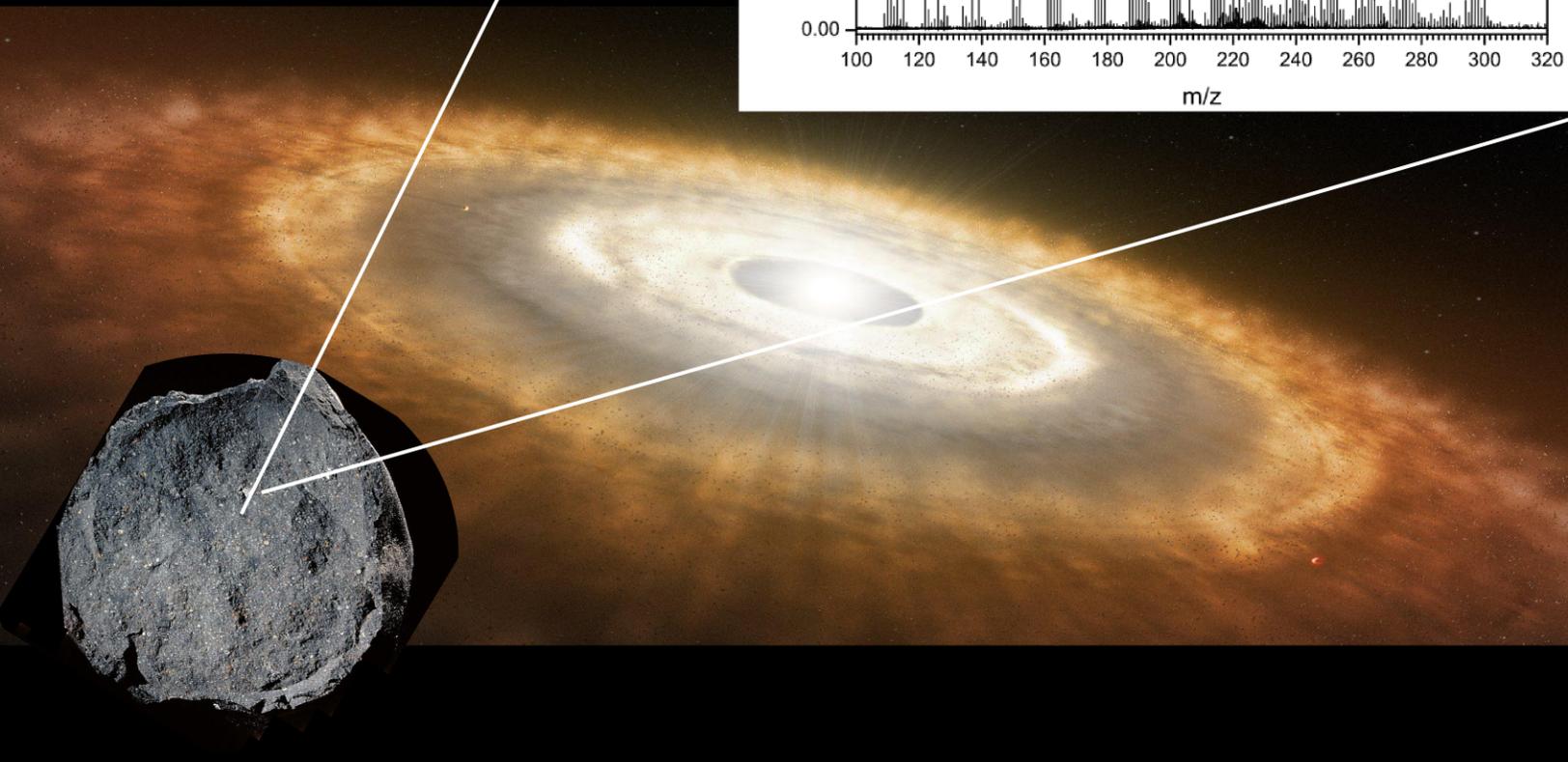
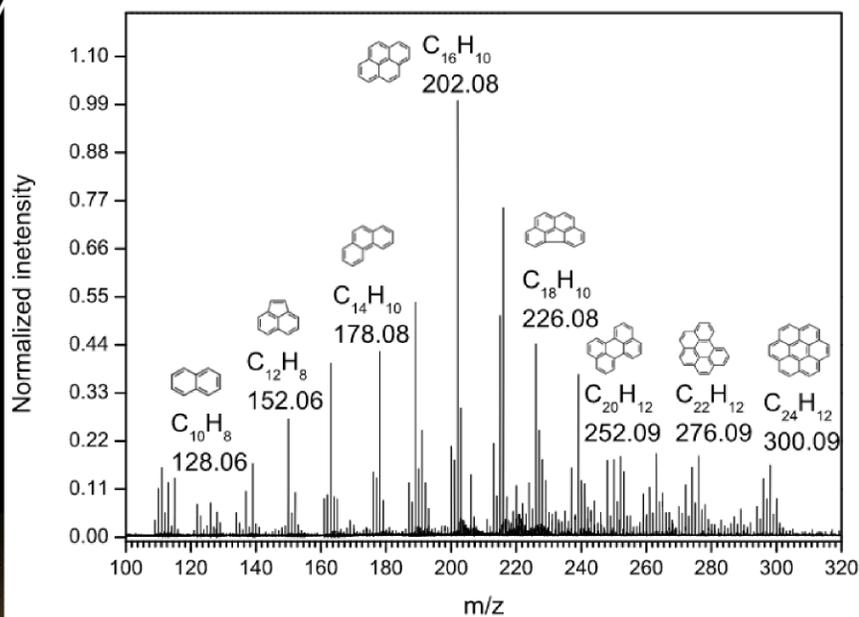


