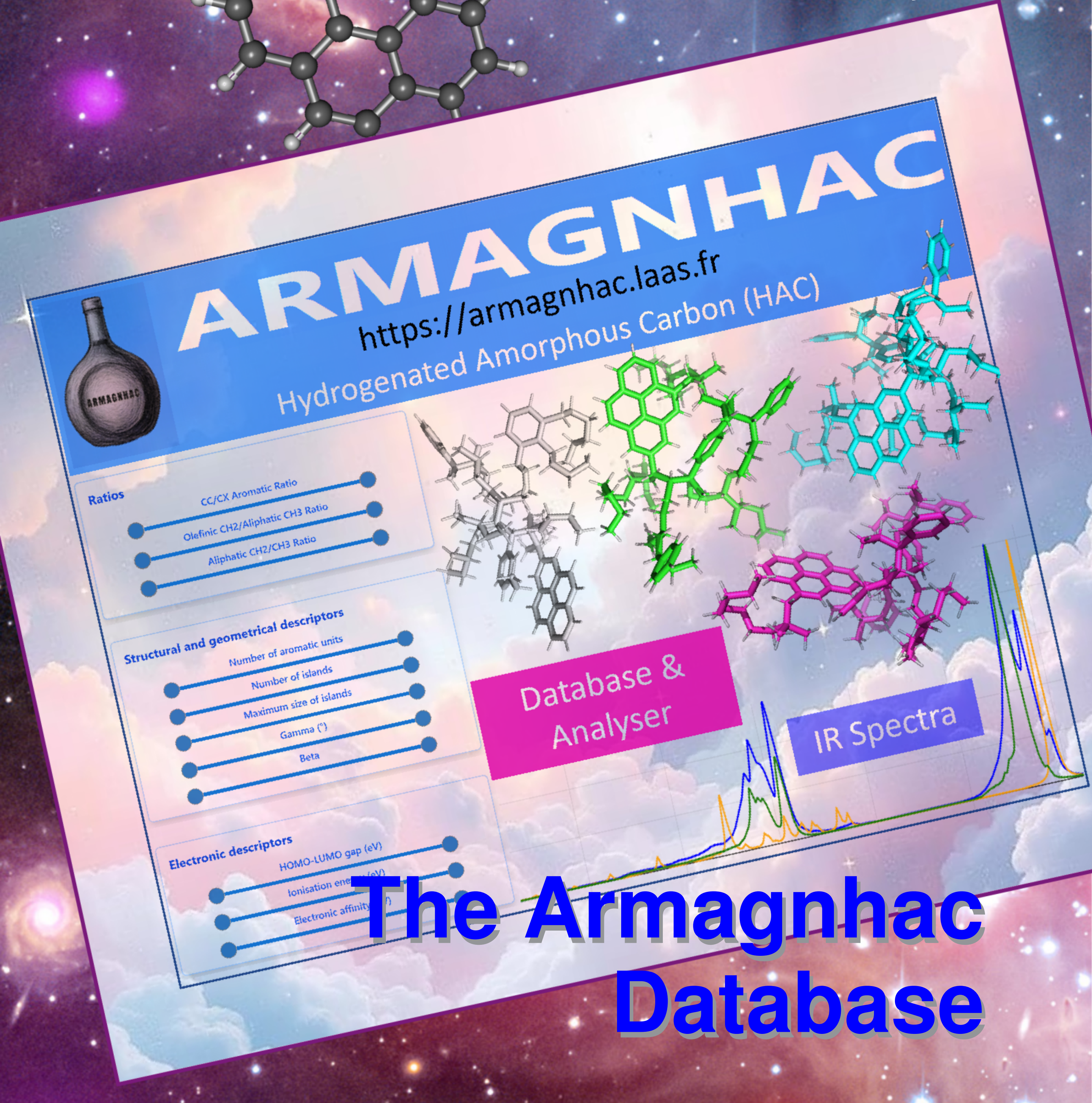
AstroPAH
A Newsletter on Astronomical PAHs

Issue 128 ● May 2026



ARMAGNHAC

https://armagnhac.laas.fr

Hydrogenated Amorphous Carbon (HAC)

Ratios

CC/CX Aromatic Ratio

Olefinic CH2/Aliphatic CH3 Ratio

Aliphatic CH2/CH3 Ratio

Structural and geometrical descriptors

Number of aromatic units

Number of islands

Maximum size of islands

Gamma (°)

Beta

Electronic descriptors

HOMO-LUMO gap (eV)

Ionisation ene (eV)

Electronic affinity

Database & Analyser

IR Spectra

The Armagnhac Database

Editorial

Dear Colleagues,

In this 127th volume of AstroPAH, the Picture of the Month and In Focus highlight the new database for hydrogenated amorphous carbons properties ARMAGNHAC. Mathias Rapacioli, Valentin Milia, Juan Cortés, and Nathalie Tarra describe ARMAGNHAC in the *In Focus*.

