

edge structure variations in interstellar PAHs

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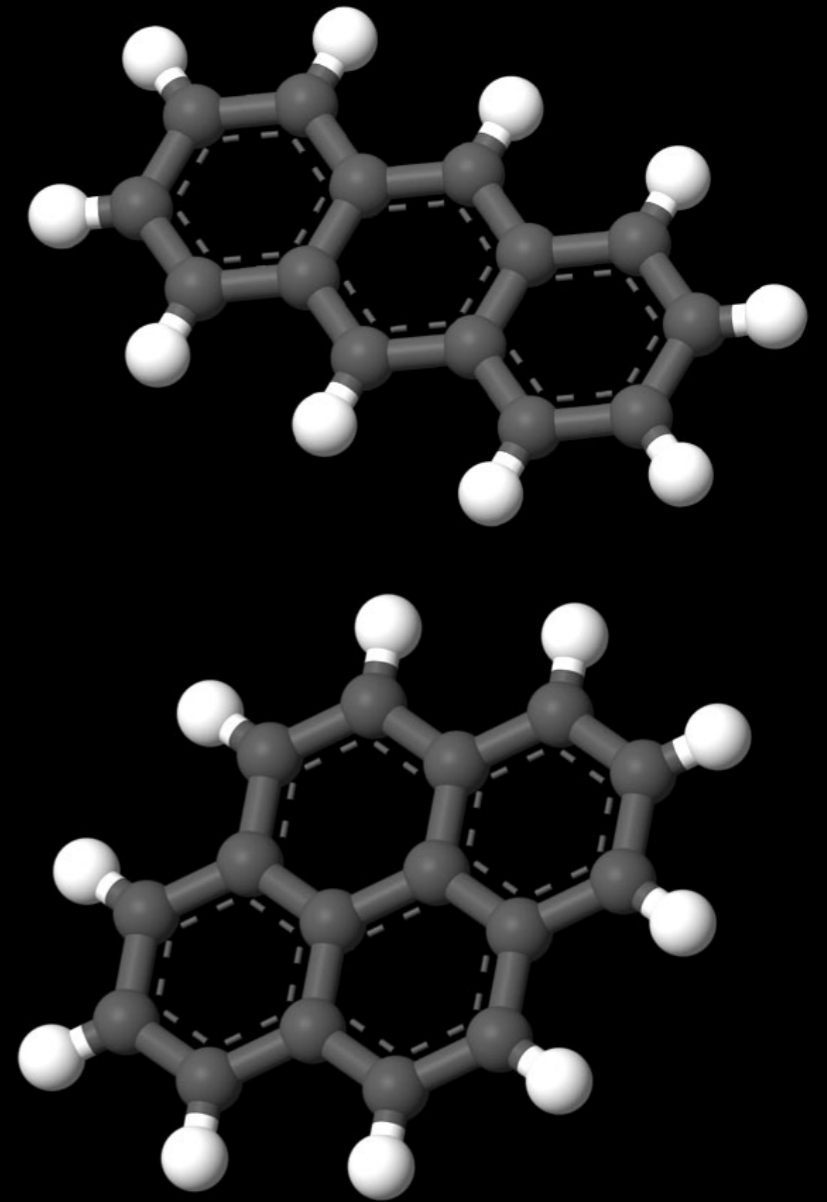
Outline

- Bay hydrogens and the 3.3 μm band
 - Spectroscopic Decomposition
- “Snowflakes” and the Diffuse Interstellar Bands
 - Out-of-plane Vibrations
 - Clar Theory
- Deprotonated PAHs and AME
 - 3.4-3.6 μm Aliphatic Vibrations?
 - PAH Rotational Spectroscopy

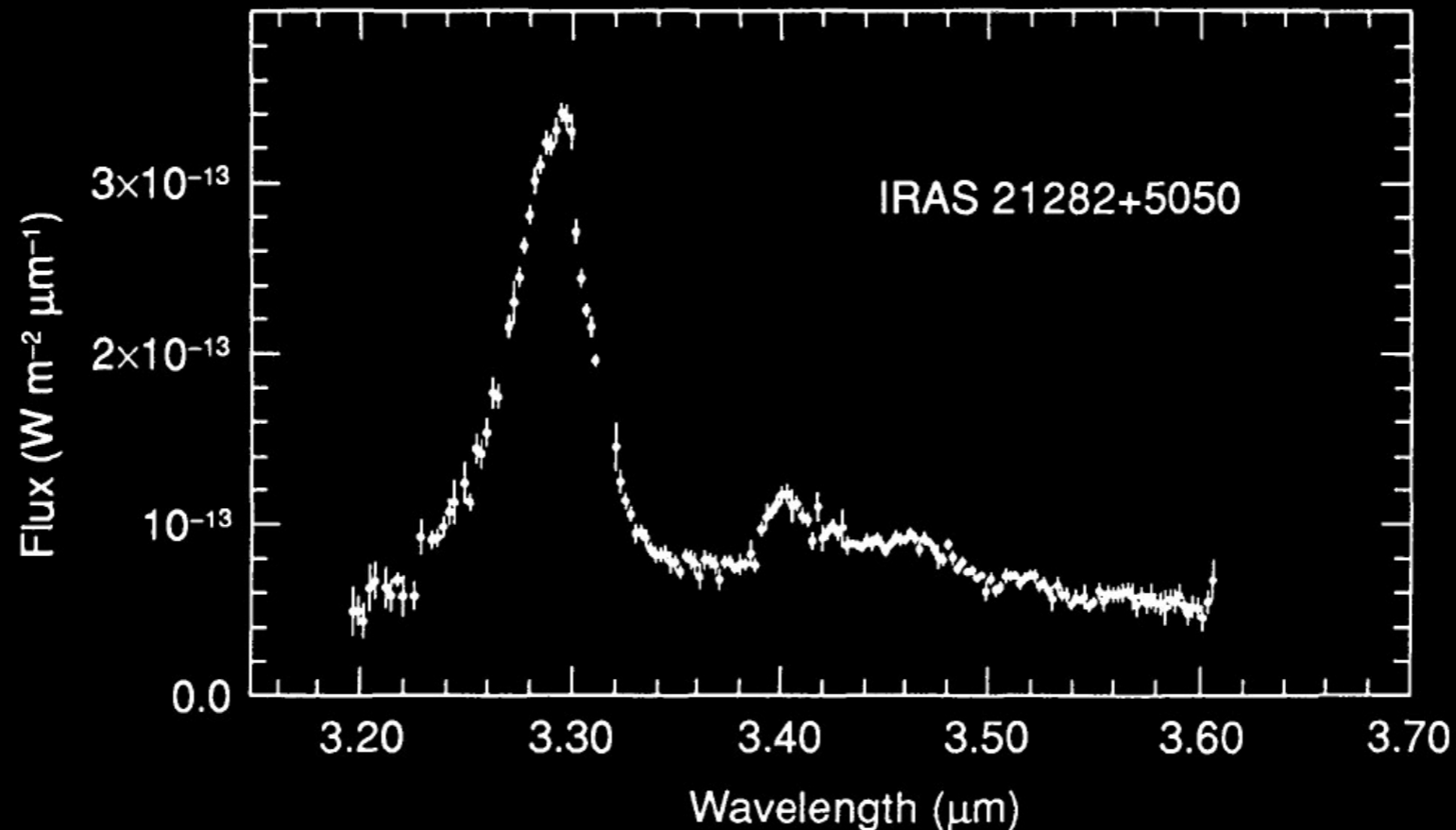


Polycyclic Aromatic Hydrocarbons

- (PAHs)
- Significant fraction of all interstellar carbon (10-20%)
- Emission – 10-15% of galaxy bolometric luminosity
- May contain hundreds of atoms
- Related to many astronomical phenomena?