AstropAH

A Newsletter on Astronomical PAHs

Issue 40 | July 2017



Editorial

Dear Colleagues,

Welcome to our summer issue of AstroPAH featuring in the cover the detection of pyrene on the Murchison Meteorite using the AROMA setup.

For everyone who ever wondered about some of the ins and outs of computing PAHs and the conundrum of making choices, we have a wonderful In Focus written by **Ryan Fortenberry**. It's worth the read!

In our abstracts section, we have a variety of papers on observations, experiment, and theory involving PAHs, fullerenes and even the call for spectra of hot molecules for super-Earths passing the review.

Check the announcement of the JWST workshop at ESAC in the Meetings section. The EPoLM-3 meeting and the Nanocosmos meeting were jointly organised on 12-16 June at the Université Paul Sabatier in Toulouse (France). You can find all information on the web site <https://epolm3-nanocosm.sciencesconf.org/>.

Next month we will take a break, thus there will be no issue of AstroPAH in August. Instead you may be able to enjoy the eclipse of the sun on Monday 21 August, either onsite or, as most of us, remotely. NASA created a very nice [website](#) as a guide with activities, events and a countdown until first contact in Oregon.

Do you want to show off your picture of the solar eclipse? We invite you to send us your photos! The best one will be chosen to feature on the September cover, with due credit of course.

AstroPAH can help you promote your science. Visit our webpage or contact us for more information. You can send us your contributions anytime. For publication in September, see the deadlines below.

We thank you all for your contributions so far! See you again in September.

The Editorial Team

**Next issue: 19 September 2017.
Submission deadline: 8 September 2017.**

AstroPAH Newsletter

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PAH Picture of the Month

The Murchison Meteorite, fallen in Murchison, Australia in 1969 is one of the most studied carbonaceous chondrites, which is known to contain complex organic compounds such as aminoacids. A recent study by Sabbah and collaborators analyzed 1 mg of powdered Murchison meteorite with the newly built AROMA setup and firmly identified pyrene from the distribution of detected PAHs (inset). For more information we refer to Sabbah et al, ApJ, 2017 843:34, in the Abstract section.

Credits: Murchison Meteorite. Chip Clark - Smithsonian Institution (Murchison Meteorite). Background ESO/L. Calçada. Image composition by Alessandra Candian.

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Computing PAHs: Good, Fast, or Cheap (Choose Two)

by Ryan C. Fortenberry

In an old carpenter's shop in the mountains of western North Carolina some time ago hung a sign that made quite an impression on this young man. The saying was new to him but seemingly older than the hills surrounding the shop. It read, "There are three ways you can have it: good, fast, or cheap. You can only pick two." The old carpenter had already figured out scientific computing. I came to realize this many years later.

The truth of such a statement is definitely applicable to the computation of quantum chemical properties, especially for polycyclic aromatic hydrocarbons. PAHs represent the penultimate challenge of quantum chemical computation with only peptides being more of a computational chemist's conceptual crisis. The planarity and pseudo-regularity are their saving graces, but only two options can still be picked from the carpenter's sign. The nature of PAHs themselves has forced one third of that decision, fast or cheap, but never both. Fast refers to the speed of the computations, and cheap refers to the amount and, hence, cost of the computer infrastructure required. Lots of computers can run many jobs making the total computation fast, but each compute node costs more money. As a result, the computations will either be slow or monetarily expensive.