This issue's *Abstracts* section features papers on the fragment-based and perturbation theories treatment of the excited benzene excimer, charge-aware machine learning for predicting infrared spectra of PAHs, the influence of aliphatic components on the aromatic emission characteristics of PAHs, and the structure and binding nature of thianaphthene dimers using gas-phase infrared spectroscopy.

The third installment of the Astrochemistry Workshop will be held at the beautiful city of Rio de Janeiro, Brazil, in July.

AstroPAH can help you promote your research. Please send your contributions to our email address.

Thank you all for your contributions!

The Editorial Team

Next issue: 18 June 2026.
Submission deadline: 5 June 2026.

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PAH Picture of the Month

ARMAGNHAC, a database for hydrogenated amorphous carbons properties (https://armagnhac.laas.fr/).

Credits: Milia et al. 2025.

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ARMAGNHAC:

A new database for hydrogenated amorphous carbons properties

**by Mathias Rapacioli[1], Valentin Milia[1,2], Juan Cortés[2],
and Nathalie Tarrat[3]**

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Background

Hydrogenated amorphous carbons (HACs) are complex, disordered forms of carbon that are of interest in various scientific fields, such as the study of air pollution, the understanding of soot particle formations and astrochemistry (see Figure 1).

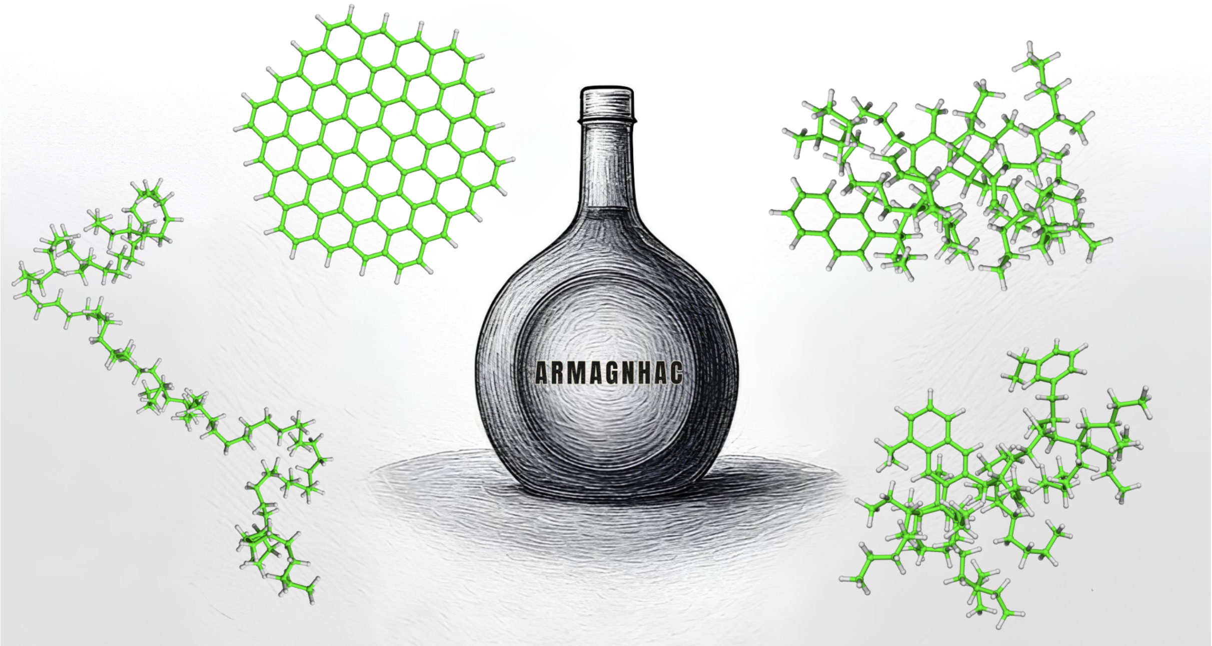


Figure 1 *– Top left: the PAH circumcircumcoronene; bottom left: an unbranched alkane structure, right: two examples of generated hydrogenated amorphous carbons.*

Unlike polycyclic aromatic hydrocarbons (PAHs), HACs contain carbonaceous chains (aliphatic or olefinic), that can be ramified or connected to one or several aromatic islands, an aromatic island being defined as one or several fused aromatic rings. The development of a database for HACs is very challenging because plenty of chemical formulae can correspond to a given stoichiometry and because these molecules are flexible, resulting in a plethora of low-energy, almost degenerate isomers. Such a database would however be precious to study the properties of these molecules and to compare models with experimental data, or to be used as references to develop machine learning-based molecular property prediction tools.