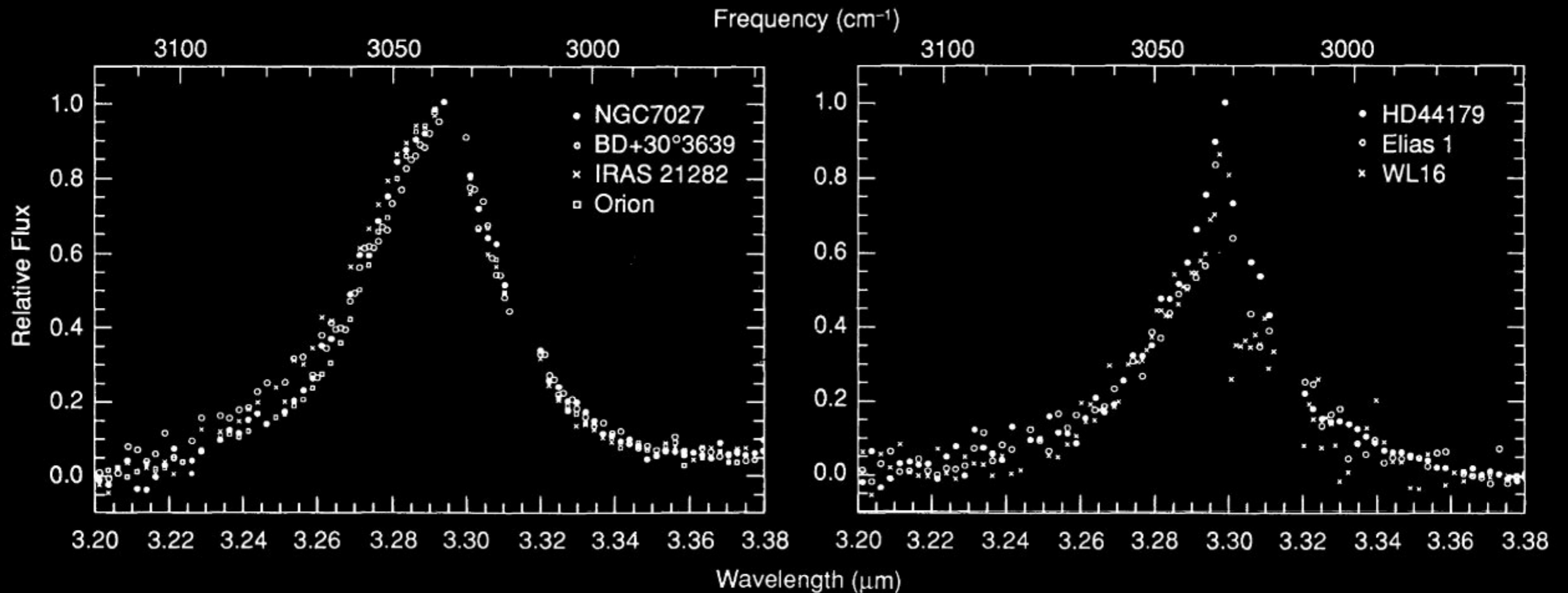


The 3 μm Complex



- C–H stretching vibrations
- Aromatic & aliphatic hydrocarbons

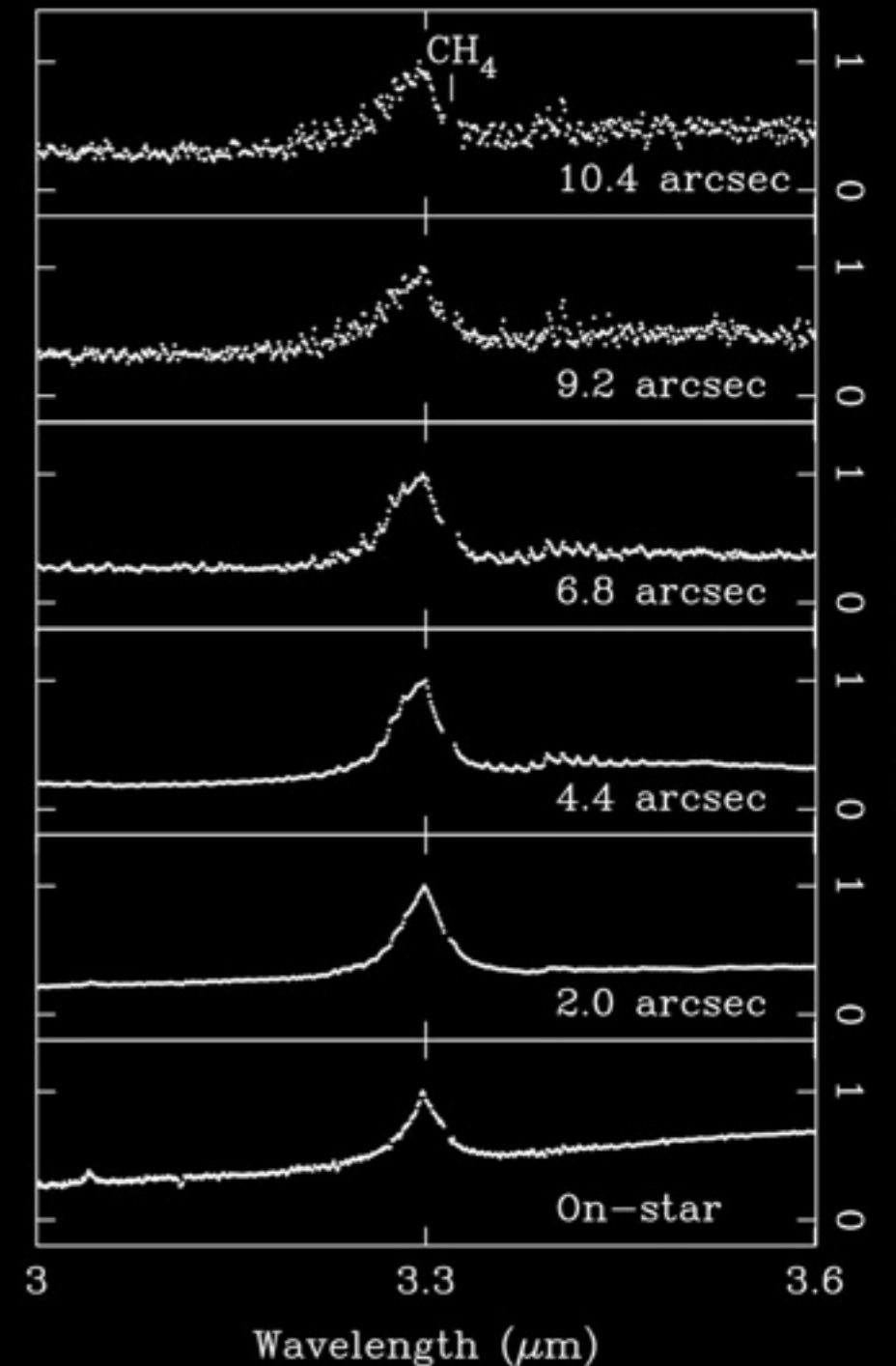
Profile Variations



- Type 1 – Common, asymmetric, broad
- Type 2 – Rare, Lorentzian profile

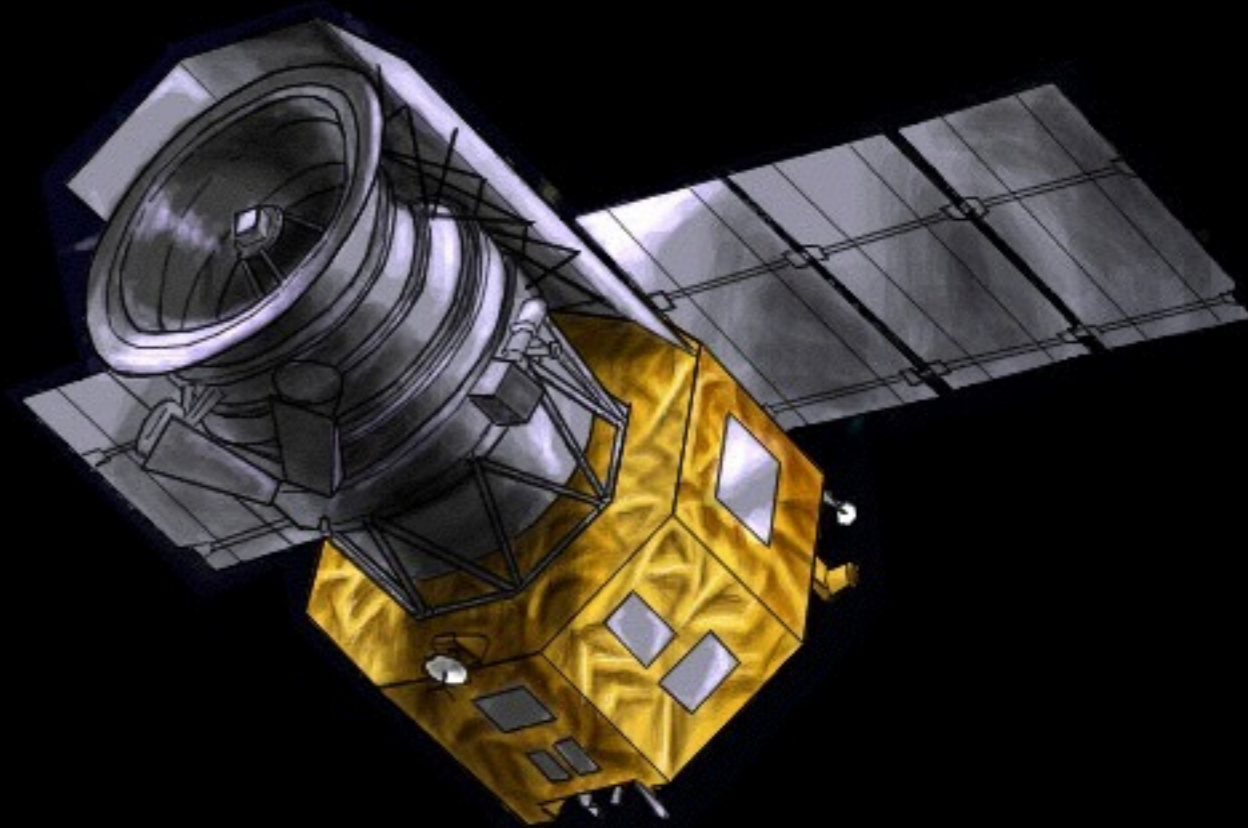
The Song et al Interpretation

- HD 44179 “Red Rectangle”
- 3.3 μm band profile varies with offset
- Composed of two sub-features
 - 3.28 μm and 3.30 μm
- 3.28 μm carrier forms further from central star