One of the issues with studying PAHs, especially experimentally, is that small isomeric changes will have small, but non-negligible changes in the physical properties. While a shift of a wavenumber is enough to offer a unique classification of a particular hydride stretch on a particular isomer, the proximity of reaction energies are often on the order of a few dozen kcal/mol. Hence, several, closely-related species are often present in the experiment each producing their own single-digit wavenumber shifts and, subsequently, a broad spectrum. While two hexagons can only be arranged one way, three can be arranged three ways, four can be arranged thirteen, and the number increases geometrically. This is not even considering charged, deprotonated, radical, functionalized, or heteroatomic species. Hence, the density of closely-related isomers approaches the confusion limit nearly immediately.

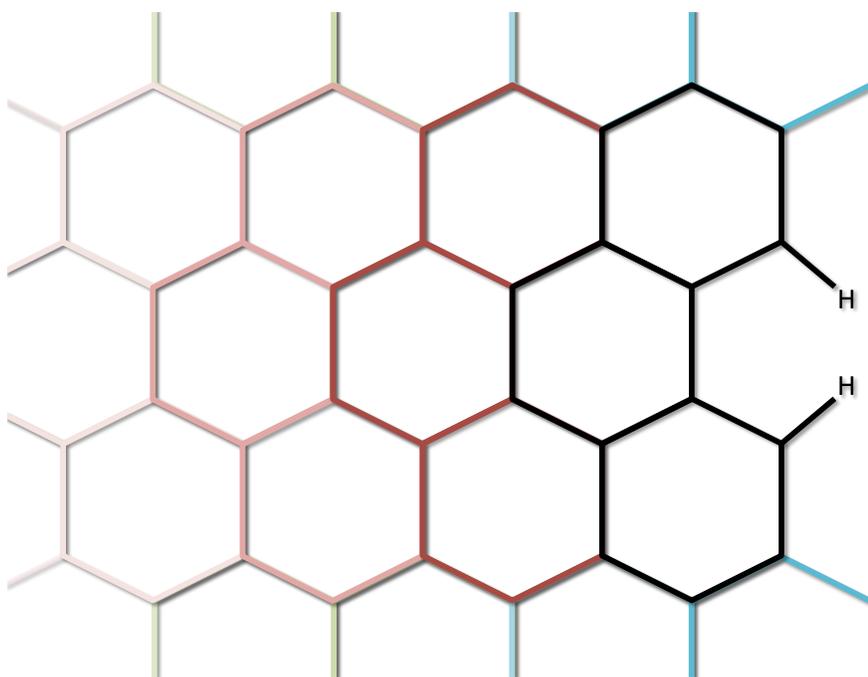


Figure 1: *The extensions of PAHs has little effect on the hydrogens in the bay region from phenanthrene (in black) up to larger structures.*

As a result, naive PAH synthetic and subsequent spectroscopic experiments will have broadly smeared features residing over a given range. This is one of the main reasons why the series of unidentified emission features in the infrared are called the unidentified aromatic bands (UABs) by some instead of the unidentified infrared bands (UIRs) by those less willing to be so convinced. Hence, much of PAH spectroscopic analysis has focused on certain regions of the molecules as classes unto themselves. Most notably, bay regions (Fig. 1) and drumbeat motions are treated similarly whether the actual species is anything from phenanthrene and triphenylene to the gargantuan asphaltenes. Even so, unique molecular classification is always the goal in order to know what the actual pixels are making up the spectral mosaic. This is computation's strong suit.

The best analogy for synthetic chemistry ever given is like that of sailing a toy boat across the pond. However, there is no remote control. All that can be done is to prep the boat as best as possible, wait for the right conditions, and pray that it floats in the desired direction often with much (useless) arm waving and mouth blowing done from the lakeshore. In other words, getting the desired product is a good bit of luck or simply picking the proper body of water to sail.

Computation does not suffer from this uncertainty. Quantum chemical results are for the molecule specified and nothing else. The input into the program is the nuclear positions as well as maybe some electronic data such as charge or spin multiplicity. Everything else is left up to the level of theory employed with "fastness" decreasing with the inclusion of more atoms in the system as well as, in turn, the number of electrons required. While experiment generates a spectrum of unknown origin, quantum chemical computation and theory, on the other hand, generates a known spectrum but of unknown accuracy. Hence, the computation can be good, fast, or cheap; choose two, almost like a Heisenberg trio instead of a Heisenberg pair.

