of various objects, different in geometry and physical conditions from the star-forming regions presented in the current work, such as planetary nebulae or protoplanetary disks. Extensions of the chemical network will also allow calculating the synthetic spectra for hotter regions: galactic nuclei and others.

Acknowledgements

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Discussion

BANDA BARRAGAN: Can PRESTALINE be adapted for use, with outputs from grid-based simulations. For example, we have a temperature map from the simulation or a column density map, can I adapt the code for a use with the simulation output as well to produce some synthetic spectra?

VAN LOOVEREN: Yes, at the moment the visualisation part and RADEX part take as an input: the column density, temperature and collision partner column density. If these are provided the different sections can work on their own. In a similar way if you have a profile of the temperature, the density and radiation field, this can be used as an input for PRESTA.