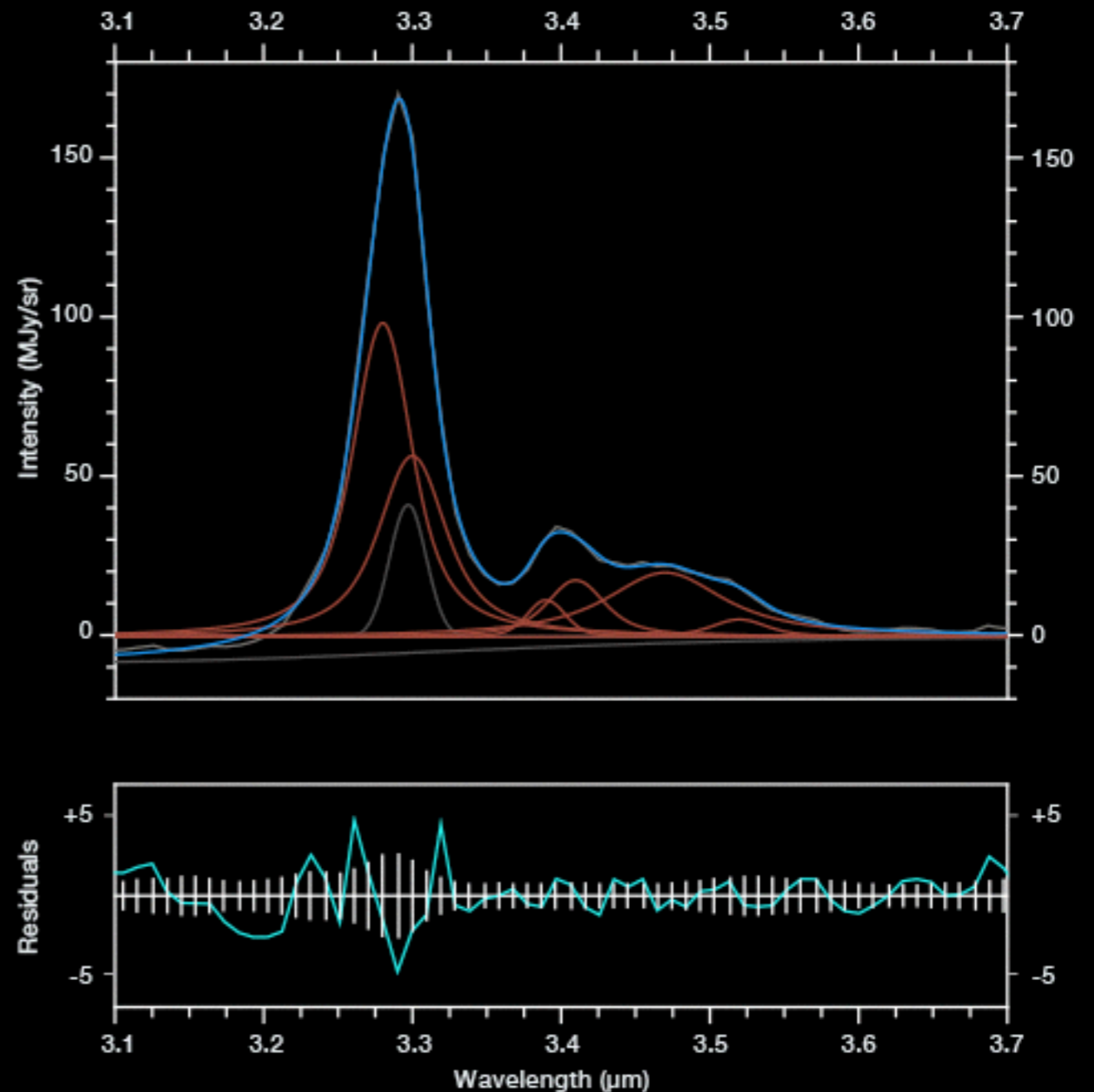
AKARI Data

- AKARI IRC grism spectra
 - 147 Nh spectra
 - 189 Ns spectra
- Selection criteria
 - Good S/N
 - H recombination/ice absorption not too strong
 - No scattered light contamination/image artefacts
- Final Sample - 136 Nh, 172 Ns - 308 total



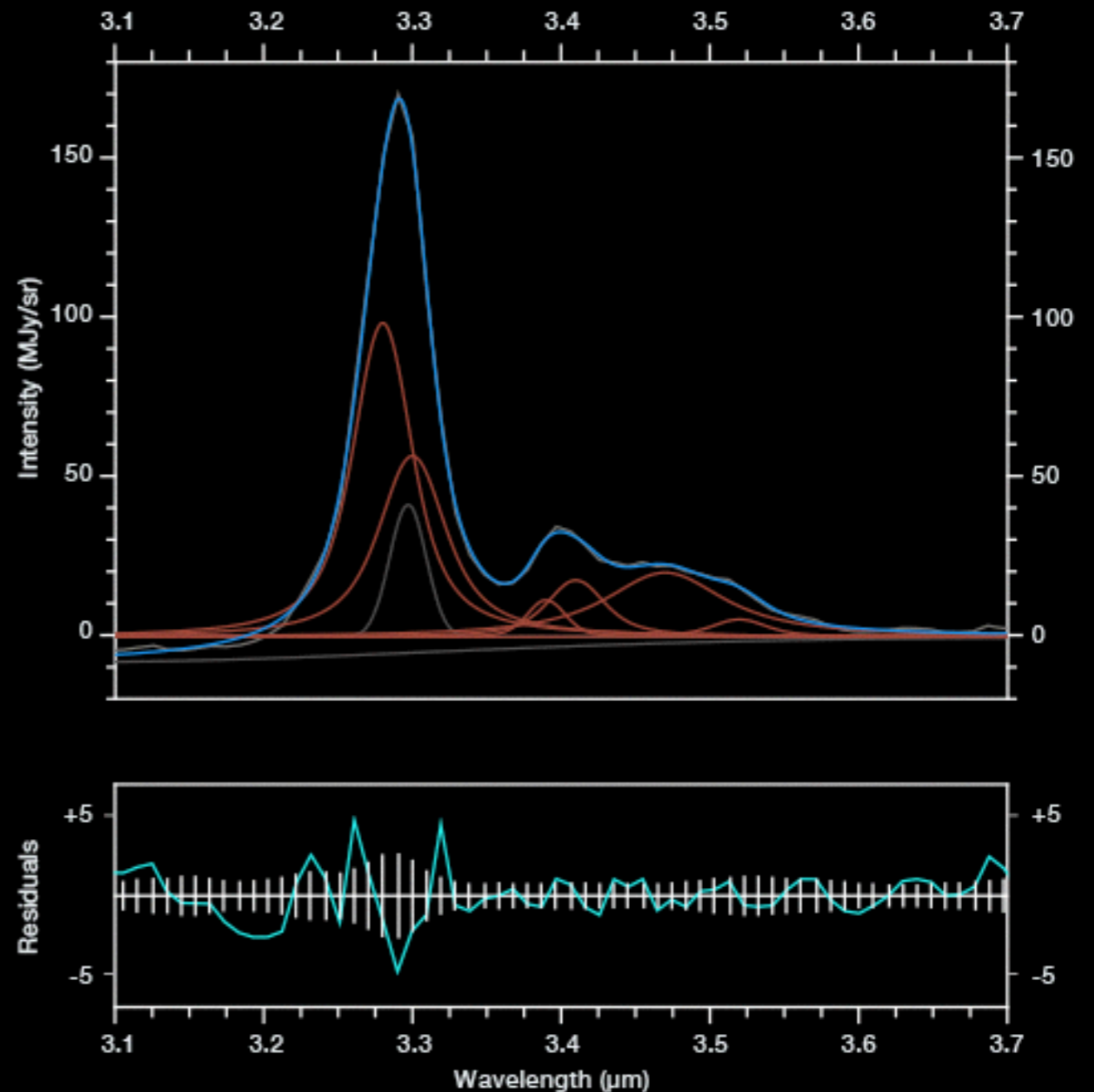
Spectroscopic Decomposition

- Most previous work:
3 Gaussian model
- Fair approximation
- 6 Voigt Profiles
- Fixed Gaussian HW
- $\chi^2_{\text{reduced}} = 2.3$
- $\text{AIC} = 2.7$



Spectroscopic Decomposition

- 3.28 μm • =CH (arom.)
- 3.30 μm • =CH (arom.)
- 3.39 μm • -CH₃ (asym.)
- 3.41 μm • -CH₂- (asym.)
- 3.47 μm • -CH₃ (sym.) ...?
- 3.52 μm • -CH₂- (sym.)