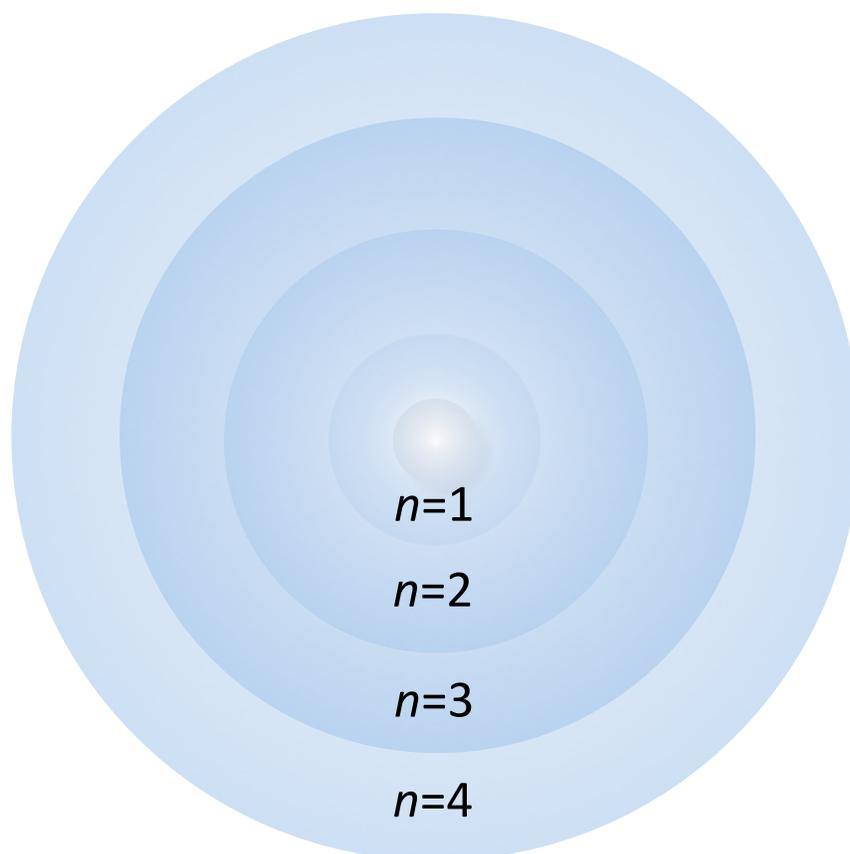


Figure 2: *The higher n values for successive s orbitals show how each higher n_s voluminously encapsulates all of the lower ones, but the quantum levels are different making them of different spaces and dimensions.*

The main delimiting factor in the tradeoffs of these three choices comes from the basis set. This term, utilized by quantum chemists to give experimentalists fireside ghost stories, is nothing more than the space the electrons are allowed to fill. Typically, sets of atomic orbitals are allowed to combine into what become molecular orbitals, and every atom adds its own number of basis functions to the total set. The quantum mechanics for such combinations are well-understood, and the overlaps produce really nice portrayals of σ bonds and π orbitals, for instance. However, some spaces occupied by the electrons in the molecule can vary wildly from where they might be found relative to the nuclei in the lone, separated atoms. Additionally, just because an orbital is not occupied in the ground state of the atom does not mean that it cannot be occupied in the molecule. Hence, more and more functions (or orbitals) must be added even if they are not occupied in order to create the space for each electron to reside in the molecule. This space is multi-dimensional since electrons may exist within the same 3-space but not the same quantum level depicted in Fig. 2. As a result, this linear combination of atomic orbitals to make molecular orbitals approximation works well, but it can get unwieldy. Luckily, there comes a point at which the space is as well-described as it is going to be, and adding more basis functions will not enhance the quality of the computation. Here, the Hartree-Fock limit is reached, but, you guessed it, the Hartree-Fock limit is not cheap.

There are three main camps within quantum chemistry: 1) force field methods, 2) density-functional theory (DFT), and 3) wave function theory. The first is fast and cheap, utilizing a minimum of basis functions, but typically not good “out of the box.” The last is good and can be cheap but will rarely be fast even with the advent of graphical processing units and multithreading due to exponential scaling of the basis set overlaps. The middle can be good, is certainly faster than wave function methods, and can be cheap. However, DFT can also be bad, especially in the most common B3LYP flavor. While DFT in general is *ab initio*, from first principles, specific methods have been parameterized to produce physically meaningful results. B3LYP gets lucky in most instances, but it can fail as happily as it can succeed in property predictions with the scientist being none-the-wiser. Even though the original B3 portion (Becke 1993) is one of the 10 most cited scientific papers of all time and the fastest to break 45,000 citations, Axel Becke (the “B” himself) has cautioned against its usage in recent years.