A new stochastic, structurally guided algorithm has been developed for the large-scale generation of atomistic models of HACs. It consists of a two-step procedure (see Figure 2): (i) the randomized generation of 2D structures using a SMILES (simplified molecular input line entry system) description, respecting user-predefined chemical constraints; (ii) the subsequent generation of 3D structures, making use of a stochastic sampling algorithm combined with local optimization. In order to explore the molecular potential energy surface, we have used algorithmic tools which were originally developed to solve path planning problems in the field of robotics and navigation. The structures of HACs, their energies and their infrared spectra have been derived from calculations performed at an approximated quantum level derived from density functional theory, namely the density functional tight binding (DFTB) method.

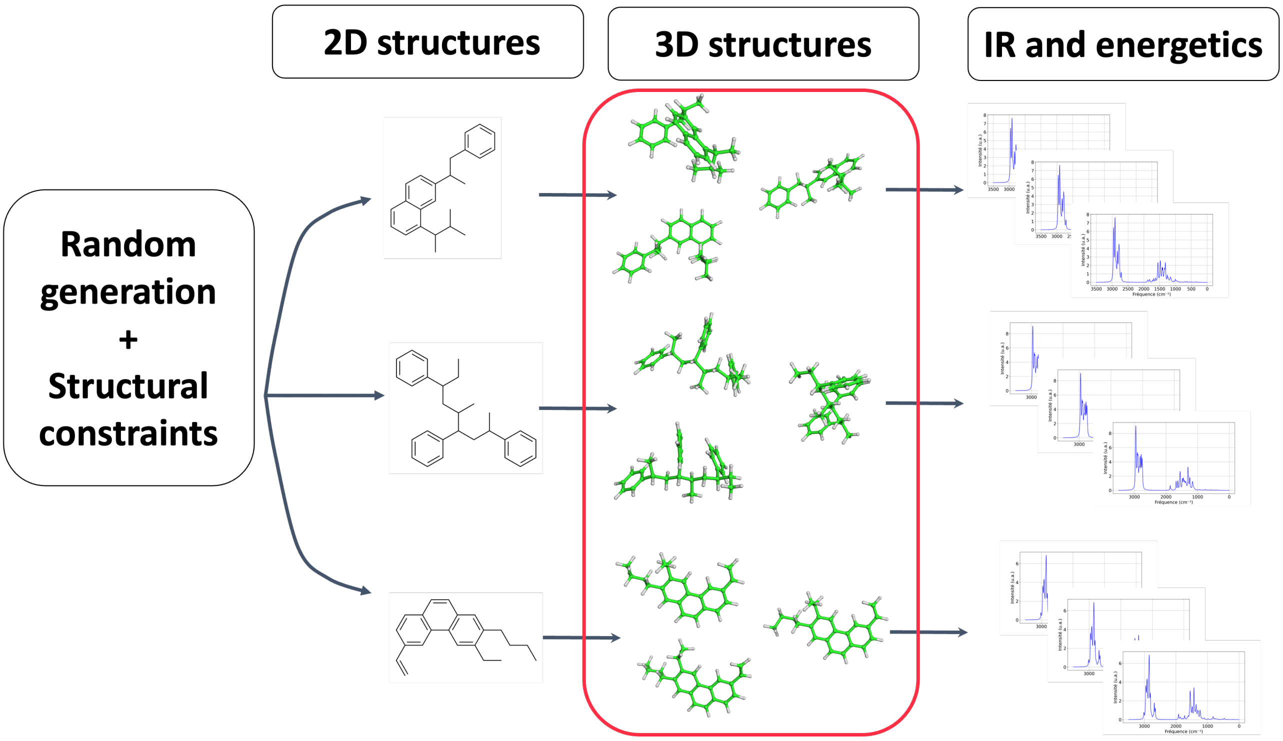


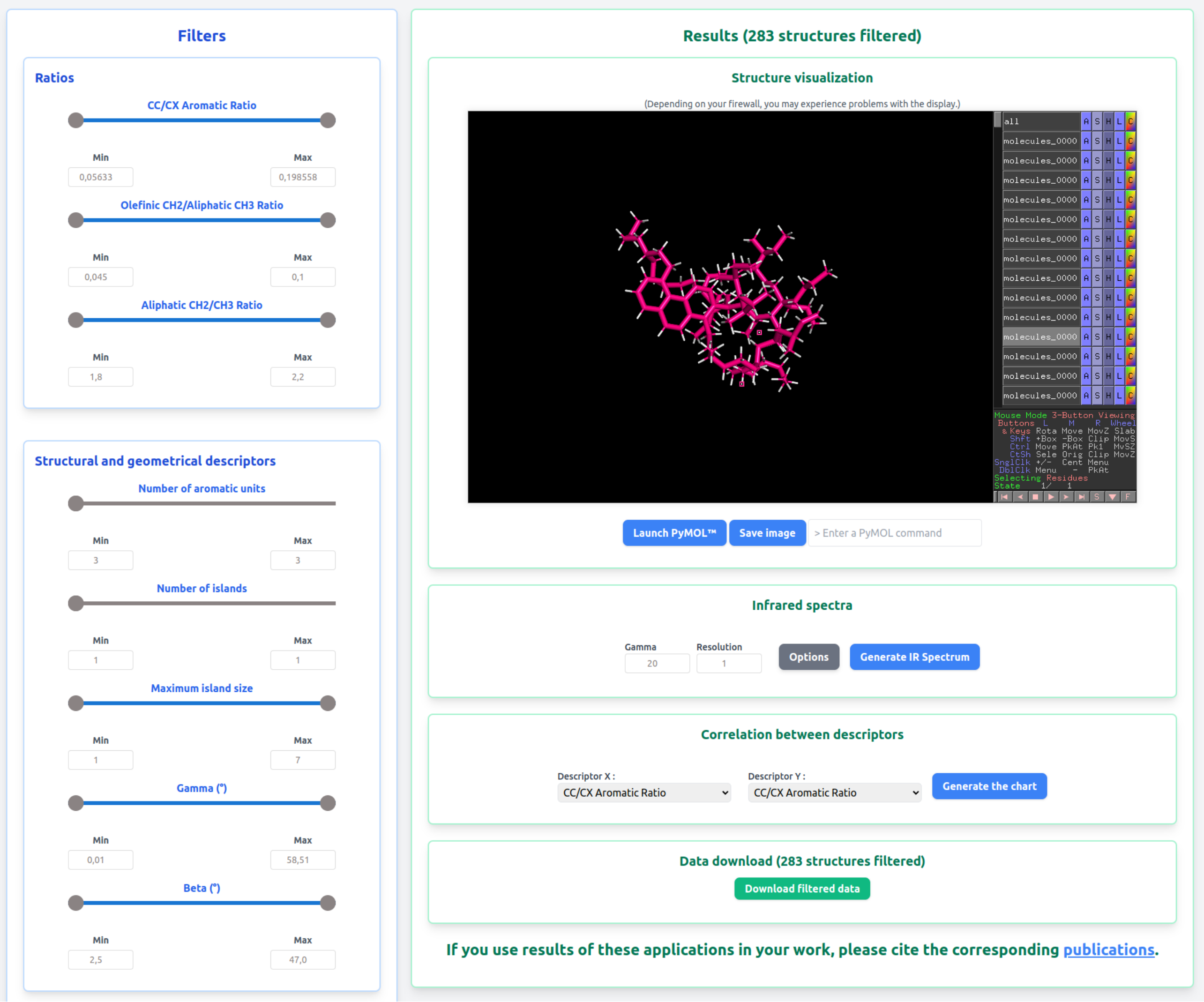
Figure 2 *– Representation of the generation scheme involving the generation of 2D structures (left), 3D structures from stochastic exploration of the potential energy surface (middle) and, finally, the properties computations (right).*

Database Overview

The method was used to generate the new HACs database named ARMAGNHAC (A Ratio-based Molecular Analyzer and Generator of Numerous Hydrogenated Amorphous Carbons). It provides structural (cartesian coordinates, functional group ratios, Hill-Wheeler parameters, and aromaticity descriptors), energetic (HOMO-LUMO gap, ionization energy, and electronic affinity), and spectroscopic properties of 4366 HACs.

A brief analysis of the ARMAGNHAC database shows that the generated HACs exhibit: (i) a rather spherical or prolate shapes, (ii) a bimodal distribution of the HOMO-LUMO gap, separating structures containing either isolated aromatic rings or larger aromatic islands, (iii) a dependence of the ionization potentials and electronic affinities on the size of the largest aromatic island. The ARMAGNHAC database was also shown to be helpful in interpreting or reinterpreting experimental measurements as optical band gaps and ionization energies of soot particles.

