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Study of the Naphthalene Vibration Properties using Density Functional Theory Modeling and its Application in Galaxies

Douglas A. da Silva, William da Silva Chaves, Dinalva A. Sales, Carlos Frajuca, & R. C. Rosa

[1] Instituto de Matemática, Estatística e Física, Universidade Federal do Rio Grande, Rio Grande 96203-900, Brazil
e-mail: douglasastrofisica@gmail.com, william.chaves.rs@gmail.com, dinalvaires@gmail.com

Abstract. Since its birth, the Universe has created complex structures from simple units, according to current studies in astrochemistry about 20% of the carbon present in the interstellar medium is found in the form of polycyclic aromatic hydrocarbons (PAHs), which family of molecules is very abundant in the Universe, and the emission of the electromagnetic spectrum of these molecules is found in the mid-infrared. In this present work we focus on the use of computational modeling of the Naphthalene molecule and allied to quantum mechanics-derived approaches, through the Gabedit platform, which is a free software that includes the following: Graphical interface for dynamic processing of packages of common molecular dynamics programs which uses a quantum approach, the Density Functional Theory, which in turn allows studying increasingly complex systems, contributing to the understanding and prediction of the properties of atoms, molecules and solids. From a theoretical point of view, the study of molecular properties has become a strong tool in the analysis of various types of physical and chemical processes. In this work, the comparison between the spectra of Starburts and Seyfert galaxies with the spectrum of the Naphthalene molecule was performed.

Resumo. Desde o seu nascimento, o Universo criou estruturas complexas a partir de unidades simples, segundo estudos atuais em astroquímica cerca de 20%, do carbono presente no meio interestelar se encontra na forma de hidrocarbonetos policíclicos aromáticos (sigla em inglês, PAHs), esta família de moléculas é muito abundante no Universo, e a emissão do espectro eletromagnético dessas moléculas se encontram no infravermelho médio. Neste presente trabalho nos detemos ao uso da modelagem computacional da molécula de Naftaleno e aliada as aproximações derivadas da mecânica quântica, através da plataforma Gabedit que é um software livre que inclui o seguinte: Interface gráfica para processamento dinâmico de pacotes de programas comuns da dinâmica molecular que utiliza uma aproximação quântica, a Teoria do Funcional da Densidade, que por sua vez permite estudar sistemas cada vez mais complexos, contribuindo para a compreensão e previsão das propriedades dos átomos, moléculas e sólidos. Do ponto de vista teórico, o estudo de propriedades moleculares vem se tornando um forte instrumento na análise de vários tipos de processos físicos e químicos. Neste trabalho foi realizado a comparação entre os espectros de galáxias Starburts e Seyfert com o espectro da molécula de Naftaleno.

Keywords. Astrochemistry – Infrared: galaxies – ISM: molecules – Methods: numerical – Techniques: spectroscopic.

1. Introduction

From a theoretical point of view, the study of molecular properties comes to making it a strong tool in the analysis of various types of physical processes and chemicals. In this work, the comparison between the spectra of galaxies was performed. Starburts and Seyfert with the Naphthalene molecule spectrum. Quantum mechanics is essential for us to understand almost all natural forces and currently the study of molecular properties is becoming a strong tool in the research of different types of chemical and physical processes of the point From a theoretical point of view, the most promising route has been via the equations of Mechanics Quantum.

Quantum mechanics has as its main focus of study the world microscopic, and had its foundations established by scientific discoveries in the end from the 19th and early 20th centuries, which were essential for Modern Physics. In this way, the study support was defined throughout the 20th century, receiving thus important contributions from several scientists. In this way, the mechanics Quantum became the theoretical and experimental support of several fields of Chemistry and from Physics (e.g. Sales et al. 2013; Joblin & Tielens 2011; Tielens, 2008). In this present work we will focus on the spectrum generated by the modes vibrational effects of the naphthalene molecule and compare with the modeling done by the AMES NASA Database project. In addition, the presence of this molecule in the mid-infrared (MIR) spectra of Starburst galaxies and Seyfert galaxies.

