Temperature determination based on molecular excitation diagrams

MSc - II Practical

I. Photodissociation regions and molecules

Astrophysical environments dominated by dissociation due to UV photons are called photodissociation regions. The region near a source of UV radiation may be considered to have a plane-parallel geometry, such that the layers of gas nearest to the UV source comprise of ionized gas (dominated by H II). Going further away from the source implies cooler conditions which allow the gas to be neutral. Such gas will host H I in large quantities. Still deeper into the cloud are regions where molecules, such as H_2 and CO, may exist.

Molecules exhibit not only electronic energy levels but also vibrational and rotational energy levels. H_2,

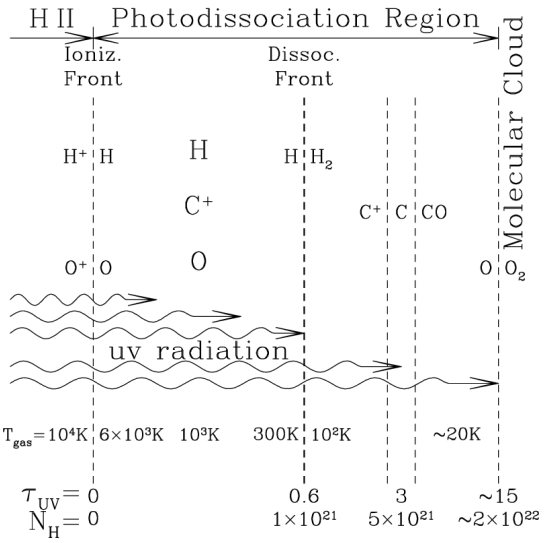

Figure 1: Structure of a photodissociation region; Credit: Draine (2011)

the most abundant molecule, may be typically detected in several different rovibrational levels. Knowing the statistical weight associated with these levels, it is possible to estimate excitation temperatures using the Boltzmann equation:

$$\frac{N_1}{N_2} = \frac{g_1}{g_2} exp \frac{-E_{12}}{kT} \tag{1}$$

Statistical weight is the product (2S+1)(2J+1), where S and J represent the nuclear spin and rotational quantum number respectively. Ortho states have odd J and I = 1, while para states have even J and I = 0. H_2 intensity or column density corresponding to different energy levels can be plotted to make an excitation diagram, that gives insight into the temperature conditions in the region hosting the H_2 gas.

The intensity and column density are related to each other through the following relation:

$$I = \frac{A \Delta E N_u}{4\pi} \tag{2}$$

Here, A is the Einstein coefficient, N_u is the column density in the upper state, and ΔE is the energy difference associated with the transition.

II. Practical exercise

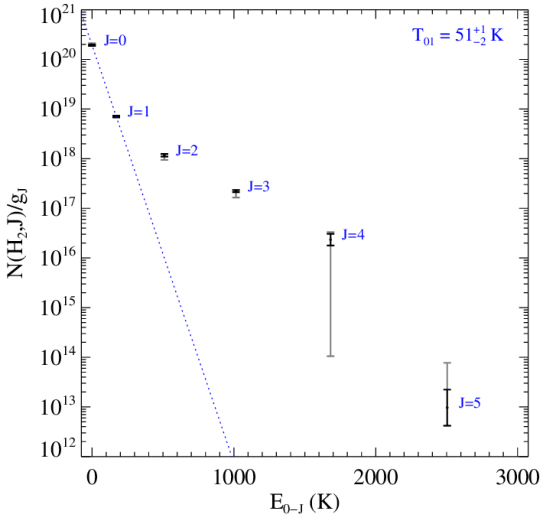

Figure 2: H_2 excitation diagram; Credit: Noterdaeme et al. (2017)

- Install the Python-based package PhotoDissocation Region Toolbox.
- Use the *Measurements* set of commands, enter the intensity values provided: 3×10^{-5}, 5×10^{-4}, 4×10^{-4}, 2×10^{-3}, 5×10^{-4}, 10×10^{-4} for S 0 to 5.
- Use the *H2ExcitationFit* set of commands to fit the temperature, first determining the column density in different H_2 levels.
- Use the *ExcitationPlot* set of commands to plot the appropriate excitation diagram. Apply two different fits to the observed data – a single component fit and a two-component fit.
- Determine the ortho-to-para ratio.

IV. References

`https://dustem.astro.umd.edu/tools.html`
`https://iopscience.iop.org/article/10.3847/1538-3881/ac9b1f`
`https://pdrtpy.readthedocs.io/en/latest/#example-notebooks`
`https://github.com/mpound/pdrtpy/tree/master`

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