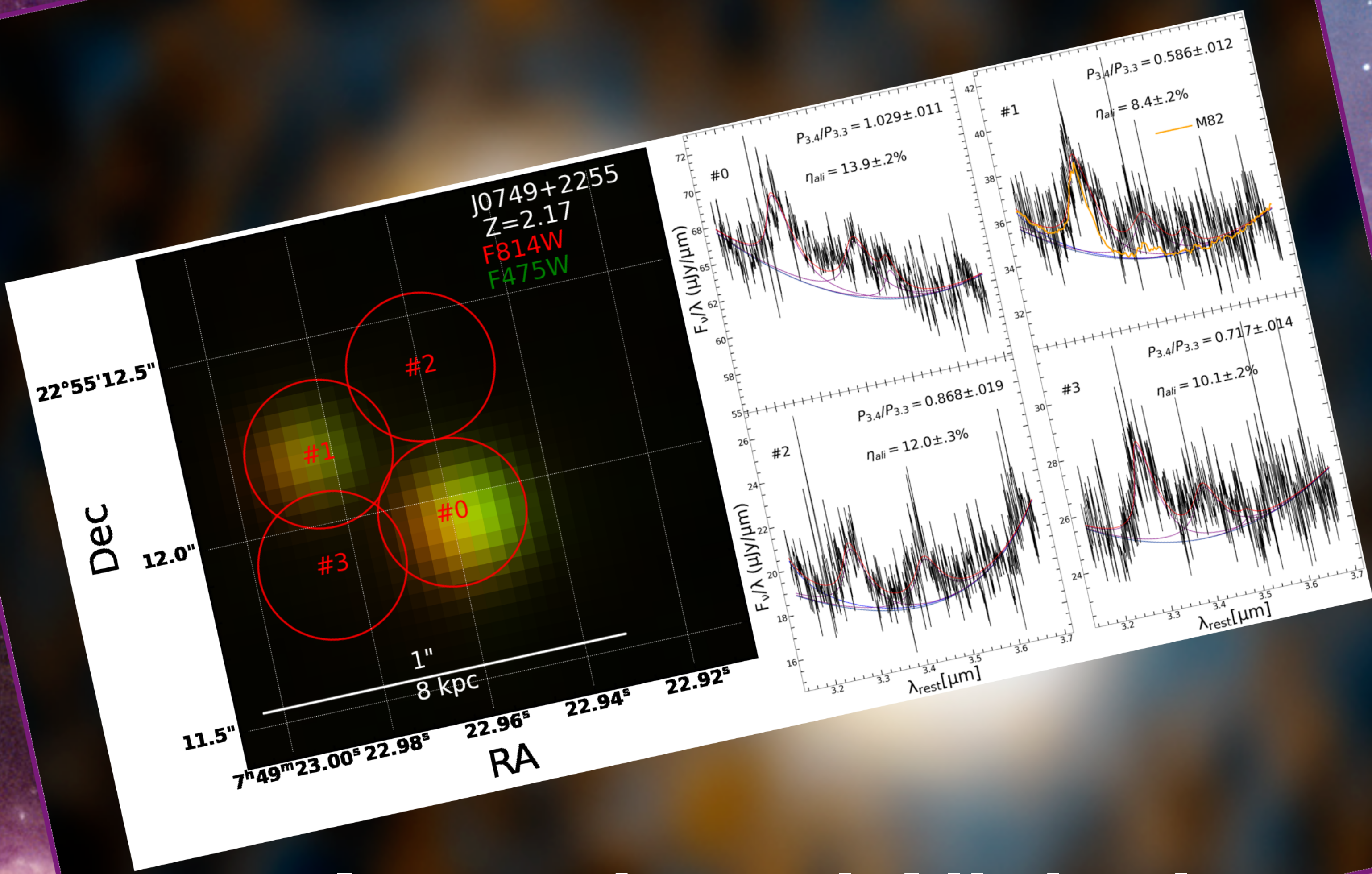
AstroPAH

A Newsletter on Astronomical PAHs

Issue 129 • July 2026



Aromatic and Aliphatic Emission at Cosmic Noon

Editorial

Dear Colleagues,

Welcome to AstroPAH #130!

