# Observational Challenges for the PAH Hypothesis

Alan T. Tokunaga<sup>1</sup>, Lawrence S. Bernstein<sup>2</sup>, Takashi Onaka<sup>3</sup>

<sup>1</sup>University of Hawaii, <sup>2</sup>Topshan, Maine, <sup>3</sup>University of Tokyo

### Introduction

We examine PAH hypothesis, which says that the Aromatic Infrared Bands (AIBs) observed at 3.3, 6.2, 7.7, 8.6, and 11.2 μm originate from gas-phase PAH molecules. We focus here on the dominant Class A sources (ref 1,2).

The core issue: the lack of spectral diversity across diverse astrophysical environments (HII regions, planetary nebulae, reflection nebulae, the diffuse ISM) suggest that there is a small set of PAH molecules with nearly source invariant compositions and UV excitation energies.

### **Key Observational Constraints**

The peak wavelengths of the AIBs are remarkably constant (ref 1,2). In addition, there are two key observational constraints in Class A sources:

- Red Wing of the 3.3  $\mu$ m AIB: The wavelength at half peak intensity of the red wing ( $\lambda_R$ ) is remarkably consistent, with an extremely small observed spread of ±0.0012 μm (see Figure 1). Since this band is emitted by small PAHs (30-50 carbon atoms) and is highly temperaturesensitive (ref 3), the constant  $\lambda_R$  implies that there are a limited set of PAH species with similar excitation temperatures across diverse astrophysical environments.
- Blue Wing of the 11.2  $\mu$ m AIB: The wavelength at half peak intensity of the blue wing ( $\lambda_{\rm R}$ ) is nearly constant, with a spread of only ±0.002 μm (see Figure 2). This band is primarily emitted by large PAHs (≥80 carbon atoms), and models using the NASA Ames PAH database show a strong species-dependent variation (see Figure 3). Thus the constant  $\lambda_R$  is very difficult to understand unless there is a very specific set of PAH species.

## Key Questions for the PAH Hypothesis

Although the PAH hypothesis has been very successful in explaining many aspects of the AIB spectrum, there are a number of open questions regarding the PAH hypothesis.

- Lack of spectral diversity. Why do sources with varying excitation conditions show a nearly identical  $\lambda_R$  and  $\lambda_R$ ? This implies two small, distinct PAH populations-- one emitting primarily at 3.3  $\mu$ m and the other at 11.2  $\mu$ m, which has consequences for interpreting the AIB band ratios.
- Conflict with current models for the AIB emission. Current modeling of the AIBs usually assume 30-50 PAH molecules of different types and sizes (see for example refs 4,5,6). How do we reconcile the constant  $\lambda_R$  and  $\lambda_R$  with current PAH emission models?
- Absence of UV/optical absorption features. Up to 20% of the IR emission of a galaxy is emitted in the AIBs, and therefore a small number of PAH species would be expected to produce strong absorption bands at 300-700 nm. Why are there no observed absorption features from PAH molecules (refs 7,8)?
- Selective Formation and Survival. Why are only a small number of gas phase PAH molecules consistently produced and preserved in the ISM?

We hope this poster will stimulate further research addressing these unresolved questions.