The database (structures and properties) is freely accessible (https://armagnhac.laas.fr/) and can be downloaded by users after registration (see Figure 3). Correlation plots between the descriptors can be generated on the website, as well as IR spectra, possibly including their evolution as a function of a given property.



Filters

Ratios

CC/CX Aromatic Ratio
Min 0,05633
Max 0,198558

Olefinic CH2/Aliphatic CH3 Ratio
Min 0,045
Max 0,1

Aliphatic CH2/CH3 Ratio
Min 1,8
Max 2,2

Structural and geometrical descriptors

Number of aromatic units
Min 3
Max 3

Number of islands
Min 1
Max 1

Maximum island size
Min 1
Max 7

Gamma (°)
Min 0,01
Max 58,51

Beta (°)
Min 2,5
Max 47,0

Results (283 structures filtered)

Structure visualization

(Depending on your firewall, you may experience problems with the display.)

Infrared spectra

Gamma 20
Resolution 1

Correlation between descriptors

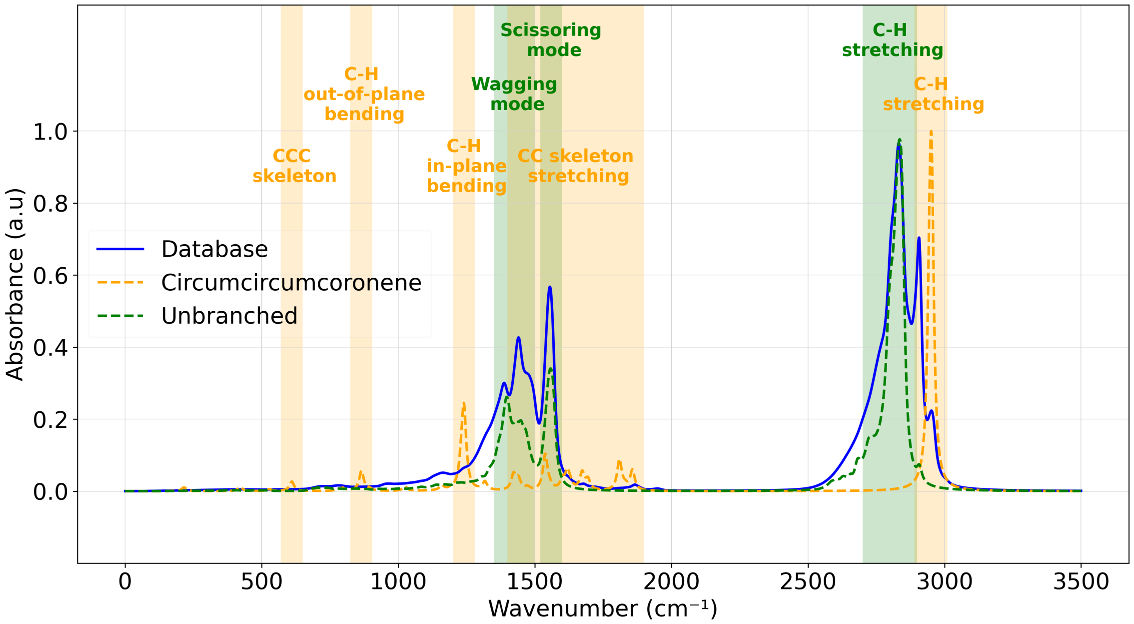
Descriptor X : CC/CX Aromatic Ratio
Descriptor Y : CC/CX Aromatic Ratio

Data download (283 structures filtered)

If you use results of these applications in your work, please cite the corresponding publications.