The one saving grace of B3LYP for PAHs, is that it was formulated for a standard set of organic molecules. Nothing is more organic, by definition, than PAHs; that’s what the “H” means! One group at the NASA Ames Research Center has been putting DFT, specifically B3LYP, through the ringer for application to PAHs. Bauschlicher, Langhoff, Ricca, and others have computed the infrared fundamentals for hundreds of PAHs over the past thirty or so years. Using a fairly standard basis set, scaled-harmonic vibrational frequencies have been computed for “small” and large PAHs, even all the way up to $C_{384}H_{48}$ (Ricca et al. 2012). Combining the spectra of certain PAHs together from both theoretical and experimental data can allow for modeling of astrophysical spectra. The NASA Ames IR PAH Spectral Database (Boersma et al. 2014) has provided a novel and highly-useful tool for smearing the pixels together to create unprecedented models of PAH IR spectra. However, the approximations (DFT, scaled-harmonics) that have to be employed in PAH computations in order to make them fast and cheap (the only way to compute data for large molecules) cannot be used to predict accurately the spectra of lone, unique molecules. These computations were not made to do such a thing and perform their designated task in large scale spectra generation quite well. The question still remains as to whether “good,” as in highly-accurate, properties can even be computed for PAHs.

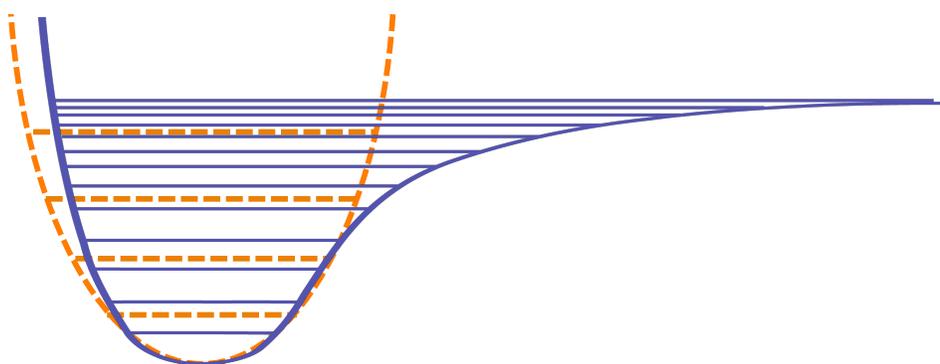


Figure 3: The harmonic potential (orange) compared with the more physical and anharmonic Morse potential (purple).

Scaled harmonic computations provide an excellent first estimate of vibrational frequencies. However, they model the bond stretching as a parabola and not as a Morse potential, shown in Fig. 3, as would be needed in anharmonic computations. Scaling the frequencies with an empirical or statistical reduction factor moves the minimum close to where the Morse potential should likely produce a minimum on the average. However, some vibrational frequencies can be positively anharmonic, have flat potential surfaces, or simply behave erratically. Hence, accurate and systematic predictions of vibrational frequencies require accurate representations for the anharmonic behavior of all atoms relative to one another. Unsurprisingly, the cheapness and the fastness of the computations reduces significantly when the goodness must increase.

The most accurate predictions of fundamental vibrational frequencies are from wave function based methods (the expensive ones from the previous discussion) with lots of basis functions fast approaching the Hartree-Fock limit (making them even more expensive). Consequently, they are good but neither fast nor cheap. With an infinite amount of time, they can be cheap, but multiple thousands of computations are required to produce the necessary data to fit the fundamental vibrational frequencies. For instance, the protonated carbon dioxide molecule (HOCO^+) has been predicted to have a O–H stretching vibrational frequency of 3376.3 cm^{-1} (Fortenberry et al. 2012) with an experimental, gas phase frequency previously reported at $3375.37413 \text{ cm}^{-1}$ (Amano & Tanaka 1985). However, these computations require more than 5500 individual quantum chemical computations with some individual computations taking as long as a day to complete in order to achieve this accuracy. Moving up from four atoms to five in protonated acetylene ($c\text{-C}_2\text{H}_3^+$) increases the number of computations to more than 11,000 (Fortenberry et al. 2014) but also with the antisymmetric C–H stretch predicted to be 3142.3 cm^{-1} and experiment indicating this value to be nearly the same at 3142.2 cm^{-1} (Crofton et al. 1989). Hence, these computations are “good” (really, they are great) and relatively cheap, but they are not fast. Each of these two sample studies took over six months from conception to completion.

Scaling up to PAHs, even simply benzene, would require several human years and several hundred or thousand computer years with this protocol. Hence, sacrifices have to be made or sheer luck employed. Linus Pauling won the Nobel Prize in 1954 for providing a better understanding of chemical bonding, and his name is synonymous with luck in quantum chemistry. The “Pauling point” is a place where theory and experiment simply happen to agree for no other reason than luck, as well as cancellation of errors. It turns out that a medium level of theory and a medium basis set can often produce exceptionally good agreement with experiment. While DFT/B3LYP has some of these hallmarks, often Møller-Plesset perturbation theory at second-order (Møller & Plesset 1934) (note the date on that publication) combined with a double-zeta basis set (that which involves two sets of functions per each angular momentum) can produce notable agreement with experiment (Zheng et al. 2009; Sherrill 2011; Fink 2016) as Pauling points. Other Pauling points include coupled cluster theory (Crawford & Schaefer III 2000; Shavitt & Bartlett 2009) at the singles and doubles level (CCSD) with a double zeta basis set (Lee & Scuseria 1995) as well as CCSD(T), inclusive of CCSD with a perturbative triples addition, with a triple-zeta basis set (Helgaker et al. 2004). Additionally, even lower levels of theory (like B3LYP) that employ explicit anharmonic treatment can produce more physically-meaningful results for a single PAH (Maltseva et al. 2015).

