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Study of the anthracene energy and temperature: the case of the canonical ensemble from the astrochemistry perspective

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Abstract. Statistical mechanics provides essentials results about the physical and chemical properties of matter at the macroscopic level, from the analysis of the microscopic components of the system of interest. This work will perform a brief description regarding the canonical formalism, as well as the essential expressions for understanding it. After deducing them, it is necessary to use the classical ideal gas approximations to obtain the internal energy. Since statistical mechanics, the temperature connects to the average energy of a system. It is possible to analyze the emission energy in the mid-infrared (MIR) by a PAH molecule as of its temperature, demonstrating the relationship between E-T. Employing ideal gas approximation work has demonstrated that PAH molecules can describe using the canonical ensemble equations and the relationship between temperature and energy.

Resumo. A mecânica estatística fornece importantes resultados sobre as propriedades físicas e químicas da matéria a nível macroscópico, a partir da análise dos componentes microscópicos do sistema de interesse. Este trabalho realizará uma breve descrição a respeito do formalismo canônico, bem como das expressões essenciais para a compreensão. Após a dedução dos mesmos, é necessário usar das aproximações do gás ideal clássico para a obtenção da energia interna. Visto que na mecânica estatística a temperatura está conectada à energia média de um sistema, é possível analisar a energia de emissão no infravermelho médio (MIR) por uma molécula de PAH e a partir de sua temperatura, demonstra a relação entre E-T. Através da aproximação do gás ideal, o presente trabalho demonstrou que moléculas de PAH podem ser descritas por meio das equações do ensemble canônico e a relação existente entre temperatura e energia.

Keywords. Astrobiology — Astrochemistry — Teaching of Astronomy — Methods: analytical

1. Introduction

Given the multi and interdisciplinary nature of astronomy, its use as a teaching tool for disciplines in the field of exact sciences, such as statistical mechanics, is coherent. This provides fundamental properties of the system, based on the analysis of the microscopic components of the object of study.

This work proposes to approach themes of statistical mechanics and suggests investigating whether the behavior of molecules in stellar environments can be described in terms of the canonical formalism, in particular, the Classic Ideal Gas. In this sense, this work seeks to integrate and establish relationships between different areas of knowledge, in addition to the use of technological tools to facilitate the teaching of physics.

2. Materials and methods

Through the description of the canonical formalism, the expressions necessary for the understanding of the Classic Ideal Gas, composed of non-interacting particles, will be discussed. After its definitions, the physicochemical characteristics of polycyclic aromatic hydrocarbons (PAHs), species with great astronomical interest, will be dealt with, as they can capture oxygen or nitrogen atoms and contribute to the formation of compounds fundamental to life in the Universe (Ehrenfreund et al. 2006).

As well as the excitation process that occurs through the interaction with ultraviolet (UV) radiation. These molecules are heated to high temperatures and enter an excited state, and as they cool, emission occurs at the MIR. The different molecular geometries that determine the vibrational excitation modes (Sales et al. 2012) and the main dimensions will also be analyzed since there are PAHs with hundreds of atoms. This work will use anthracene (Figurae1) that will go compared to the ideal gas. Literature indicates that small species can reach temperatures above 1000K, cool down to 10K seconds later and, remain so until absorbing another UV photon (Tielens 2008)

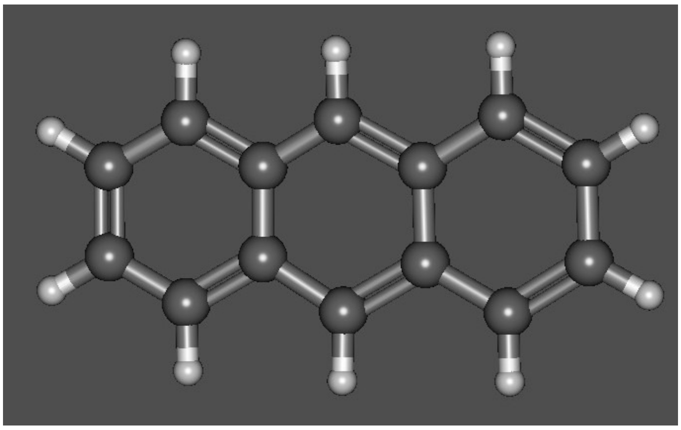

Figure 1. Anthracene molecule.

3. Results and discussions

The Z partition function allows obtaining other physical quantities within the canonical formalism as the expression of the internal energy of the ideal gas. As they are non-interacting particles, the internal energy is equal to the average kinetic energy of each particle. In this event, as anthracene is will be treated as a gas, the 24 atoms will be the component particles.

Through the equipartition of energy, we get the mean square velocity. In addition, the system's probability distribution makes it possible to deduce the most likely velocity expressions and the

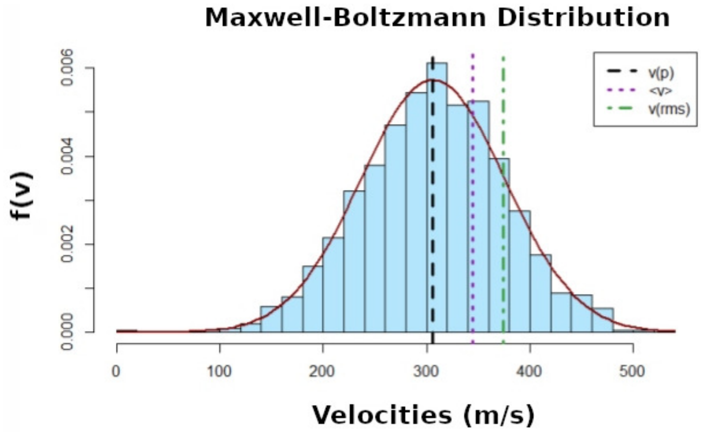

Figure 2. Distribution of velocities.

mean velocity value. As the temperature measures the degree of agitation of the particles, it is possible to infer the possible velocities that the PAH will reach during the emission process after the absorption of a UV photon.

Figure 2 presents the characteristic graph of the Maxwell-Boltzmann distribution, where the most probable velocity is equal to $v_p = 305.42\ m/s$ a and is found at the peak of the graphic, indicating the high probability of finding particles in this velocity. Next comes the mean value of velocity, equal to $\langle v \rangle = 344.64\ m/s$. Finally, the mean square velocity designates the mean velocity of all particles and has a value of a $v_{rms} = 374.07\ m/s$.

4. Summary And Conclusions

This work presented deductions regarding ideal gases, using research objects from astronomy. This shows the possibility of using interdisciplinary means to awaken students' attention and motivation. It is noteworthy that this work used approximations and treated a molecule as a gas, just for better understanding. Furthermore, it allowed us to infer that despite having different physical properties from ideal gases, it is possible to describe the relationship between temperature and kinetic energy of a PAH.

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