Figure 3 *– The ARMAGNHAC database website (https://armagnhac.laas.fr/)*

Infrared Spectra



Spectrum by Maximum size of islands

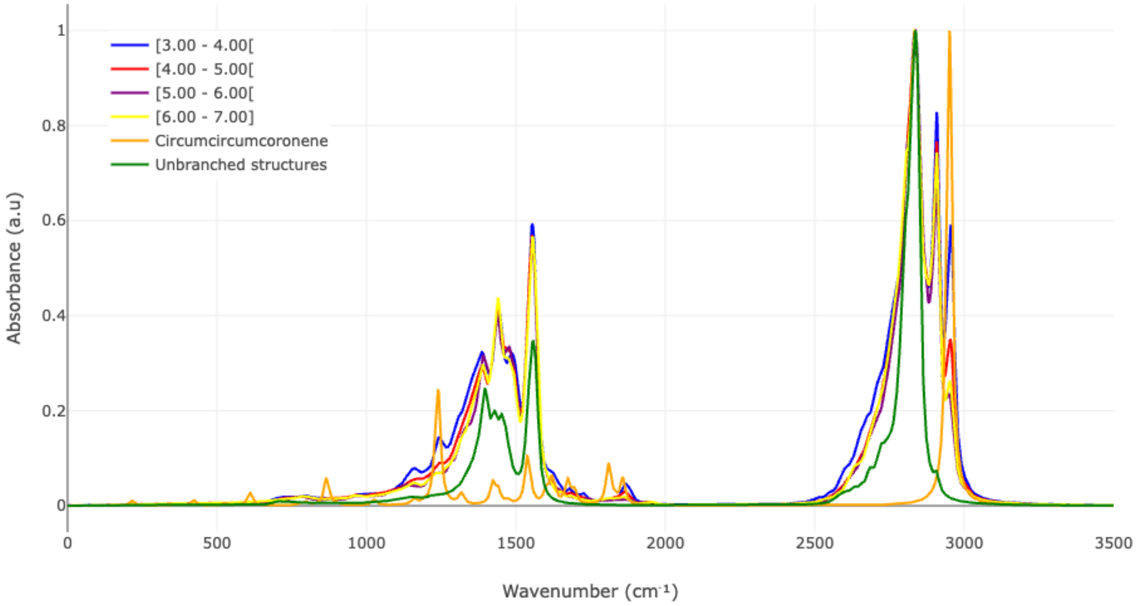


Figure 4 *– Top: IR harmonic spectra computed for a PAH (circumcircumcoronene) and average spectra for 3 unbranched alkane structures and for the 4366 database HACs. Bottom: Evolution of the IR spectra for HACs containing 10 aromatic rings split as a function of the maximum size of aromatic islands (values in brackets from 3 to 7).*

As an example, Figure 4 (top) reports the IR spectrum of unbranched structures of the PAH circumcircumcoronene. The characteristic PAH IR features appear in the circumcircumcoronene spectrum, i.e., C-H stretching and CC skeleton stretching modes (sometimes also containing C-H bending modes contributions), C-H out-of-plane and in-plane bending modes, and the CCC skeleton vibration modes. A band at 2700-2900 cm^{-1} corresponding to CH_3 and CH_2 stretching modes dominates the unbranched structures' IR spectrum. One peak at ($\approx$ 1560 cm^{-1}) corresponds to the scissoring mode and a broader feature (1350-1500 cm^{-1}) is associated with wagging modes. Averaging all the IR spectra of the HAC molecules of the database provides the blue curve, dominated by the three features identified for unbranched structures. Another significant contribution is present around 2900 cm^{-1}, corresponding to antisymmetric stretching of CH_3 groups. An additional contribution is present at 2950 cm^{-1}. The latter results from aromatic C-H stretching modes.

A strength of the ARMAGNHAC website is that users can apply filters to simulate the evolution of IR spectra as a function of specific criteria. Figure 4 (bottom) reports such a case where the IR spectrum has been split as a function of the maximum size of aromatic islands. To do this, we used the website tools to first select only the structures containing 10 aromatic units and, second, to subdivide this isomer pool as a function of the size of the largest aromatic island. The produced picture shows, for instance, that increasing maximum size of aromatic islands results in a decrease of the aromatic C-H stretching mode intensity.

This work paves the way for future studies aiming to derive relationships between structure, energetic, and spectral properties of HACs, which are essential to interpret interstellar medium spectral observations and experimental measurements. At the moment, the ARMAGNHAC database contains 4366 HACs with 96 carbon atoms and it is expected to be continuously extended by incorporating data for a wider range of systems.

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The ARMAGNHAC Database: A Ratio-based Molecular Analyzer and Generator of Numerous Hydrogenated Amorphous Carbons V. Milia, M. Rapacioli, C. Zanon, J. Cortés, and N. Tarrat, J. Phys. Chem. A 2025, 129, 45, 10358–10367

https://doi.org/10.1021/acs.jpca.5c04941
https://armagnhac.laas.fr/

The fragment-based and perturbation theories treatment of the excited benzene excimer

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The non-orthogonal product approach (NOPA) was combined with complete degenerate active space perturbation theory (CDAS-PT2) in order to investigate the excited electronic states of the benzene dimer molecule (Bz_2), which is supposed to play a precursor role in the chemical growth of polycyclic aromatic hydrocarbons in the interstellar gas medium. The fraction contribution of Rydberg and charge-transfer states into the total electronic density of low-lying exciton states of Bz_2 was analyzed in the framework of the NOPA. A general mechanism of the photo-induced formation of the Bz_2 excimer states, their subsequent stabilization due to a vibrational relaxation to the minimum of the optically inactive states plus the parallel predissociative decay caused by the intramolecular coupling with repulsive states manifold, is considered.