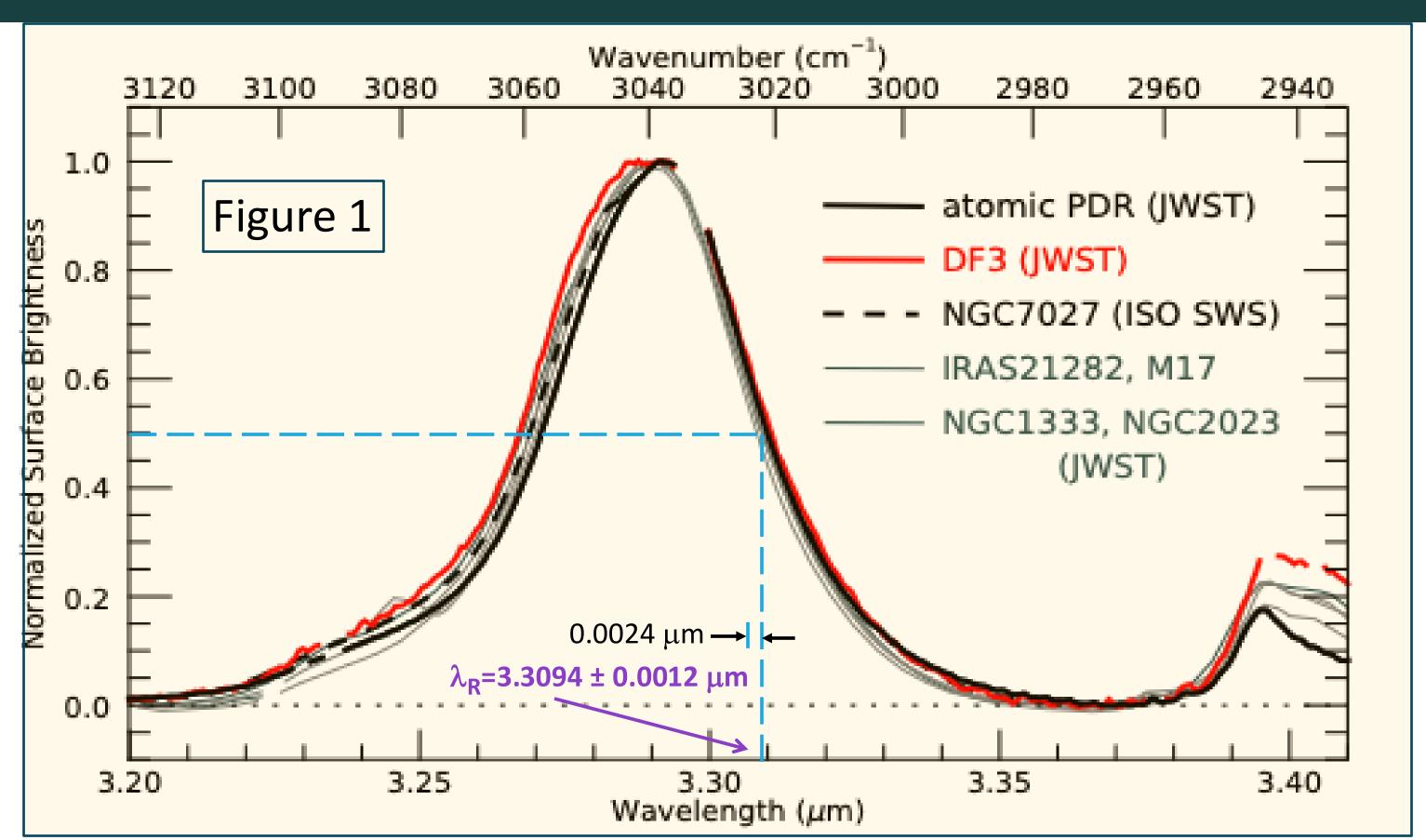


Figure 1. Normalized JWST spectra of the atomic PDR region and DF3 regions of the Orion Bar (ref 9) compared to the normalized ISO spectrum of NGC 7027 (ref 10) and the JWST spectra of IRAS 21282, M17, NGC 1333, and NGC 2023 (ref 11; grey solid lines). The continuum, plateau, and emission lines were removed.