Our cover image this month highlights a remarkable discovery: the detection of aromatic and aliphatic hydrocarbon emission from a dual quasar observed during the epoch of cosmic noon. Dual quasars are rare astronomical phenomena in which two quasars, each hosting a supermassive black hole, are found in close proximity, typically within interacting or merging galaxies. JWST/MIRI observations revealed a widespread presence of aromatic and aliphatic hydrocarbon emission at rest-frame 3.3 and 3.4 micron in SDSS J074922.96+225511.7, a dual quasar at redshift z = 2.17, corresponding to a cosmic age of 3 billion years after the Big Bang, a time period known as the ”cosmic noon”when star formation and black hole growth peak. This is the most distant object to date in which both aromatics and aliphatics have ever been detected. As PAH emission has been widely used as a diagnostic of the relative roles of starbursts and AGNs in galaxies, dual quasars provide a valuable opportunity to explore the effects of quasar-driven shocks and galaxy-merging-induced starbursts on the excitation and destruction of PAH molecules.

The Editorial Team

Next issue: 17 September 2026.
Submission deadline: 4 September 2026.

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PAH Picture of the Month

JWST/MIRI observations revealed a widespread presence of aromatic and aliphatic hydrocarbon emission at rest-frame 3.3 and 3.4 μm in SDSS J074922.96+225511.7. This is the most distant object to date in which both aromatics and aliphatics have ever been detected. The cover shows a colour composite image (left) of the dual quasar J0749+2255 at $z \approx 2.17$, and JWST/MIRI rest-frame spectra (right) extracted from its brightest inner regions.

Credits: Image from: C.E. Mentzer, Aigen Li, & X.J. Yang, 2026, ApJL, 1005, L38. Background image: Dual Quasar J0749+2255 (NASA, ESA, Yu-Ching Chen (UIUC), Hsiang-Chih Hwang (IAS), Nadia Zakamska (JHU), Yue Shen (UIUC)).

This newsletter is edited in LaTeX. Newsletter Design by: Isabel Aleman. Image Credits: Background image in this page: NASA, ESA, and the Hubble Heritage Team (STScI/AURA). Headers background: X-ray and optical image composition. X-ray by Chandra: NASA/CXC/Univ.Potsdam/L.Oskinova et al; Optical by Hubble: NASA/STScI; Infrared by Spitzer: NASA/JPL-Caltech.

AstroPAH Questionnaire

Help us serve the PAH community better

Dear AstroPAH readers,

As our board continues to evolve in this exciting JWST era, we are actively exploring ways to enhance the newsletter's value for the community. We discussed several initiatives, including the transition to a more automated submission process via Google Forms to streamline the parsing of abstracts into LaTeX format.

Furthermore, we are expanding our ***In Focus*** section to include ***Expert Perspectives*** from senior researchers. We are also looking to recruit new editor(s), particularly those with an observational background, to ensure a balanced multidisciplinary approach. Your feedback is crucial as we implement these new processes and strive to bridge the communication gap between laboratory, theoretical, and astronomical research.

Please click here or scan the QR code below to fill up the questionnaire for us. It would only take 2 – 3 minutes!

Thank you for your contribution!

The AstroPAH Editorial Board

Abstracts

Full-Spectrum Machine Learning: Reading PAH Spectra Beyond the Band Ratio

Zhao Wang

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Traditional PAH diagnostics have long relied on empirical band ratios. However, this approach suffers from fundamental degeneracies that complicate interpretation. Moreover, the apparent accuracy of ratio-based models is often a byproduct of sample selection rather than physical universality.