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Charge-aware machine learning for predicting infrared spectra of PAHs

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Interstellar polycyclic aromatic hydrocarbons (PAHs) emit characteristic infrared (IR) light that is sensitive to hosting environments, making them excellent astrophysical probes. However, detailed spectral analysis has been limited by the high computational cost of quantum chemistry methods like density functional theory (DFT), which has hindered systematic studies of how features such as the aromatic infrared bands (AIBs) depend on a PAH's charge state and molecular structure. To overcome this, we developed a machine learning model, specifically a multi-layer perceptron (MLP) neural network, that predicts IR spectra for PAHs across four charge states with near-DFT accuracy but at orders-of-magnitude faster speed (see Figure 5). The model was trained on over 12,599 PAHs, of which 9,731 came from the NASA PAHdb library. Our model reliably handles PAHs with up to 150 carbon atoms, including anions, neutrals, cations, and di-cations, though predictions for larger molecules are currently limited by training data. This work also reassessed how ionization affects PAH spectra and found that anions emit strongly across multiple bands, often matching or exceeding cation intensities, while the 11.2 micron band shows a distinct charge dependence.

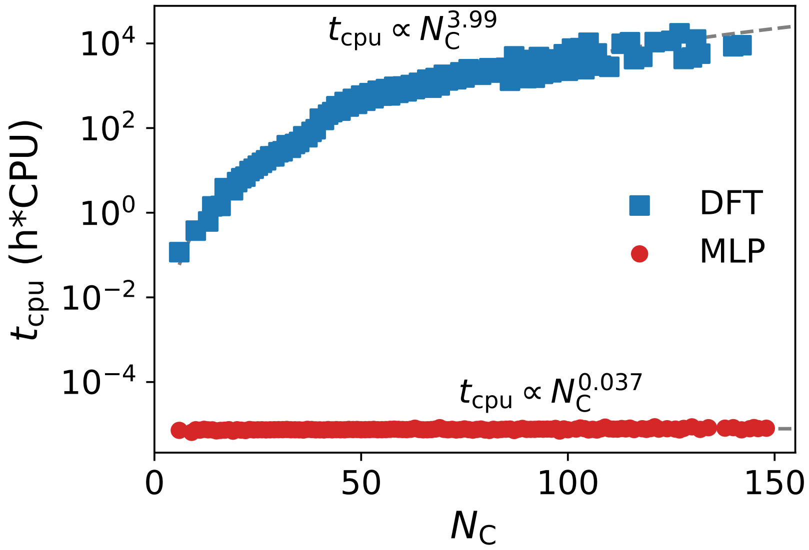

Figure 5 *– Mean computational time for computing an IR spectrum vs PAH size ($N_{\rm C}$). Results compare the NN model with DFT calculations at B3LYP/6-311+g level.*

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The Influence of Aliphatic Components on the Aromatic Emission Characteristics of Polycyclic Aromatic Hydrocarbons

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Intensity ratios of aromatic emission features are widely used to diagnose the size and ionization state of polycyclic aromatic hydrocarbons (PAHs) in astronomical environments. However, PAHs are known to typically carry aliphatic side chains, a structural feature that may compromise the reliability of traditional diagnostic methods. This study systematically investigates the effects of aliphatic components on the aromatic emission properties of PAHs. Based on theoretical data from the NASA Ames PAH IR Spectroscopic Database, we compare the emission behavior of purely aromatic PAHs with those containing aliphatic substituents, revealing that aliphatic functionalization may modify the intensity ratio of the 11.2 µm band relative to the 7.7 µm and 3.3 µm bands. This potentially leads to misidentification of their ionization state if molecular structural effects are neglected. Further analysis indicates that the impact of aliphatic components on diagnostic band ratios strongly depends on PAH size: small PAHs exhibit significant emission ratio shifts, deviating from traditional size/ionization trends, while larger PAHs are minimally affected. Despite these shifts, the classic $I_{11.2/7.7}$ versus $I_{11.2/3.3}$ diagnostic grid remains largely applicable to mixed aromatic-aliphatic PAHs, although some systematic calibration may be needed. Our findings emphasize the necessity for caution when interpreting PAH band ratios in aliphatic-rich environments, as variations in PAH molecular composition may distort inferences about physical conditions.