One of the promising approaches for treating PAHs lies in the third camp of quantum chemistry, semiempirical methods. These methods either neglect or empirically parameterize algebraic treatment of the electron-electron repulsion (or, equivalently, two-electron) integrals within the Schrödinger equation. As mentioned above, this can make them really fast and really cheap but not good. The “goodness,” however, is a matter of perspective. For computing turns of DNA, such methods are fine as they are the only tractable means of computing such properties. However, semiempirical methods can be tuned for a given set of properties, as well. One idea being developed by myself and collaborators from the University of St. Thomas (MN), NASA Ames, and the University of Leiden is to train molecular mechanics methods to treat PAHs. It remains to be seen if such an approach is viable, but the regularity of PAHs makes them a natural fit for such cheap and fast methods trained to be good.

In summary, the truth of good, fast, or cheap is definitely true of computing PAHs. They are already “big” in the first place, from a quantum chemical standpoint. Hence, they either will not be fast or will not be cheap. In theory, they can still be good, but, typically, sacrifices are made in the fast department as grants and research dollars are limited forcing them to be cheap and, as a result, often less good. Most of us balance the game of good versus fast. Pauling points can give surprisingly good answers as can scaled harmonics, but both are known to fail at times. More consistent, accurate, and precise spectroscopic and structural predictions require more expensive, higher-level quantum chemical computations that are not fast at all. However, cutting-edge methods are cutting the corners of the three constraints making methods that are cheap and fast (as required to study PAHs) but also good. Human creativity combined with advances in scientific computing will continue to push the study of PAHs into the silicon environment. Only within a single molecular simulation can the unique properties of individual PAHs be constructed so that the trees begin to emerge the infrared forest.

Acknowledgments

RCF acknowledges NASA Grant NNX17AH15G for supporting this work. He also acknowledges Drs. Timothy J. Lee and Xinchuan Huang of NASA Ames and the SETI Institute, respectively, for their tutelage and training as well as Prof. Joshua P. Layfield of the University of St. Thomas for help in editing this document. RCF also is thankful to the editors of this publication for the opportunity to submit this piece.



In theory, the author is a chemist. At some point in the recent past, he obtained a Ph.D. in theoretical chemistry from Virginia Tech before becoming a “fellow” of the NASA Postdoctoral Program at the NASA Ames Research Center which is definitely not in Iowa. Ryan dreams of surpassing the assistant nature of his current professorship to become an associate-type of the sort, hopefully this upcoming academic year. He previously earned a Bachelor’s of Science in mathematics and a Master’s of Science in communication at Mississippi College. Being from Mississippi, Ryan naturally hates wearing shoes and typically puts too many syllables in his words. He does enjoy bad jokes, mountains, soccer, yoga, his family, and hearing himself talk even when the audience left ten minutes ago.

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References

- Amano, T., & Tanaka, K. 1985, *J. Chem. Phys.*, 82, 1045
- Becke, A. D. 1993, *J. Chem. Phys.*, 98, 5648
- Boersma, C., Bauschlicher, Jr., C., Ricca, A., et al. 2014, *Astrophys. J. Suppl. Ser.*, 211, 8
- Crawford, T. D., & Schaefer III, H. F. 2000, in *Reviews in Computational Chemistry*, ed. K. B. Lipkowitz & D. B. Boyd, Vol. 14 (New York: Wiley), 33–136
- Crofton, M. W., Jagod, M.-F., Rehfuss, B. D., & Oka, T. 1989, *J. Chem. Phys.*, 91, 5139
- Fink, R. F. 2016, *J. Chem. Phys.*, 145, 184101
- Fortenberry, R. C., Huang, X., Crawford, T. D., & Lee, T. J. 2014, *J. Phys. Chem. A*, 118, 7034
- Fortenberry, R. C., Huang, X., Francisco, J. S., Crawford, T. D., & Lee, T. J. 2012, *J. Chem. Phys.*, 136, 234309
- Helgaker, T., Ruden, T. A., Jørgensen, P., Olsen, J., & Klopper, W. 2004, *J. Phys. Org. Chem.*, 17, 913
- Lee, T. J., & Scuseria, G. E. 1995, in *Quantum Mechanical Electronic Structure Calculations with Chemical Accuracy*, ed. S. R. Langhoff (Dordrecht: Kluwer Academic Publishers), 47–108
- Maltseva, E., Petrigani, A., Candian, A., et al. 2015, *Astrophys. J.*, 814, 23
- Møller, C., & Plesset, M. S. 1934, *Phys. Rev.*, 46, 618
- Ricca, A., Charles W. Bauschlicher, J., Boersma, C., Tielens, A. G. G. M., & Allamandola, L. J. 2012, *Astrophys. J.*, 754, 75
- Shavitt, I., & Bartlett, R. J. 2009, *Many-Body Methods in Chemistry and Physics: MBPT and Coupled-Cluster Theory* (Cambridge: Cambridge University Press)
- Sherrill, C. D. 2011, *Rev. Comput. Chem.*, 26, 1
- Zheng, J., Zhao, Y., & Truhlar, D. G. 2009, *J. Chem. Theory Comput.*, 5, 808