Wang (2026) introduces a paradigm shift. Instead of focusing on a few discrete features, the machine-learning model treats the complete infrared spectrum as a high-dimensional fingerprint. By leveraging the full spectral morphology, the model captures correlated information across all wavelengths simultaneously. This allows it to disentangle overlapping physical effects, such as size, charge, and excitation conditions, that individual band ratios cannot separate. The full-spectrum approach also reduces sensitivity to the specific molecular subsets used for calibration, mitigating the sample-selection biases inherent to ratio-based methods.

Using a random forest classifier trained on ∼19,000 spectra across four charge states, the model achieves an overall accuracy exceeding 95% across 12 size-charge categories. The model was validated on synthetic mixtures of molecules that the model had never "seen" before, as well as on real JWST MIRI observations. These results underscore its potential as a robust tool for interpreting interstellar PAH emission in the JWST era.

The source code and training data are publicly available at AstroPAH-MLDiag.

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Ultraviolet Interstellar Extinction toward High Galactic Latitudes

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Nearby high Galactic latitude clouds provide a unique laboratory to study the physics and structure of the Galactic interstellar medium (ISM) and the properties of the interstellar dust. In this work, we select 32 sightlines toward reddened background stars at high Galactic latitudes with $|b| > 20^{\rm o}$, for which high-quality spectra from the $International\ Ultraviolet\ Explorer$ are available. We utilize the "pair-method" to derive the ultraviolet interstellar extinction curves for these sightlines. We examine the extinction properties of these sightlines and find no systematic variations with the Galactic latitudes, although they do show appreciable sightline-to-sightline variations.

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The Astrophysical Journal (Accepted)

https://arxiv.org/abs/2607.03923

Widespread Detection of Aromatic and Aliphatic Emission in the Dual Quasar J0749+2255 at Cosmic Noon

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Based on the integral field observations made with the *Mid Infrared Instrument* (MIRI) aboard the *James Webb Space Telescope* (JWST), we report a widespread detection of aromatic and aliphatic hydrocarbon emission at rest-frame 3.3 and 3.4 μm in SDSS J074922.96+225511.7 (hereafter J0749+2255), a dual quasar at redshift $z \approx 2.17$, corresponding to a cosmic age of $\sim$3 billion years after the Big Bang, a time period known as the "cosmic noon" when star formation and black hole growth peak. With the 3.3 μm emission ascribed to aromatic C–H stretches of small polycyclic aromatic hydrocarbon (PAH) molecules and the 3.4 μm emission assigned to aliphatic C–H stretches of aliphatic sidegroups attached to PAHs, we utilize the observed intensities of the 3.3 and 3.4 μm emission features to estimate the aliphatic fractions of PAHs and their spatial variations across J0749+2255, which is, to our knowledge, the most distant object to date in which both aromatics and aliphatics have ever been detected. We find that both the 3.3 and 3.4 μm emission features are pronounced and the aliphatic fractions are surprisingly high in the most luminous regions centered on the two quasar nuclei, suggesting that not only small PAHs (of $\sim$20–30 carbon atoms) but also their attached aliphatic sidegroups survive in extreme starburst activities and quasar-driven shocks.

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The Astrophysical Journal Letters, **1005**, L38 (10 pages) (2026)

https://arxiv.org/abs/2607.03913

Theoretical and Experimental IR Spectra of Astronomical PAHs and PANHs in the 2000-1650 cm^{-1} Range ($\sim$5-6 μm)