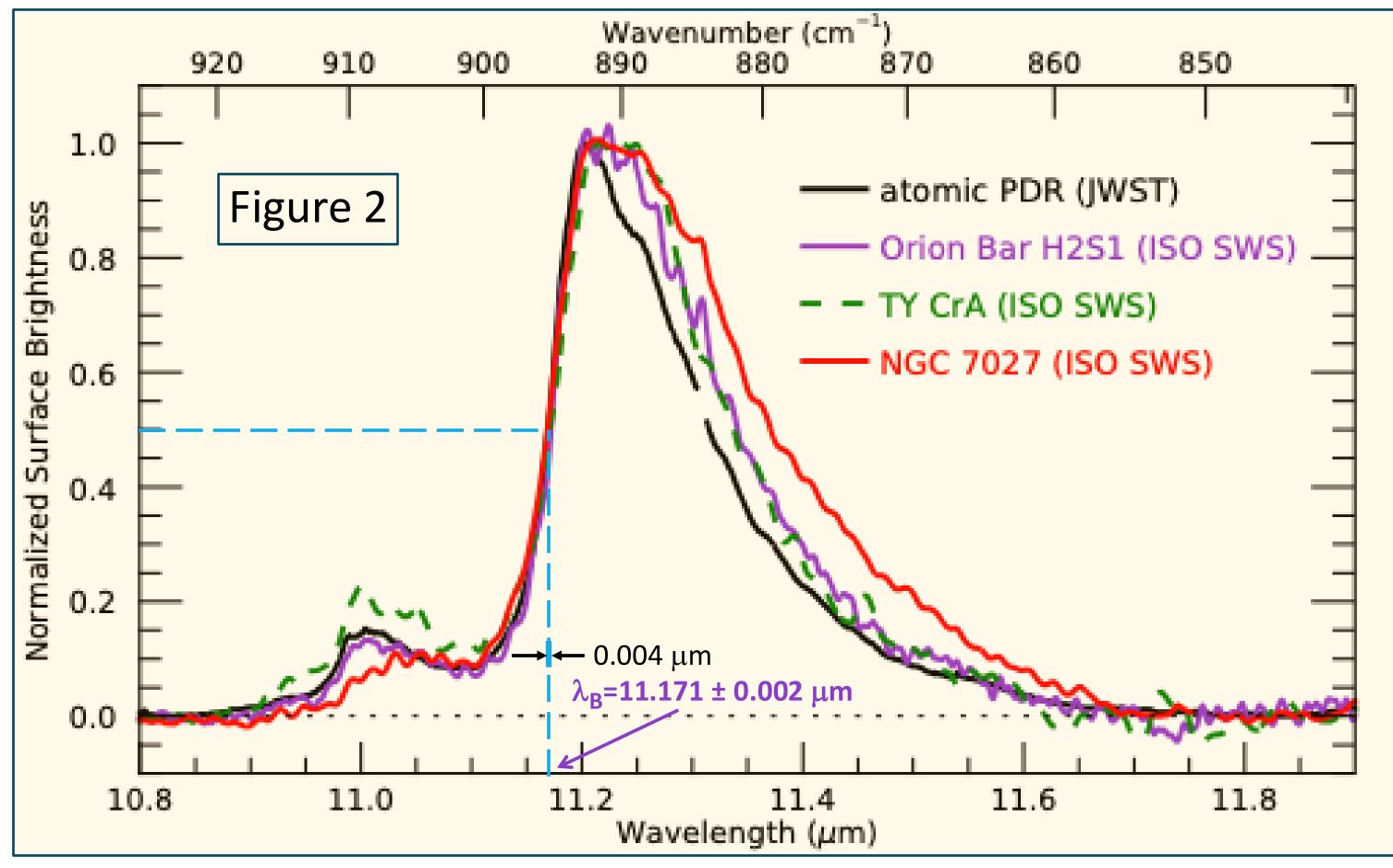


Figure 2. Normalized spectra of the atomic PDR regions of the Orion Bar compared to the ISO SWS spectra of the Orion Bar H2S1, TY CrA, and NGC 7027. The continuum, plateau, and emission lines were removed. The DF3 Orion Bar spectrum is a Class B type and is not shown.