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http://doi.org/10.1093/mnras/stag751

Elucidating the structure and binding nature of thianaphthene dimers using gas-phase infrared spectroscopy

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[3]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

Crucial for many biological systems, in astrochemistry, and for fundamental chemistry in general, the conformations adopted by weakly bound complexes of polycyclic aromatic hydrocarbons (PAHs) have been the focus of debate for decades. Still, there are great challenges in forming such complexes in the laboratory, measuring accurate spectroscopic information sensitive to structure, and computing molecular properties for systems subtly bound by dispersive interactions. Here, we employ a combination of gas-phase infrared spectroscopy with extensive density functional theory (DFT) calculations to unambiguously determine the preferred conformation adopted by dimers of neutral thianaphthene, a PAH composed of one six- and one five-membered ring with an incorporated sulfur atom. A very wide spectral range from 350 to 3150 cm^{-1} is covered, allowing a determination of the effect of complexation on fingerprint vibrations as well as C–H stretches. A comparison of the recorded infrared spectra of monomers and dimers in combination with detailed vibrational calculations assigns a π-stacked configuration for the complex. This agrees with energetic arguments, where DFT predicts the isomeric T-shaped configuration to be 0.13 eV higher in energy. The potential energy surface of the complex is explored using the nudged elastic band (NEB) method and the nature of the interaction between neutral monomers is investigated based on the local energy decomposition (LED) analysis. The π-stacked dimer is overwhelmingly stabilized by π-π dispersion, an interaction that is much weaker in the T-shaped configuration, despite the effect of C-H–π forces. The methodology applied here to thianaphthene is extendable to dimers without a permanent dipole moment, hence invisible to microwave spectroscopy, as well as larger clusters of PAHs.

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Phys. Chem. Chem. Phys., **28**:10364-10372 (2026)

https://pubs.rsc.org/en/content/articlehtml/2026/cp/d6cp00544f

III Astrochemistry Workshop:

Astrochemistry Across Scales – From Molecular Processes to Cosmic Environments

Rio de Janeiro, Brazil
6 - 18 July, 2026

Workshop de
Astroquímica

https://sites.google.com/fat.uerj.br/iii-workshop-astro/p%C3%A1gina-inicial

Dear AstroPAH community,

On behalf of the Scientific Organizing Committee, we are pleased to announce the **III Astrochemistry Workshop: Astrochemistry Across Scales – From Molecular Processes to Cosmic Environments**, which will take place from July 6 to 8, 2026, at the Salão Nobre of the Center for Mathematical and Natural Sciences (CCMN), Federal University of Rio de Janeiro (UFRJ), Rio de Janeiro, Brazil.

Following the two previous editions, the workshop aims to bring together researchers, students, and collaborators working across the broad and interdisciplinary field of astrochemistry. The program will include invited talks, oral communications, and poster presentations covering observational, experimental, theoretical, and computational approaches to the chemistry of astronomical environments.

The event will provide an opportunity to discuss recent developments in astrochemistry, foster new collaborations, and strengthen interactions within the Brazilian and international astrochemistry communities.

Important dates:

- Registration without abstract submission: until June 19, 2026
- Registration with simple abstract submission: until June 19, 2026
- Expanded abstract for publication in AIDASCO: Participants interested in submitting an expanded abstract should first register with a simple abstract by June 19, 2026, and then send the expanded abstract by July 8, 2026 to: workshopastroquimica@gmail.com

Further information, including registration details and templates, is available on the workshop website:

https://sites.google.com/fat.uerj.br/iii-workshop-astro/p%C3%A1gina-inicial

The detailed program will be announced soon.

Best regards,

The Scientific Organizing Committee

III Astrochemistry Workshop

Ricardo Oliveira — Institute of Chemistry, Federal University of Rio de Janeiro (UFRJ)
Leonardo Baptista — Rio de Janeiro State University (UERJ)
Alexandre Bergantini — Federal Center for Technological Education Celso Suckow da Fonseca (CEFET-RJ)
Breno Galvão — Federal Center for Technological Education of Minas Gerais (CEFET-MG)
Diana Andrade — Valongo Observatory, Federal University of Rio de Janeiro (UFRJ)
Karín Menéndez-Delmestre — Brazilian Center for Research in Physics (CBPF)
Leticia Dobler — Institute of Chemistry, Federal University of Rio de Janeiro (UFRJ)
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AstroPAH Newsletter

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