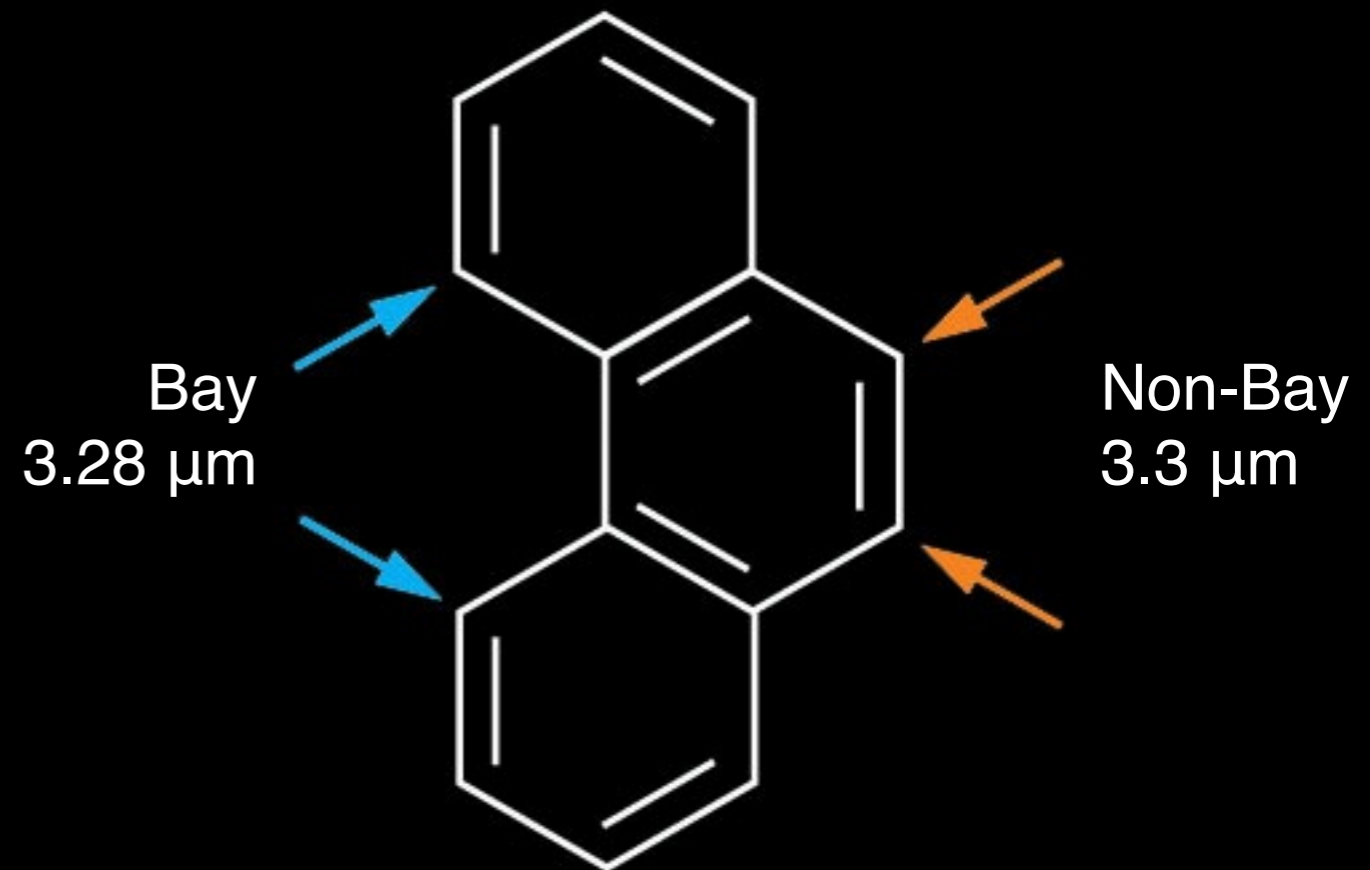
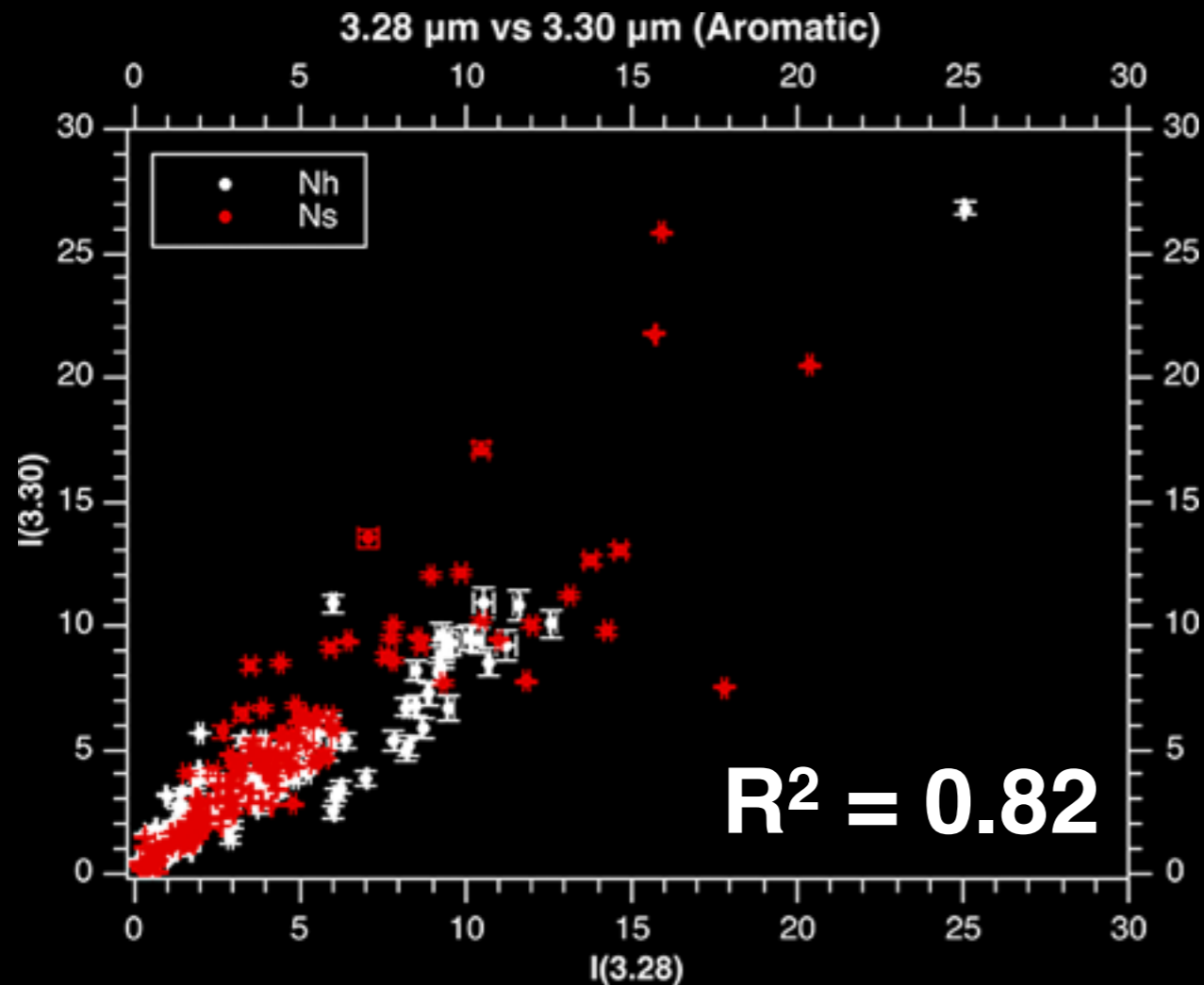
AKARI IRC data

Fit performed using fitted software - Wojdyr (2010)

Assignments based on Gaddallah+ (2012)/Sloan+ (1997)/etc...

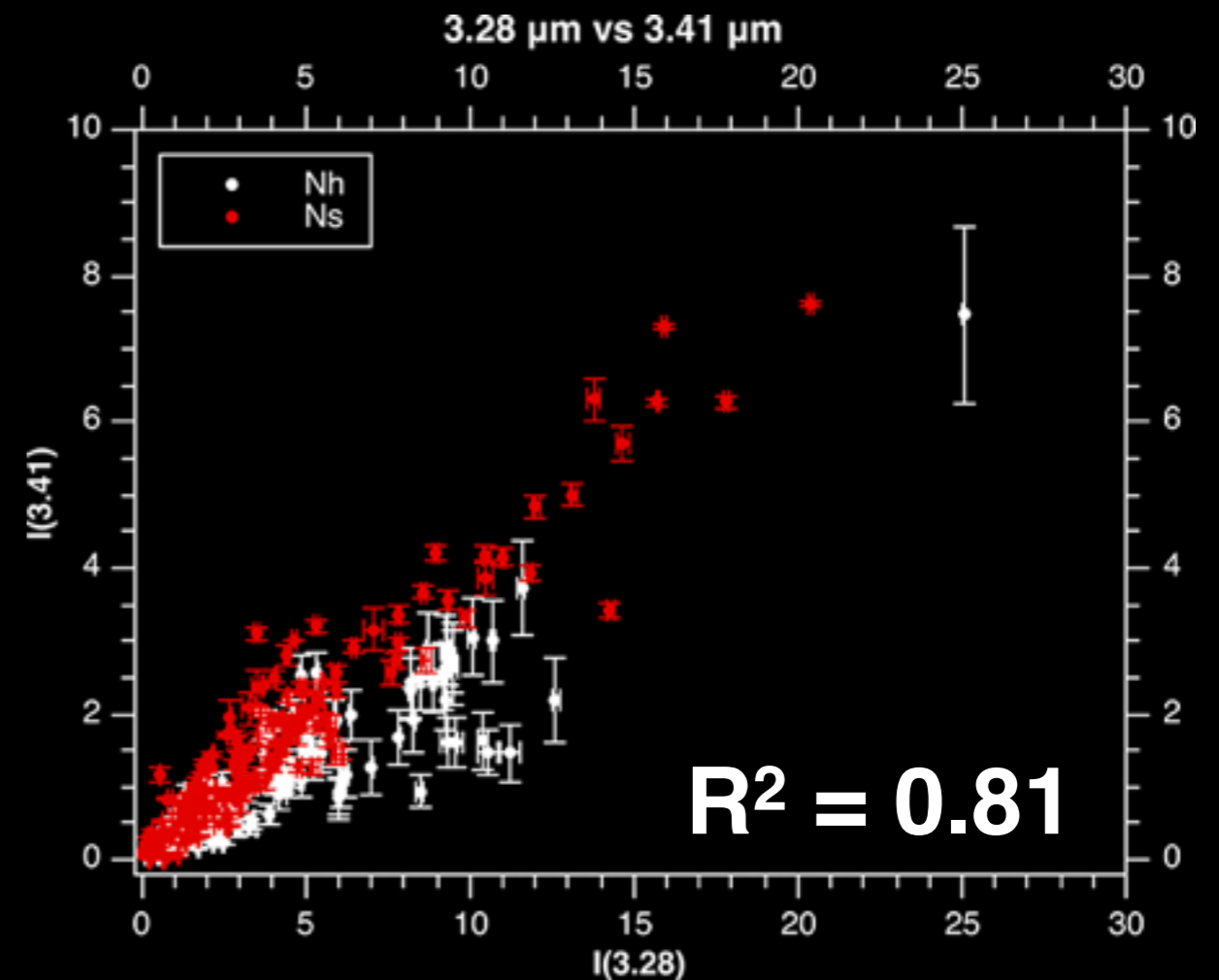
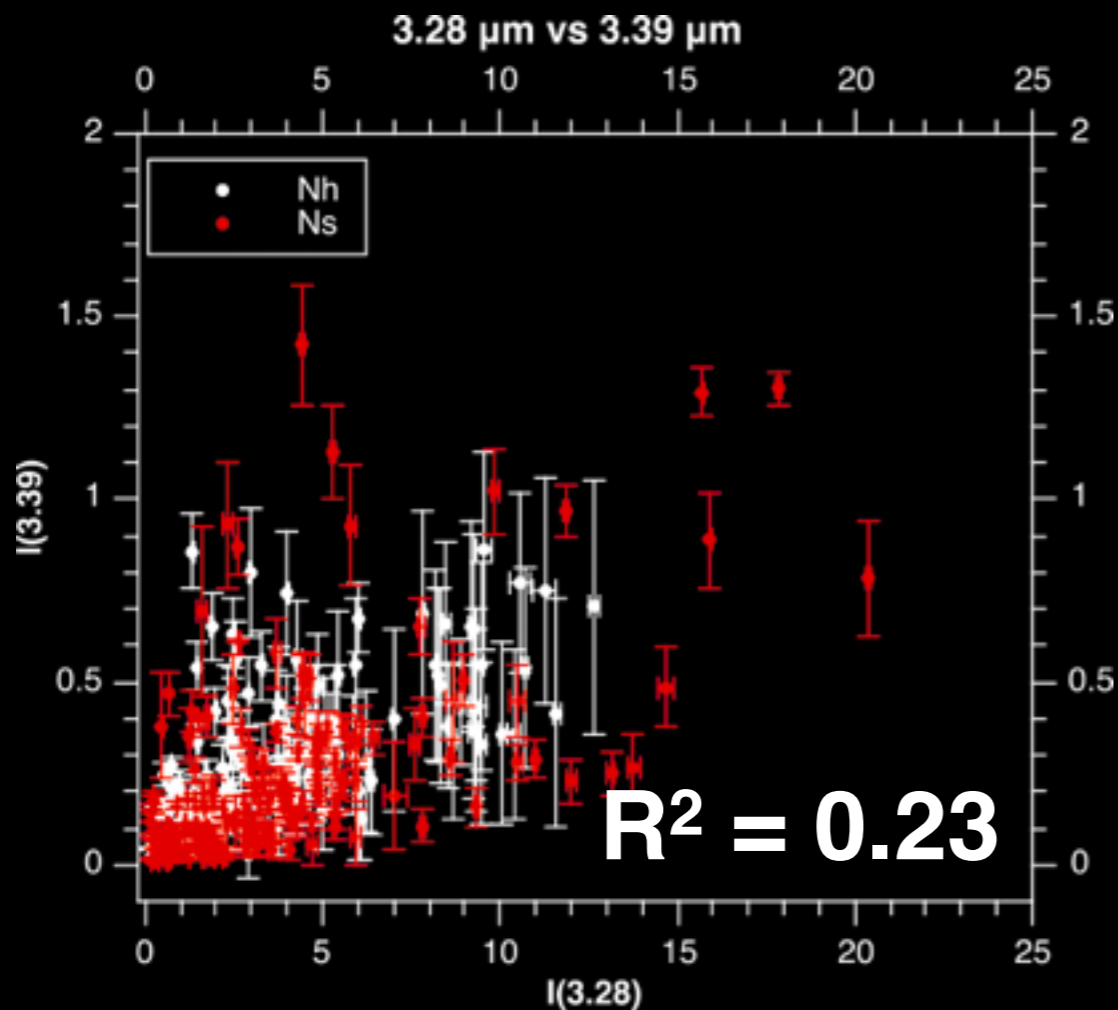
The 3.3 μm Band