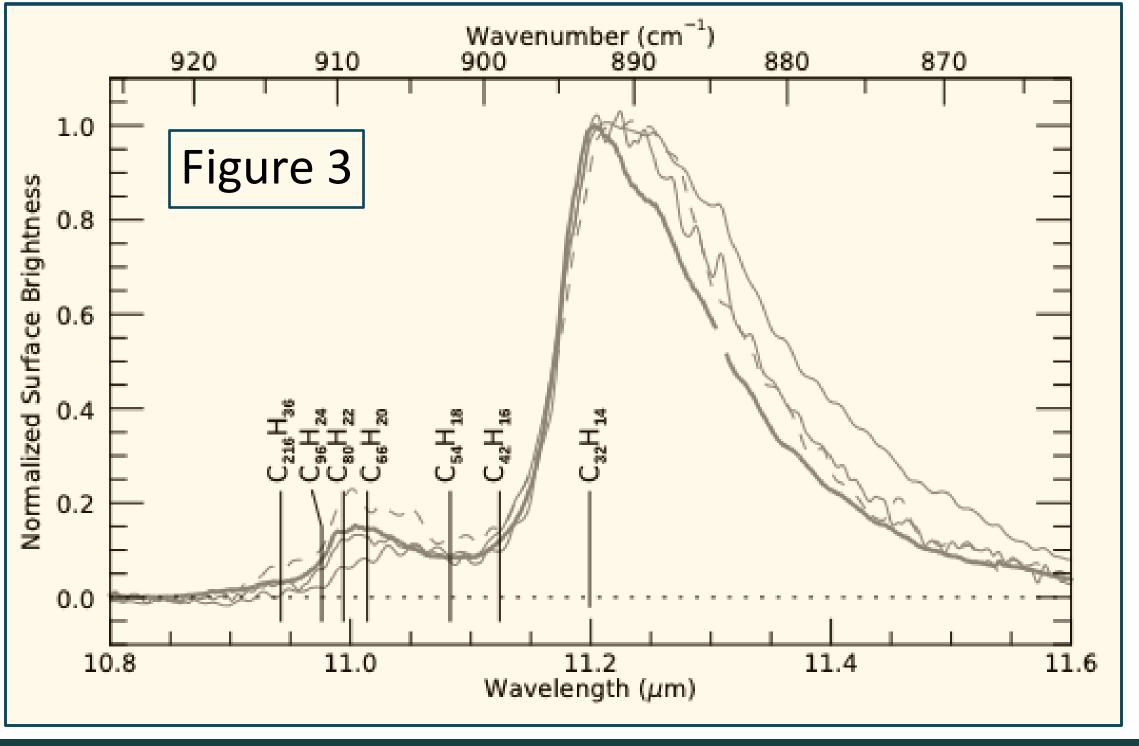


Figure 3. Vertical lines show the out-of-plane bending mode wavelengths for symmetric, compact PAHs from the NASA Ames PAH database (ref 12, 13), without corrections for anharmonic or temperature effects. The narrow range of  $\lambda_R$  places tight constraints on which PAH species can exist. Although not shown, isomers also need to be taken into account.

#### Contact

Get a copy of this poster:

Alan Tokunaga University of Hawaii Email: tokunagaa001@gmail.com



Read our paper: https://arxiv.org/abs/2510.26970

MNRAS, in press



### References

Peeters, E., et al., 2002. The rich 6 to 9 µm spectrum of interstellar PAHs. A&A 390, 1089.

Introduction of Multiple Scaling Factors. ApJS 234, 32.

- van Diedenhoven, B., et al., 2004. The Profiles of the 3-12 Micron Polycyclic Aromatic Hydrocarbon Features. ApJ 611, 928.
- 3. Joblin, C., et al., 1995. Infrared spectroscopy of gasphase PAH molecules. II. Role of the temperature. A&A 299, 835. 4. Andrews, H., et al., 2015. PAH Emission at the Bright Locations of PDRs: the grand PAH Hypothesis. ApJ 807, 99.
- 5. Bauschlicher, C.W., et al., 2018. The NASA Ames PAH IR Spectroscopic Database: Computational Version 3.00 with Updated Content and the Introduction of Multiple Scaling Factors. ApJS 234, 32.
- 6. Ricca, A., et al., 2024. Role of Polycyclic Aromatic Hydrocarbons with Edge Defects in Explaining Astronomical Infrared Emission Observations. ApJ 968, 128.
- Gredel, et al., 2011. Abundances of PAHs in the ISM: confronting observations with experimental results. A&A 530, A26. 8. Steglich, M., et al., 2012. The smoothness of the interstellar extinction curve in the UV. Comparison with recent laboratory measurements of PAH mixtures. A&A 540, A110.
- 9. Chown, R., et al., 2024. PDRs4All. IV. An embarrassment of riches: Aromatic infrared bands in the Orion Bar. A&A 685, A75. 10. Tokunaga, A.T., Bernstein, L.S., 2021. The 3.3 μm Infrared Emission Feature: Observational and Laboratory Constraints on Its Carrier. ApJ 916, 52.

11. Boersma, C., et al., 2023. JWST: Deuterated PAHs, PAH Nitriles, and PAH Overtone and Combination Bands. I. Program Description and First Look. ApJ 959, 74.

12. Boersma, C., et al., 2014. The NASA Ames PAH IR Spectroscopic Database Version 2.00: Updated Content, Web Site, and On(Off)line Tools. ApJS 211, 8 13. Bauschlicher, C.W., Jr., Ricca, A., Boersma, C., Allamandola, L.J., 2018. The NASA Ames PAH IR Spectroscopic Database: Computational Version 3.00 with Updated Content and the

Website: https://people.ifa.hawaii.edu/faculty/bio/alan-tokunaga/