Due to the degree of complexity of some systems, it is necessary use computer simulations to understand processes molecular structures, one of the most widely used techniques to study structures complex is the Density Functional Theory (DFT) . In DFT, the fundamental quantity is the Electronic Density. In Quantum Mechanics, the product $|\Psi(r)|^2$ is interpreted as the probability to find an electron whose physical state, at a certain moment, is described by the Wave Function $\Psi(r)$, the electron density is then interpreted as the electron charge times the probability density $\rho(r) = e\Psi(r)$. doing some approximations it is possible to describe the behavior of systems with many electrons as atoms and molecules, for that we start with the Schrödinger equation regardless of time.

After the calculations performed by the Gabedit software, it can be viewed in the figure 1 the characteristic vibrational modes of the naphthalene molecule and its electromagnetic spectrum, the spectrum is normalized by the highest emission peak. In Figure 1, it is possible to identify the existence of emission bands in the region corresponding to 12.445 μm, highlighted by the red solid line and that can be related to the presence of naphthalene, we can also infer the presence of this molecule in the 3 galaxies in which the spectra are compared.

The investigation of molecular properties has become a strong instrument in the analysis of different types of physical and chemical processes, for the analysis of these properties,

from a theoretical point of view, the most favorable way is using the equations of Quantum Mechanics. the main emission bands of the electromagnetic spectrum are in the mid-infrared region, characteristic of Emission by Molecular Vibration. This work aimed to study the electromagnetic spectrum of the Naphthalene molecule, and to infer its presence in Seyfert galaxies. The results obtained through the use of DFT, with two base sets, proved to be satisfactory. Since the computational modeling of the Naphthalene molecule identified contributions in wavelengths in the medium range, the same ones observed in Seyfert galaxies. In this sense, we can conclude that this molecule can be present in extragalactic objects.

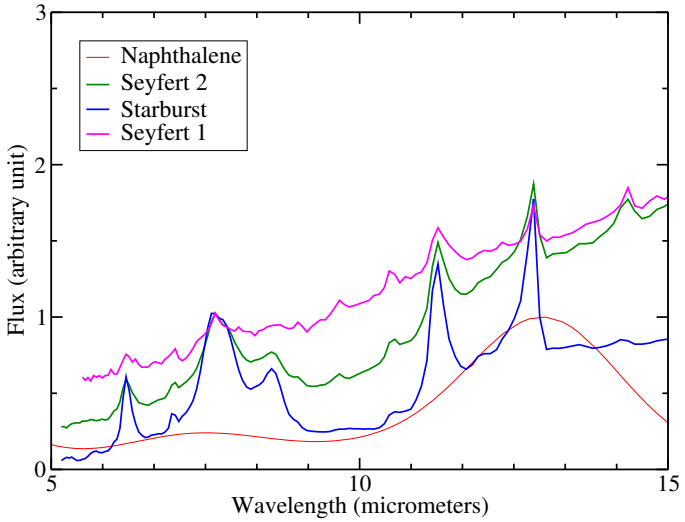

Figure 1. Mid-Infrared spectra of Seyferts and Starburst galaxies observed with Spitzer telescope. Modeled naphthalene molecule is shows in red line.

Functional B3LYP is the one that best suits the modeling of organic molecules and is what we use in this work.The energy calculation was done in the neutral state, since a large part of the contribution of emission in galaxies comes from neutral species and also due to the optimization of computational time. The choice of a base function allows greater precision in the calculation of the molecule's electronic structure, in this work Gaussian functions (GTFs) were used because in the literature they are considered to have more advantages over other bases, and it is one of the sets database used by NASA Ames PAH IR Spectroscopic Database (PAHdb)

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References

Andrews, H. et al. *PAH emission at the bright locations of PDRs: the grandpah hypothesis. The Astrophysical Journal*, v. 807, n. 1, p. 99, 2015.

Joblin, C.; Tielens, A. G. G. M. *PAHs and the Universe: A Symposium to Celebrate the 25th Anniversary of the PAH Hypothesis, EAS Pub.*

Sales et al. 2013, MNRAS, 429, 2634.

Tielens, A. 2008, Physics and chemistry of the interestelar medium, (New York: Cambridge)

Woods, Peter M. et al. *The chemistry of protoplanetary nebulae.* Astronomy & Astrophysics, v. 402, n. 1, p. 189-199, 2003.