Bay Hydrogens



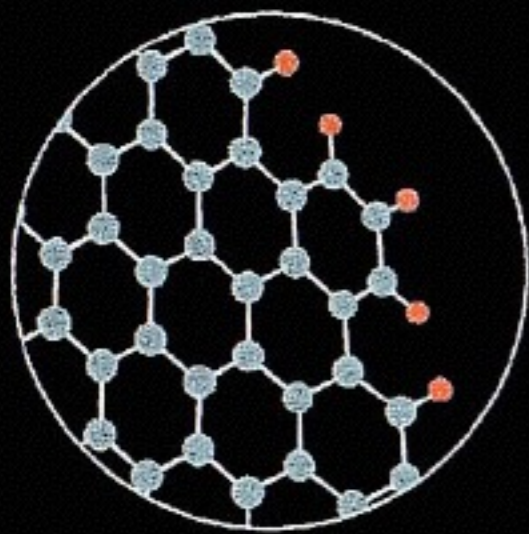
- $I(3.28)$ vs $I(3.30)$ correlate well
- $I(3.28)/I(3.30)$ frequently at unity or above!

Bays and Methylene Groups



- No link with methyl
- Good correlation with methylene!

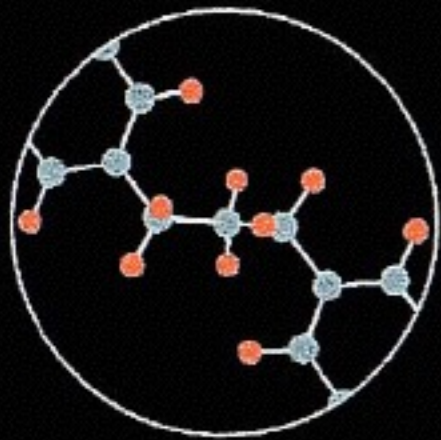
Dust Formation?