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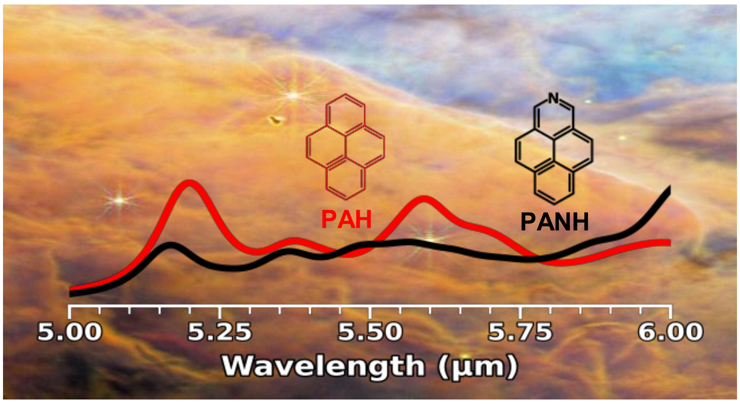
Recent James Webb Space Telescope observations reveal unprecedented detail in the 2000–1650 cm^{-1} ($\sim$5–6 μm) region, including the well-known 5.25 and 5.75 μm bands. This range, dominated by overtone and combination bands mainly involving C–H out-of-plane (CH_{oop}) bending fundamentals, provides a powerful yet underexplored probe of astronomical polycyclic aromatic hydrocarbons (PAHs) and their nitrogen-containing analogues (PANHs). We present a combined experimental and theoretical investigation of 27 neutral PAHs and PANHs using matrix-isolation spectroscopy and second-order vibrational perturbation theory to disentangle effects of PAH structures and nitrogen substitution in the 2000–1650 cm^{-1} region. Coupling among the underlying fundamentals subdivides this region accommodating the distinct characteristics of the 5.25 and 5.75 μm bands. The higher-frequency subregion (2000–1870 cm^{-1}; 5.00–5.35 μm) reflects PAH edge topology, where the highest-frequency band shifts from quartet+bay structures ($\sim$5.13 μm) to quartet+solo ($\sim$5.18 μm) and pericondensed PAHs ($\sim$5.20 μm), consistent with the relatively stable astronomical 5.25 μm band. The lower-frequency subregion (1870–1650 cm^{-1}; 5.35–6.06 μm) shows greater structural variability, consistent with the composite 5.75 μm band. Nitrogen substitution broadens the spectral distribution by shifting bands by $\sim$10 cm^{-1}. From our neutral PAHs/PANHs set, we infer that the 5–6 μm region reflects contributions from neutral astronomical PAHs, dominated by pericondensed PAHs, with secondary contributions from catacondensed PAHs with limited quartets and increasing solos. Contributions from irregular edges containing quartets C-H groups and nitrogen-substitution are modest. A corresponding study of cations is needed to fully characterize the 5–6 μm emission, disentangling cation and neutral contributions from CH_{oop} region.



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ACS Earth and Space Chemistry, **10**, 1685-1701 (2026)

https://pubs.acs.org/doi/full/10.1021/acsearthspacechem.6c00033

Benzene formation on interstellar dust grain analogues via single-atom Fe catalysis

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Benzene has been detected across a range of astrophysical environments, though the primary mechanism underpinning its formation has not yet been constrained and the extreme conditions of the interstellar medium often necessitate the need for grain-surface mediated reactions. However, while interstellar grains are known to enhance encounter rates and dissipate energy from exothermic reactions, their potential as chemical catalysts remains less explored. Here we aim present mechanistic insights into the formation of benzene through successive cyclotrimerisation of space abundant acetylene under astrophysical conditions, using single-atom Fe-containing silica surfaces as interstellar heterogeneous catalysts. Periodic quantum chemical calculations were performed to identify stationary points and transition states to construct a reaction potential energy surface, whilst binding energy and transition state theory rate calculations were also performed to evaluate the catalytic efficiency and identify plausibility across a range of astrophysical environments. Our results identify a thermodynamically favourable exergonic processes with small activation energy barriers, offering a novel route that can explain the presence of benzene across diverse astrophysical regions where current models cannot reproduce observational quantities.