PAH features within few hundred parsecs of active galactic nuclei

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Spectral features from poly-cyclic aromatic hydrocarbon (PAH) molecules observed in the mid-infrared (mid-IR) range are typically used to infer the amount of recent and ongoing star formation on kiloparsec scales around active galactic nuclei (AGN) where more traditional methods fail. This method assumes that the observed PAH features are excited predominantly by star formation. With current ground-based telescopes and the upcoming JWST, much smaller spatial scales can be probed and we aim at testing if this assumption still holds in the range of few tens to few hundreds of parsecs. For that, we spatially map the emitted 11.3 μm PAH surface flux as a function of distance from 0.4-4 arcsec from the centre in 28 nearby AGN using ground-based high-angular resolution mid-IR spectroscopy. We detect and extract the 11.3 μm PAH feature in 13 AGN. The fluxes within each aperture are scaled to a luminosity-normalised distance from the nucleus to be able to compare intrinsic spatial scales of AGN radiation spanning about 2 orders of magnitude in luminosity. For this, we establish an empirical relation between the absorption-corrected X-ray luminosity and the sublimation radius in these sources. Once normalised, the radial profiles of the emitted PAH surface flux show similar radial slopes, with a power-law index of approximately -1.1 , and similar absolute values, consistent within a factor of a few of each other as expected from the uncertainty in the intrinsic scale estimate. We interpret this as evidence that the profiles are caused by a common compact central physical process, either the AGN itself or circumnuclear star formation linked in strength to the AGN power. A photoionisation-based model of an AGN exciting dense clouds in its environment can

reproduce the observed radial slope and confirms that the AGN radiation field is strong enough to explain the observed PAH surface fluxes within $\sim 10\text{-}500$ pc of the nucleus. Our results advice caution in the use of PAH emission as a star formation tracer within a kpc around AGN.

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Accepted for publication in MNRAS

<https://arxiv.org/abs/1706.04811>

Identification of PAH Isomeric Structure in Cosmic Dust Analogs: The AROMA Setup

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We developed a new analytical experimental setup called AROMA (Astrochemistry Research of Organics with Molecular Analyzer) that combines laser desorption/ionization techniques with ion trap mass spectrometry. We report here on the ability of the apparatus to detect aromatic species in complex materials of astrophysical interest and characterize their structures. A limit of detection of 100 femto-grams has been achieved using pure polycyclic aromatic hydrocarbon (PAH) samples, which corresponds to 2×10^8 molecules in the case of coronene ($\text{C}_{24}\text{H}_{12}$). We detected the PAH distribution in the Murchison meteorite, which is made of a complex mixture of extraterrestrial organic compounds. In addition, collision induced dissociation experiments were performed on selected species detected in Murchison, which led to the first firm identification of pyrene and its methylated derivatives in this sample.

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<https://doi.org/10.3847/1538-4357/aa73dd>

<https://arxiv.org/abs/1705.09974>

Detection of Buckminsterfullerene emission in the diffuse interstellar medium

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Emission of fullerenes in their infrared vibrational bands has been detected in space near hot stars. The proposed attribution of the diffuse interstellar bands at 9577 and 9632 Å to electronic transitions of the buckminsterfullerene cation (i.e. C_{60}^+) was recently supported by new laboratory data, confirming the presence of this species in the diffuse interstellar medium (ISM). In this letter, we present the detection, also in the diffuse ISM, of the 17.4 and 18.9 μm emission bands commonly attributed to vibrational bands of neutral C_{60} . According to classical models that compute the charge state of large molecules in space, C_{60} is expected to be mostly neutral in the diffuse ISM. This is in agreement with the abundances of diffuse C_{60} we derive here from observations. We also find that C_{60} is less abundant in the diffuse ISM than in star-forming regions, supporting the theory that C_{60} can be formed in these regions.