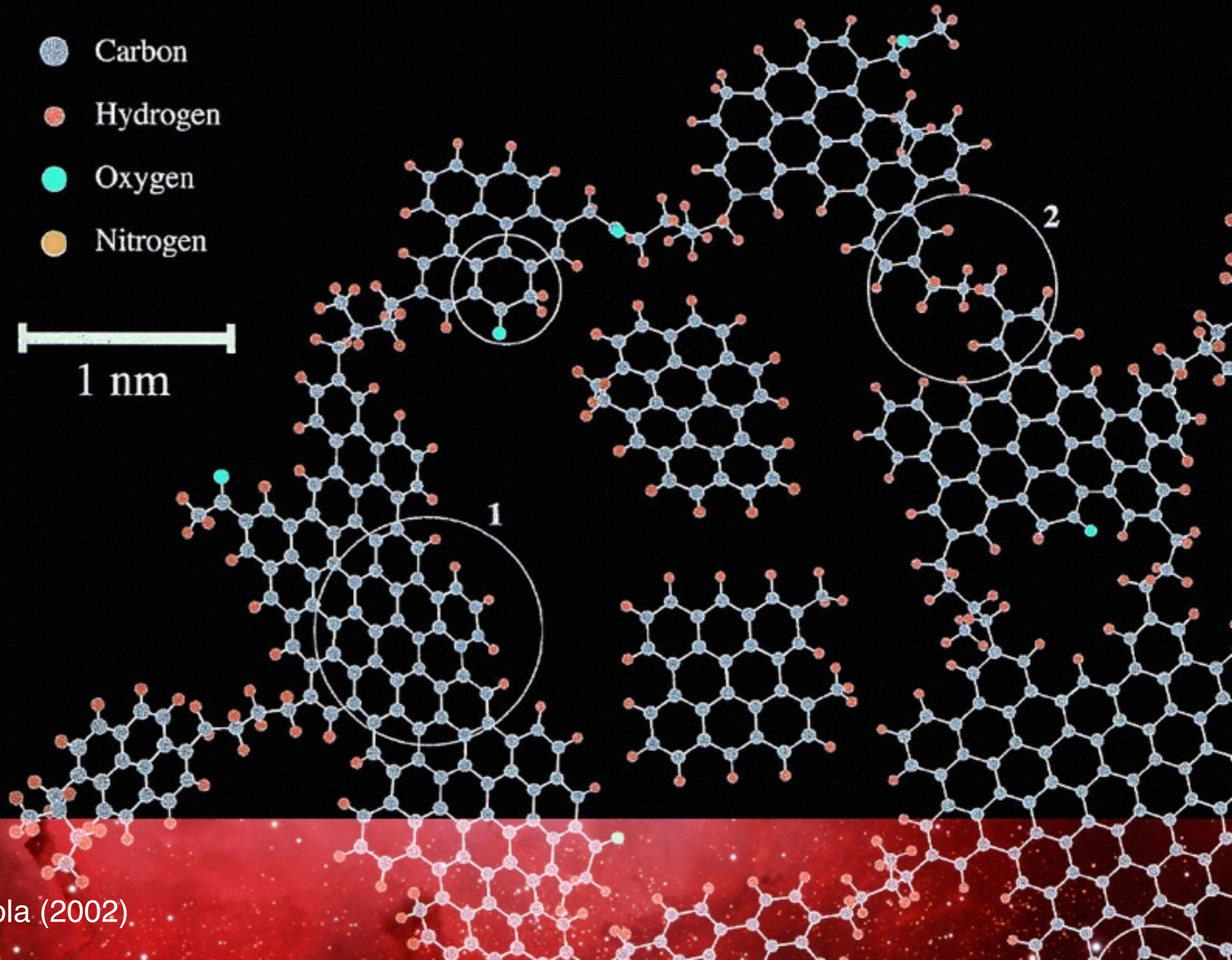
1. Aromatic network

- Carbon
- Hydrogen
- Oxygen
- Nitrogen

1 nm

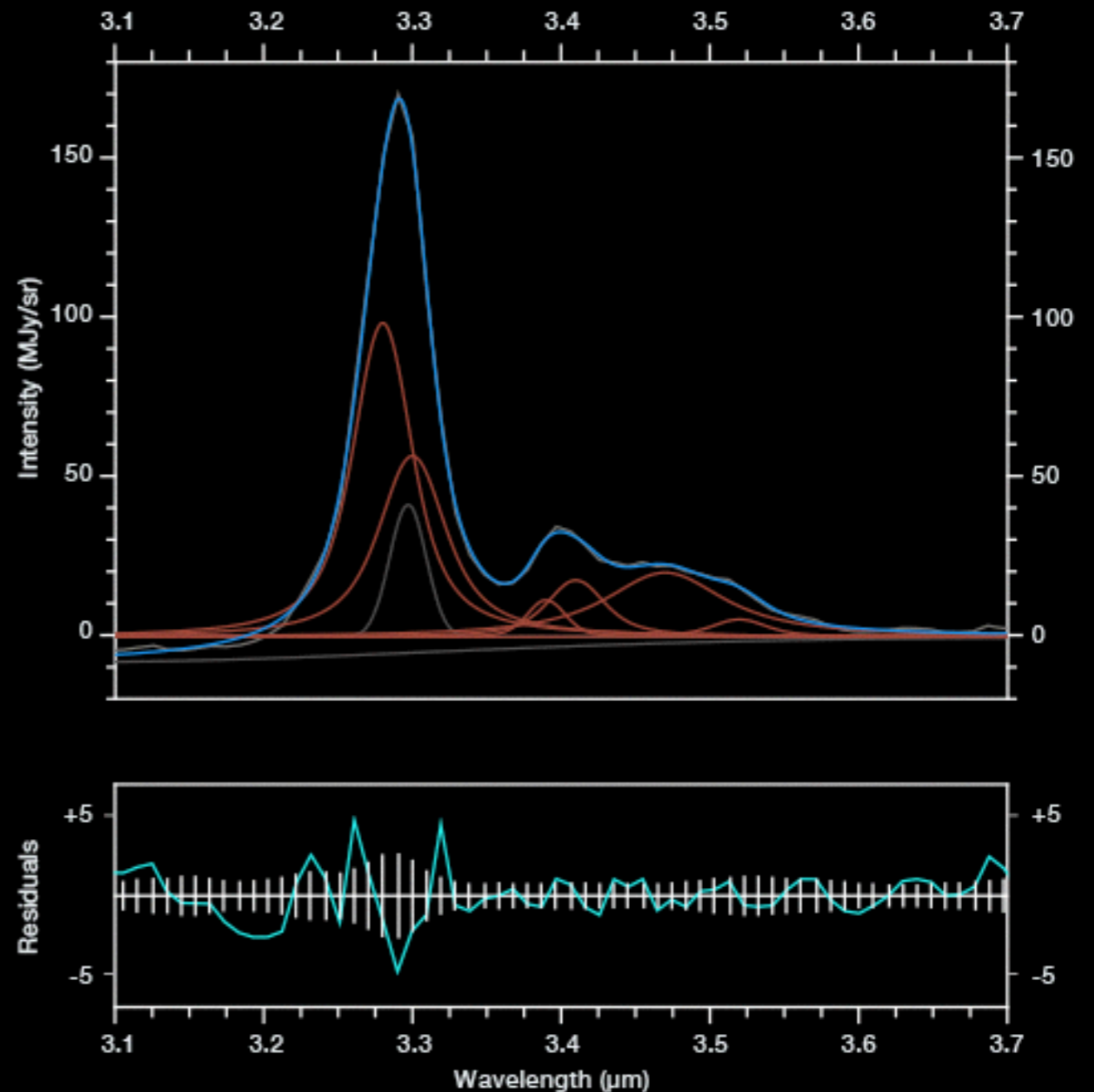


2. Aliphatic bridge

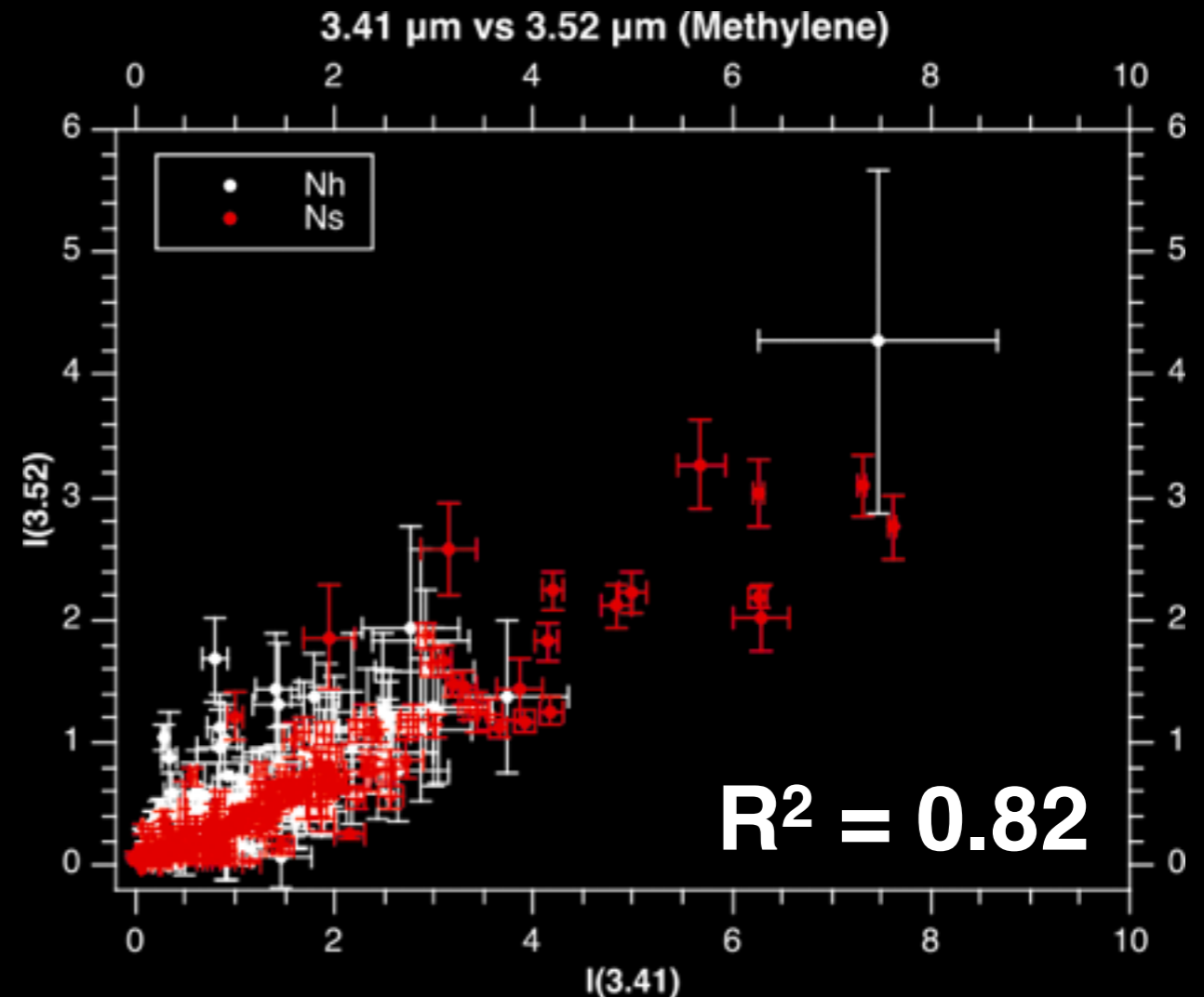
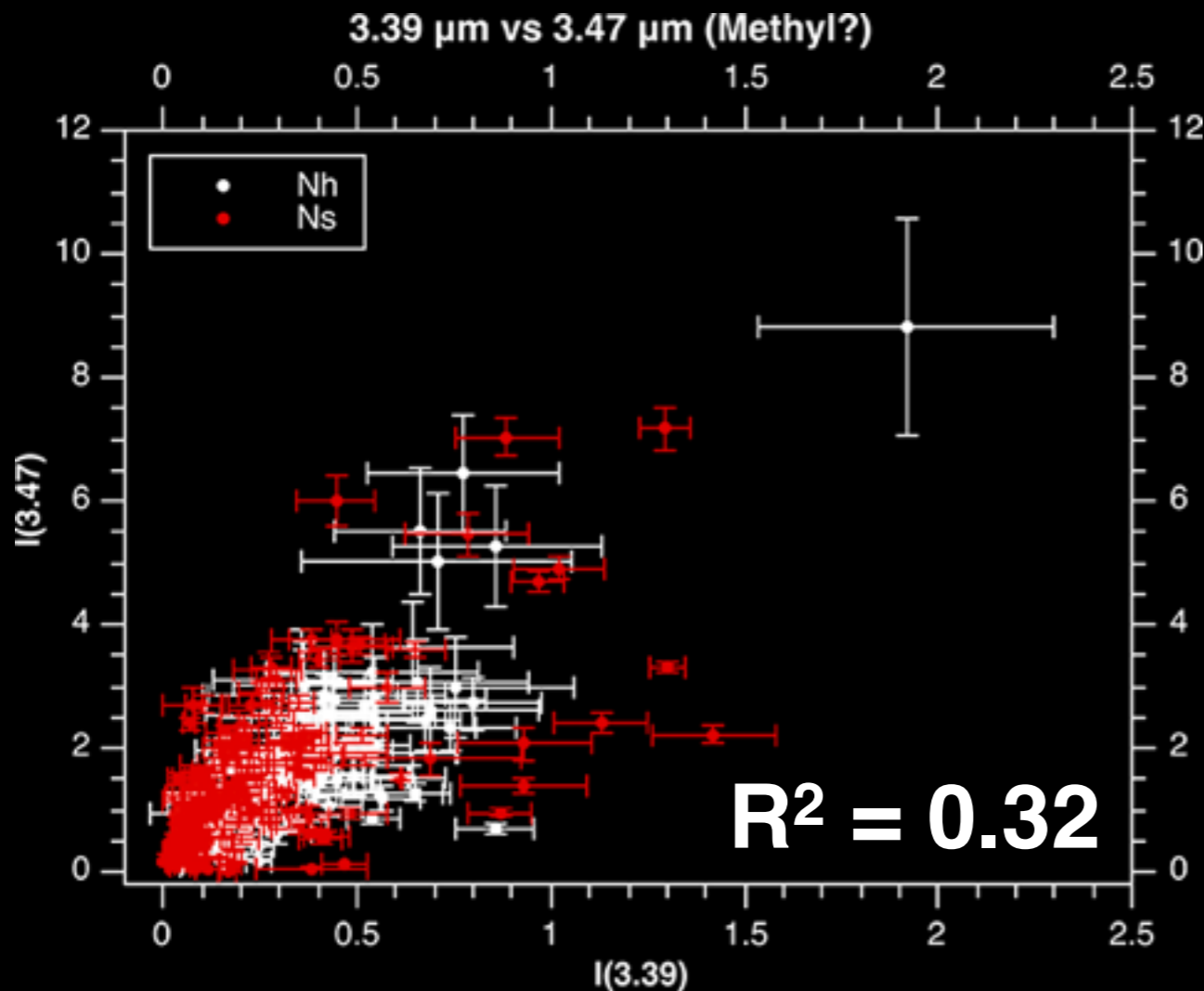


The Aliphatic Stretches

- Methyl (...?)
 - 3.39 μm
 - 3.47 μm
- Methylene
 - 3.41 μm
 - 3.52 μm
- Should give two correlations!