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Monthly Notices of the Royal Astronomical Society, **550**, stag1202 (2026)

https://doi.org/10.1093/mnras/stag1202

Vibrational Carbon Character Analysis of Astronomical PAHs

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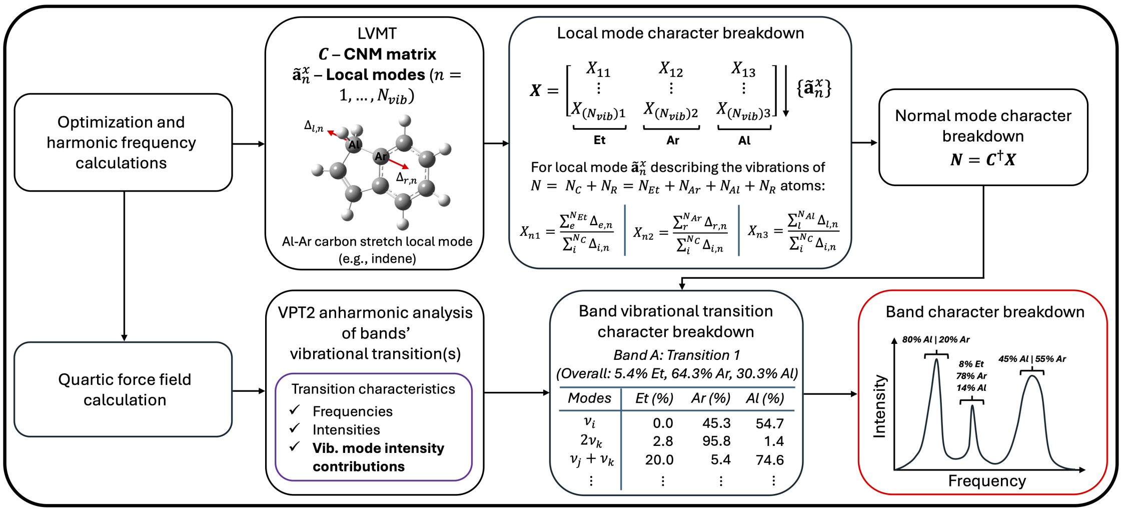
Emission features of astronomical spectra typically attributed to aromatic and aliphatic portions of polycyclic aromatic hydrocarbons (PAHs) should not be so clearly binned as previously ascribed. Vibrational carbon character analysis (VCCA) herein shows that the 3.4 μm aromatic infrared emission band (AIB), typically labeled as "aliphatic," possesses more than 45% non-aliphatic (i.e., aromatic) character for the test case of indene, the smallest astronomically detected PAH. Significant non-aliphatic character is seen as well for the 6.85 and 7.25 μm emission bands of indene, which are also considered to be markers of aliphaticity. VCCA predicts similar behavior for all three emission bands in the case of 2-ethynyltoluene, the proposed interstellar precursor of indene. Although the typical aromatic emission bands (i.e., 3.3 and 6.2 μm bands) exhibit slight aliphatic character for both indene and 2-ethynyltoluene, these bands are primarily aromatic. While these are only two example molecules, if significant character mixing occurs for the emission bands of most potential AIB carriers, current aliphatic/aromatic AIB attributions must be reconsidered. Reprinted from *J. Chem. Phys.*, 165, 034104 (2026), with the permission of AIP Publishing.



Workflow of the VCCA method for calculating the VCC of AIB carrier emission bands. Et, Ar, and Al refer to ethynyl, aromatic, and aliphatic, respectively. See the text for further explanation of the workflow. Reprinted from J. Chem. Phys., 165, 034104 (2026), with the permission of AIP Publishing.