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<https://arxiv.org/abs/1706.06803>

Laboratory spectra of hot molecules: Data needs for hot super-Earth exoplanets

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The majority of stars are now thought to support exoplanets. Many of those exoplanets discovered thus far are categorized as rocky objects with an atmosphere. Most of these objects are however hot due to their short orbital period. Models suggest that water is the dominant species in their atmospheres. The hot temperatures are expected to turn these atmospheres into a (high pressure) steam bath containing remains of melted rock. The spectroscopy of these hot rocky objects will be very different from that of cooler objects or hot gas giants. Molecules suggested to be important for the spectroscopy of these objects are reviewed together with the current status of the corresponding spectroscopic data. Perspectives of building a comprehensive database of linelist/cross sections applicable for atmospheric models of rocky super-Earths as part of the ExoMol project are discussed. The quantum-mechanical approaches used in linelist productions and their challenges are summarized.

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Molecular Astrophysics, Volume 8, September 2017, Pages 1-18

<http://www.sciencedirect.com/science/article/pii/S240567581730012X>

Detection of Polarized Infrared Emission by Polycyclic Aromatic Hydrocarbons in the MWC 1080 Nebula

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Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous in astrophysical environments, as revealed by their pronounced emission features at 3.3, 6.2, 7.7, 8.6, 11.3, and 12.7 μm commonly ascribed to the C–H and C–C vibrational modes. Although these features have long been predicted to be polarized, previous searches for PAH polarization led to null or, at best, tentative detections. Here we report the definite detection of polarized PAH emission at 11.3 μm in the nebula associated with the Herbig Be star MWC 1080. We measure a polarization degree of $1.9 \pm 0.2\%$, which is unexpectedly high compared to models. This poses a challenge in the current understanding of the alignment of PAHs, which is required to polarize the PAH emission but thought to be substantially suppressed. PAH alignment with a magnetic field via a resonance paramagnetic relaxation process may account for such a high level of polarization.

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Accepted for publication in ApJ

<https://arxiv.org/abs/1706.02015>

Meetings

Mastering the science instruments and the observing modes of the JWST: get set

European Space Astronomy Centre (ESAC), Madrid, Spain

4 - 6 October 2017

In anticipation of the first JWST call for proposals in November 2017 the European Space Agency is organizing workshops to engage and inform the astronomical community about the JWST Proposal Planning process. This workshop will take place at the ESA's European Space Astronomy Center (ESAC) near Madrid on October 4-6, 2017.

The main goal of this workshop is to present all the available tools in support of the proposal preparation and submission and to provide ample hands-on teaching for the the JWST Target Visibility Tools, the JWST Exposure Time Calculator (ETC), and the JWST Astronomer's Proposal Tool (APT).

This is the second workshop of the series "On your Mark, Get Set - Go!" The first workshop in this series took place at ESAC on September 26-28, 2016 and its main goal was to help prospective JWST users to select the best observing modes to achieve their science goals. All the material presented at the workshop, including videos of the presentations, is available at <https://www.cosmos.esa.int/web/jwst-2016-esac>.

E-mail for contact: jwst_workshop@sciops.esa.int

Webpage: <https://www.cosmos.esa.int/web/jwst-2017-esac>

Announcements

PhD opening in experimental (astro)molecular spectroscopy

University of Amsterdam, The Netherlands

Closing date: 4 September 2017

We are looking for excellent candidates with a high affinity to experimental chemical physics and/or laser physics.

This PhD project involves the experimental investigation of the spectroscopy and photochemistry of polycyclic aromatic hydrocarbon (PAH) species. The PhD candidate will determine the branching and the kinetics involved in the fragmentation and cooling of PAHs upon UV excitation. This includes the branching between fragmentation and alternative decay channels such as ring opening. Furthermore, he/she will measure the corresponding signatures required for observations.

Multiple molecular-beam and ionic spectroscopy techniques will be used, such as IR-UV double resonance spectroscopy, velocity map imaging, and ion mobility spectrometry. This project is highly experimentally oriented, involving state-of-the-art spectroscopic setups. It is therefore important that the PhD candidate has an affinity with the development, construction, and implementation of challenging experimental approaches.

The PhD candidate will be appointed at the University of Amsterdam within the framework of the Dutch Astrochemistry Network. He/she will perform the experimental studies within a small research team and at the same time be part of collaborative network of theoretical, astronomical, and other experimental groups.

Interested? Find additional information about the vacancy and apply [here](#).

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AstroPAH Newsletter

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Submission deadline: 8 September 2017