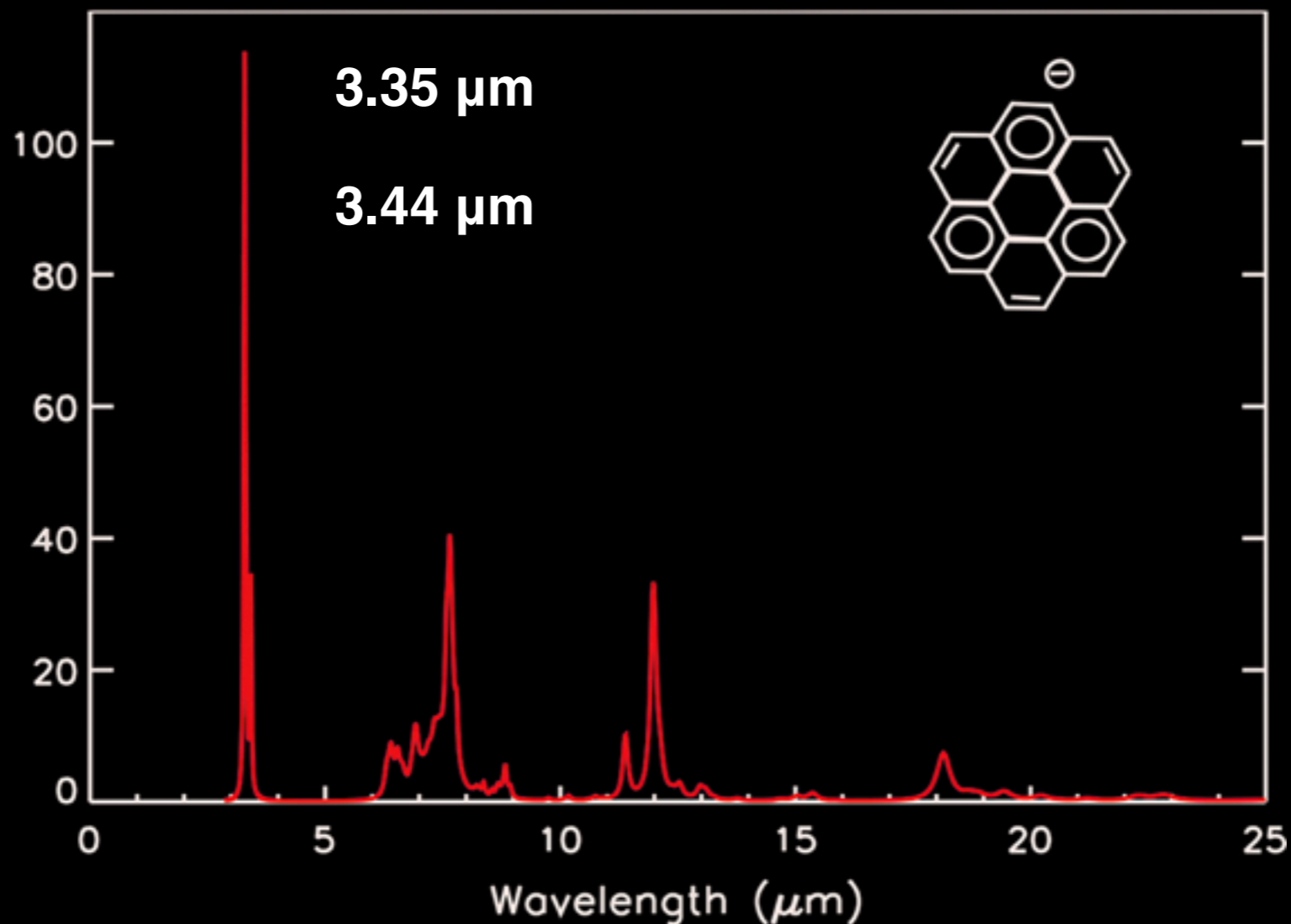


3.47 μm Band Contamination



- Contamination in broad 3.47 μm band?
- Anharmonicity? Other edge structures?

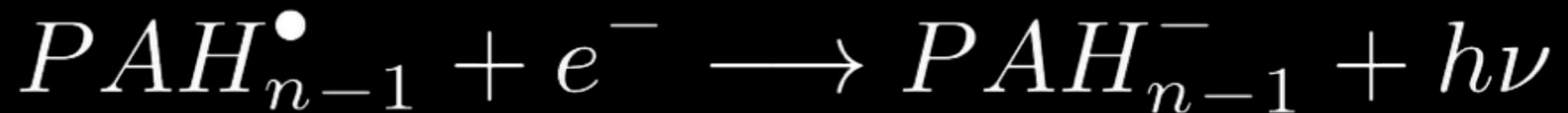
Deprotonated PAHs



- Redward shift on C–H stretches adjacent to deprotonation site

Deprotonation

- Removal of a single proton

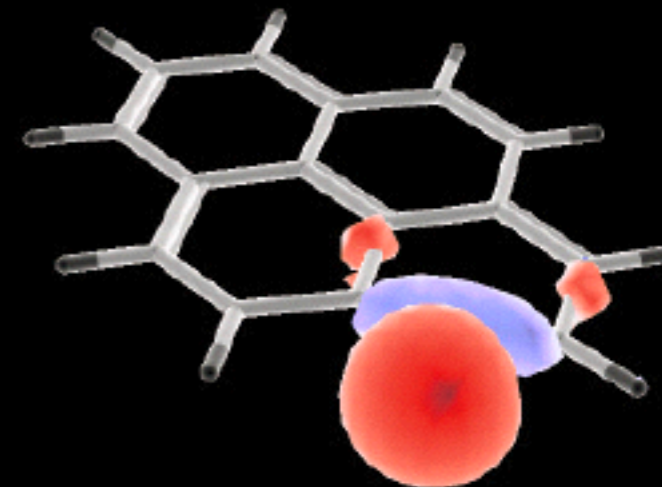


- 2 step mechanism
 - Dehydrogenation (~5-6 eV)
 - Radiative association (~1-2 eV)

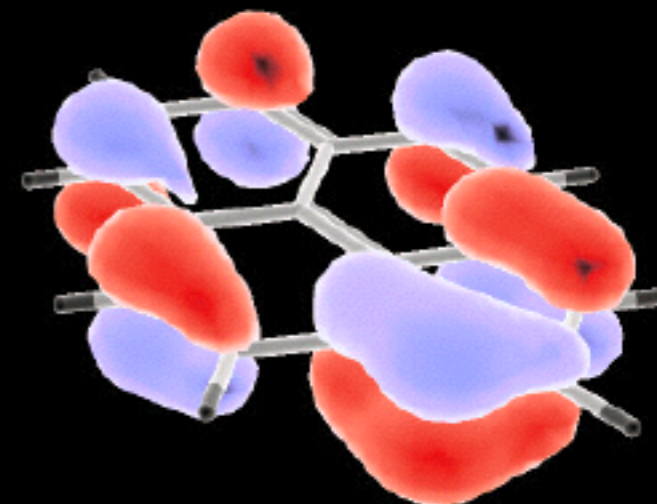
Electronic Structure

- Anionic
- Charge highly localised
- Huge dipole moment!

—
-0.463 eV



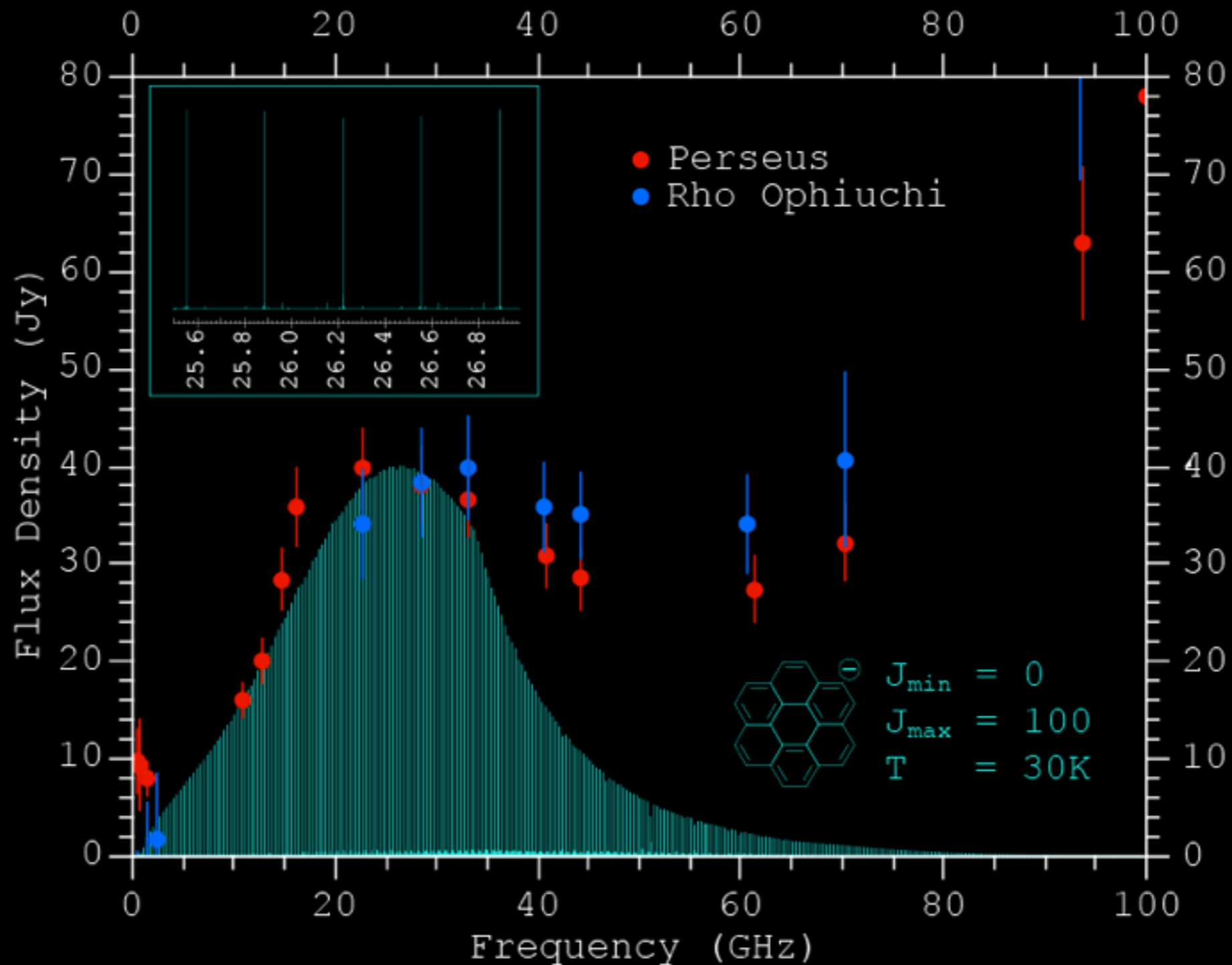
—
-1.578 eV



Dipole Moments

Molecular Anion	H-L Gap (eV)	Detachment Energy (eV)	Dipole Moment (D)
Anthracenyl	2.041	1.45	8.238
Tetracenyl	2.068	1.74	4.990
Pentacenyl	1.878	1.89	3.370
Pyrenyl	1.959	1.26	7.710
Ovalenyl	2.041	1.99	7.792
Circumpyrenyl	2.090	2.09	9.750
Triphenylenyl	2.204	1.45	7.300
Dibenzopyrenyl	2.014	1.64	7.801
Hexabenzocoronenyl	1.252	2.63	12.636
Coronenyl	2.095	1.68	9.929
C ₆ H ⁻	4.381	3.62	7.21