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The Journal of Chemical Physics, **165**, 034104 (2026)

https://doi.org/10.1063/5.0331629

Anharmonic Infrared Emission of Cyano-Substituted Polycyclic Aromatic Hydrocarbon Molecules: Cyano-naphthalenes as a Case Study

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The recent radio-spectroscopic detection of nitrile-bearing aromatic species, has identified cyano-substituted polycyclic aromatic hydrocarbons (cyano-PAHs) as key tracers of nitrogen heterocycles in the interstellar medium (ISM). Despite this, their infrared (IR) identification remains a challenge, requiring high-fidelity anharmonic vibrational radiative models that account for dynamic cooling processes in diverse astrophysical environments. We aim to provide IR cascade model emission spectra for the anion, neutral, and cation states of 1- and 2-cyanonaphthalene (1- and 2-CNN) in representative astrophysical regions. We investigate how charge states and substitution sites (1- vs. 2-position) modulate the anharmonic vibrational profiles and energy redistribution during the IR cascade process. We employed B3LYP/N07D in conjunction with the Second-order Vibrational Perturbation Theory (VPT2). To simulate the emission under astrophysical conditions, we utilized an optimized microcanonical sampling algorithm to determine the vibrational density of states and generate IR cascade emission spectra for different astrophysical environments. Our results reveal that, compared to neutrals, the intensity of the CN nitrile band of anions is dramatically enhanced by an order of magnitude, while the CN band intensity of cations is somewhat weaker than that of neutrals. We show that 1- and 2-CNN exhibit distinct isomeric signatures: 1-CNN induces a complex "red-wing" structure in the 3.3 μm C-H stretch due to peri-hydrogen interactions, whereas 2-CNN displays a more symmetric profile. We evaluated the fractional energy emitted via the CN stretch relative to the total IR cascade intrinsic emissivity for neutral, cationic, and anionic 1- and 2-CNN in different astrophysical environments, and demonstrated how they, combined with the observationally detected CN stretch flux, can be used to quantitatively probe their presences in space. By bridging the gap between static laboratory benchmarks and dynamic interstellar emission, this work provides accurate anharmonic cascade emission spectra for cyanonaphthalenes. The spectral fingerprints for different charge states and isomers offer essential tools for interpreting high-resolution observations from the James Webb Space Telescope.

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Accepted for publication in *Astronomy & Astrophysics*

https://arxiv.org/abs/2607.20015

Interstellar X-ray Absorption and Scattering

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Accurate estimates of the absorption of X-rays by interstellar gas and dust are of crucial importance for the analysis and interpretation of almost all astronomical soft X-ray observations. However, the present X-ray absorption data extensively used by the community were derived from a reduced interstellar abundance ($\sim$70% of solar) and ignoring dust scattering. Therefore, these X-ray absorption data, although highly popular, could have been substantially underestimated. Here we update the interstellar X-ray absorption and scattering by making use of updated atomic cross sections, updated interstellar abundances, and realistic X-ray dust physics, and appropriately distributing metal elements in gas and dust. The resulting X-ray absorption and scattering data are publicly available on `GitHub`: https://github.com/yanll-xray/xray-extinction-model.

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The Astrophysical Journal, **1004**, pp 253 (2026)

https://arxiv.org/abs/2605.08981

Announcements

PAHdb Releases 2 New Libraries:

Computed Anharmonic IR PAH Spectra and Laboratory Gas-phase IR PAH Spectra

Advertised by Christiaan Boersma and the PAHdb Team

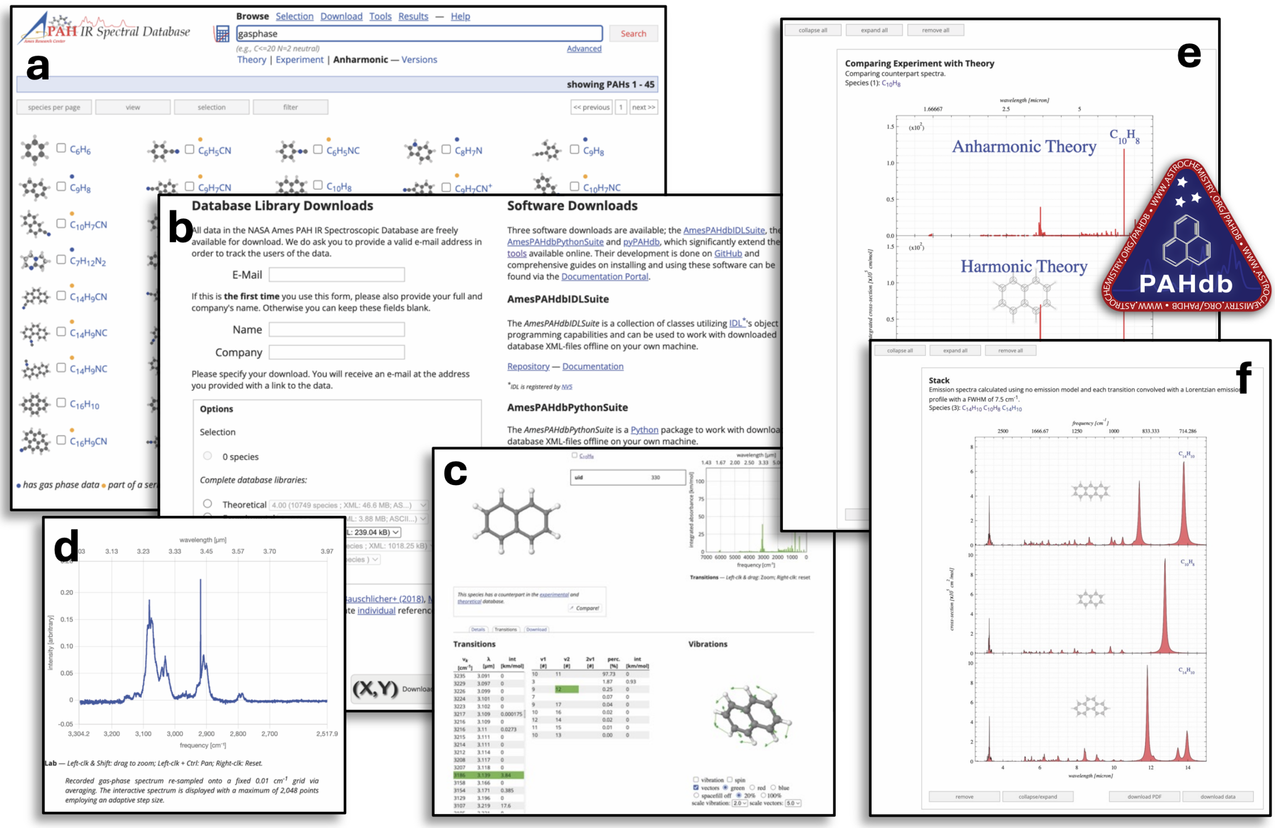

Figure 1 *– PAHdb website with the redesigned (**a**) browse, (**b**) download, and (**c**) transitions pages as well as (**d**) the new adaptive zoom interface, (**e**) a cross-library comparison of the data on naphthalene, and (**f**) the stack tool comparing generated emission spectra.*

After many years in the making, the NASA Ames PAH IR Spectroscopic Database (PAHdb) Team is proud to announce the release of two new libraries. Namely, the libraries of *Computed Anharmonic* and *Laboratory Gas-phase* spectra[1]. The inaugural versions of the computed and laboratory library offer 45 and five spectra, respectively. These libraries will be expanded with additional spectra as they become available. The PAHdb website

[1]Computational and laboratory data by V.J. Esposito and S. Bejaoui, respectively.

has been updated and redesigned to accommodate the two new libraries, where they can be browsed, used in simple analysis, and downloaded (see Figure). For the newly added anharmonic data, each overtone/combination band is broken down into contributing modes and the fundamental visualized. Also, substitution patterns are organized into linked series. The newly added high-resolution gas-phase laboratory measurements are found next to the anharmonic data, where spectra are presented using an adaptive zoom interface (see Figure 1).

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Webpage: https://www.astrochemistry.org/pahdb/

AstroPAH Newsletter

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