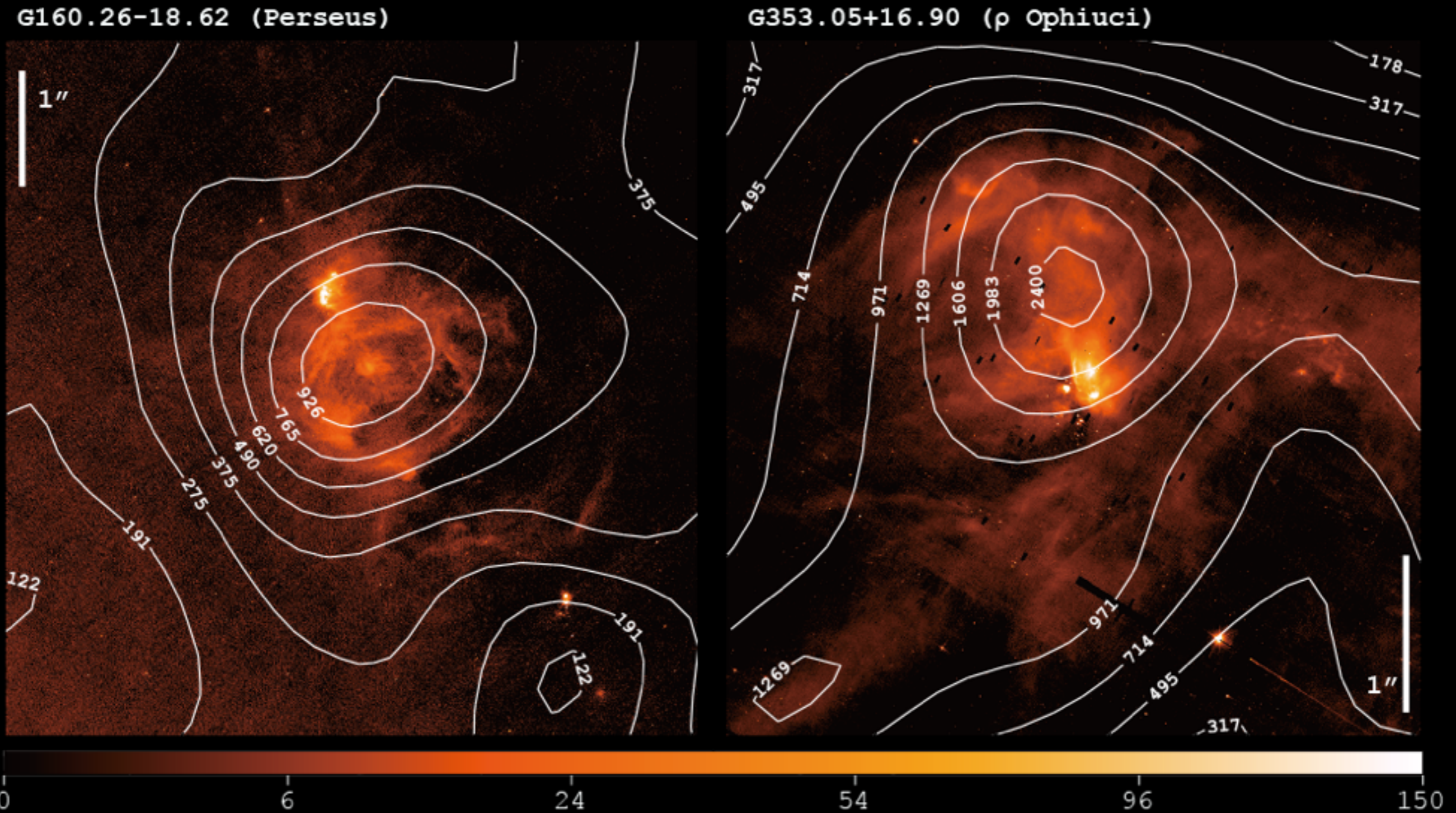
Rotational Spectroscopy



Rotational spectrum calculated using PGOPHER
AME data from Planck Collab. XV (2014)

Deprotonated PAHs and AME

AME Distribution



AKARI IRC 9 μm survey – Ishihara+ (2010)
AME data from Planck Collab. X (2015)

Deprotonated PAHs and AME

Excitation Mechanisms...

- AME vs PAH
 - Spatial distribution comparable
 - Intensities do not correlate
- Different excitation mechanism expected
 - UV photons excite IR emission...
 - ...but destroy anions
 - Anion collisional excitation?

Summary

- Strong contribution from 3.28 μm subfeature in PAHs
 - Probably due to aromatic bay sites
- Also related to 3.41 μm methylene emission
 - Dust formation?
- Deprotonated PAHs have strong rotational emission
 - Potential AME carrier?



Mahalo nui loa!

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with the AKARI and Planck projects.

Quantum chemistry calculations
were performed using the
University of Nottingham HPC Facility

Image credit:

Lagoon Nebula (M8)

ESO/S. Guisard

有り難う御座ります



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THE UNIVERSITY OF TOKYO

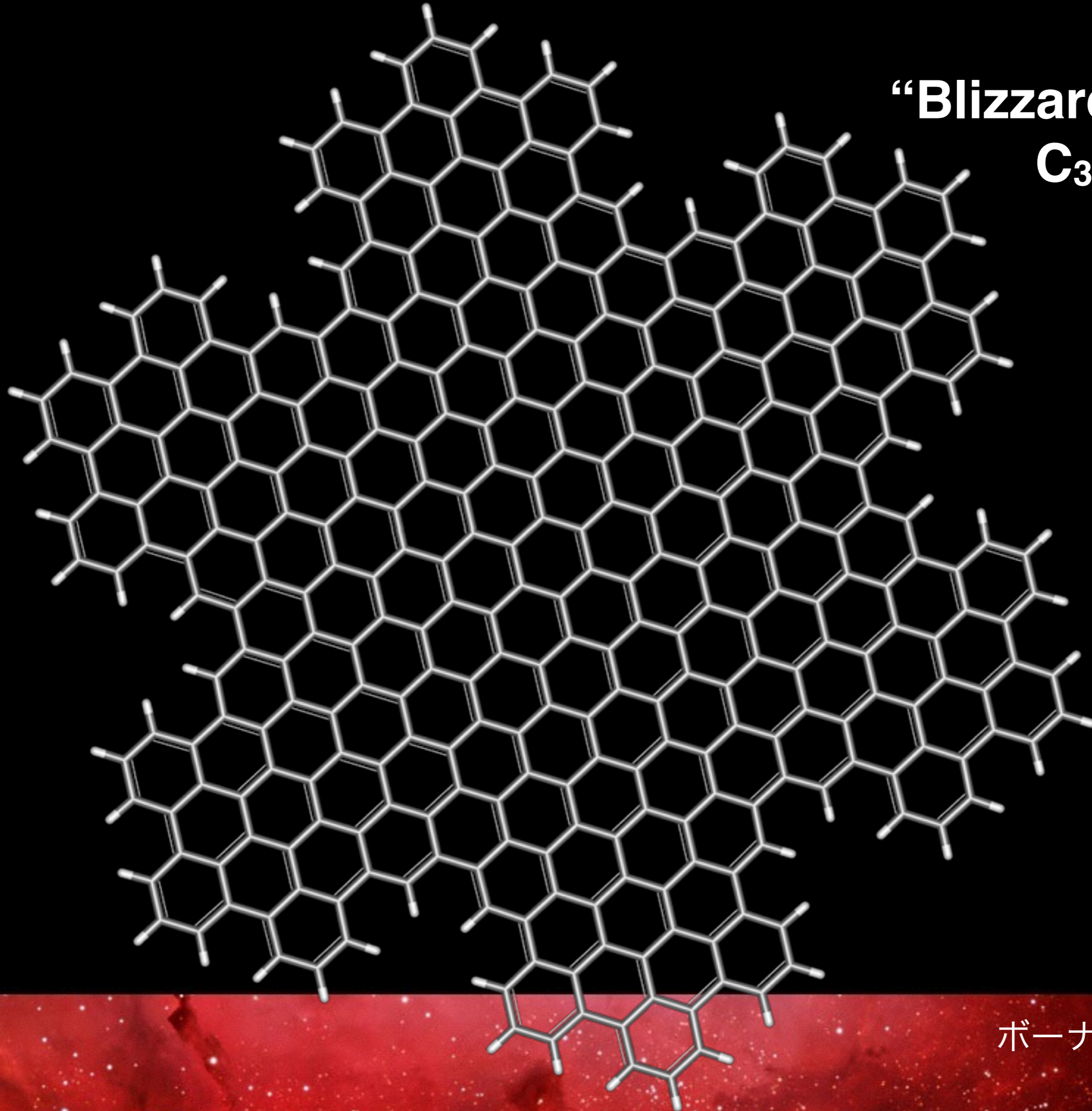


A vibrant, multi-colored nebula, primarily in shades of red and pink, with a dense field of bright stars. The nebula's structure is complex, with various filaments and regions of higher intensity. The stars are scattered throughout, with some appearing as sharp points of light and others as soft, glowing spheres. The overall scene is a rich, cosmic display of interstellar dust and gas.

Bonus Slides!

“Blizzardene”

C₃₃₀H₆₆



ボーナス・スライド

Statistics

	3Gf	4Gf	5L	6L	7Lf	3Vf	5Vf	6V
χ^2	266	284	222	164	118	112	124	266
χ^2_{red}	4.4	5.6	4.4	3.2	2.3	2.2	2.4	2.3
赤 _{corr}	4.8	6.0	4.7	3.6	2.7	2.6	2.8	2.7

- Voigt models perform best
- 3Vf (Voigt analog of Geballe+ 1985)
- 6V a good compromise of statistics and information obtained