

# Interstellar PAHs

## *Observations*

Andrew Burkhardt, Sergei Kalenskii  
Anthony Remijan

## *Modeling*

Christopher Shingledecker, Andrew Burkhardt  
Eric Herbst

## *Laboratory*

K. L. Kelvin Lee, Michael McCarthy

Pre-SOFIA



Brett A. McGuire  
NRAO Hubble Fellow

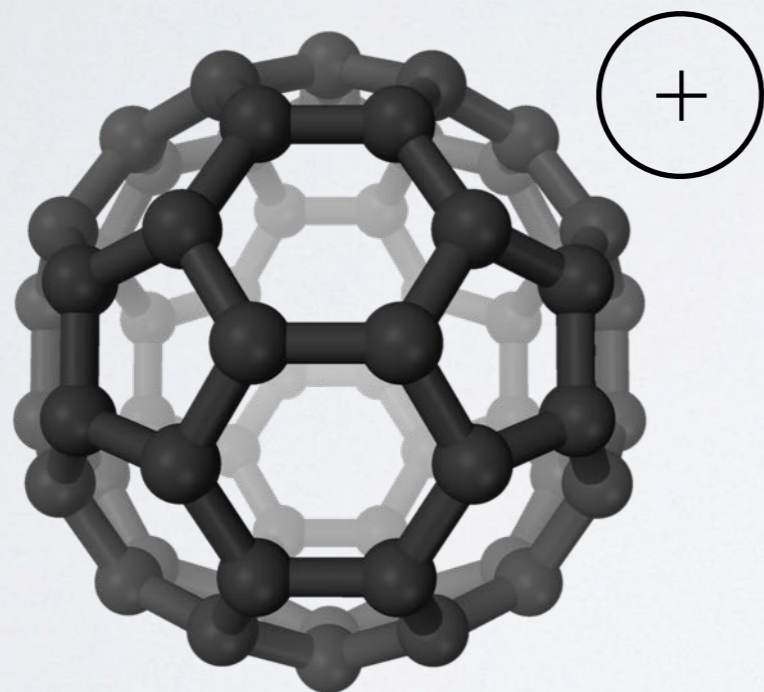


# LETTER

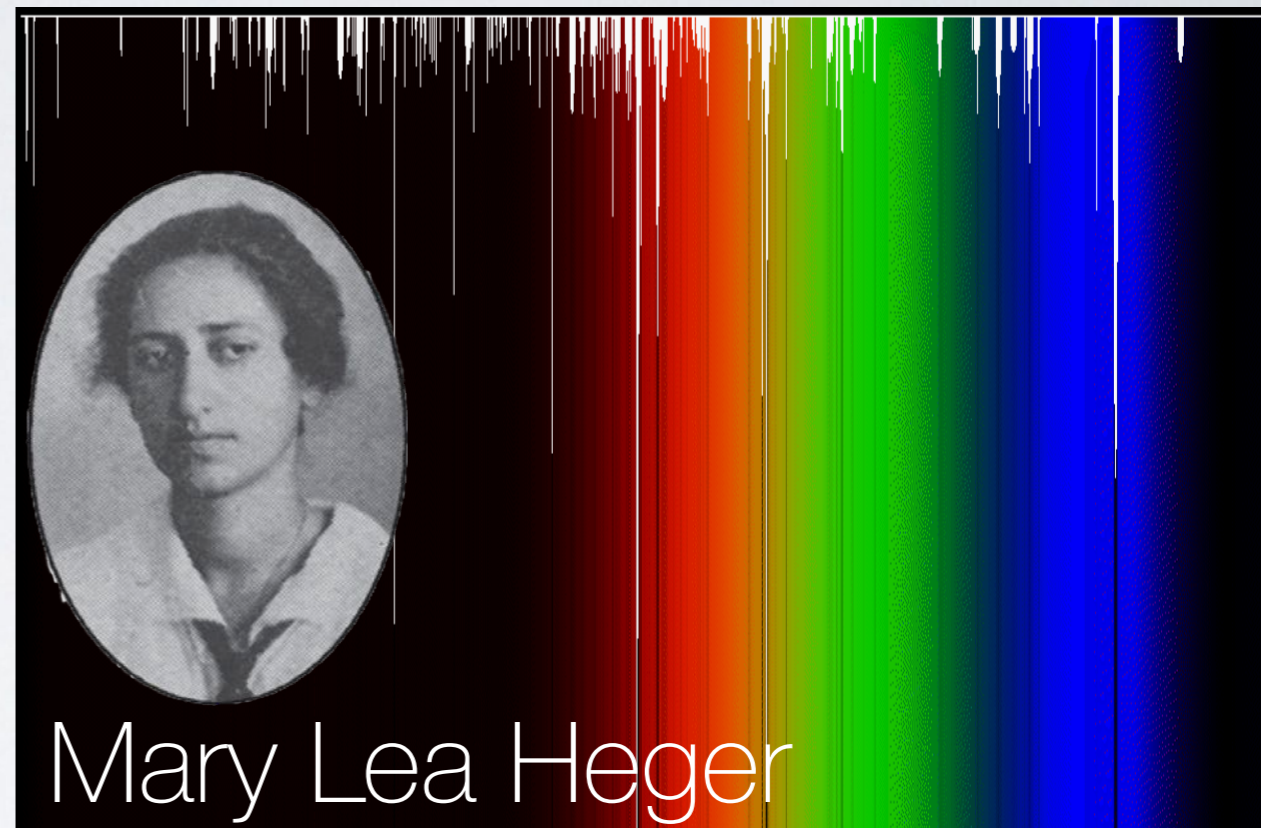
doi:10.1038/nature14566

## Laboratory confirmation of $C_{60}^+$ as the carrier of two diffuse interstellar bands

E. K. Campbell<sup>1</sup>, M. Holz<sup>1</sup>, D. Gerlich<sup>2</sup> & J. P. Maier<sup>1</sup>



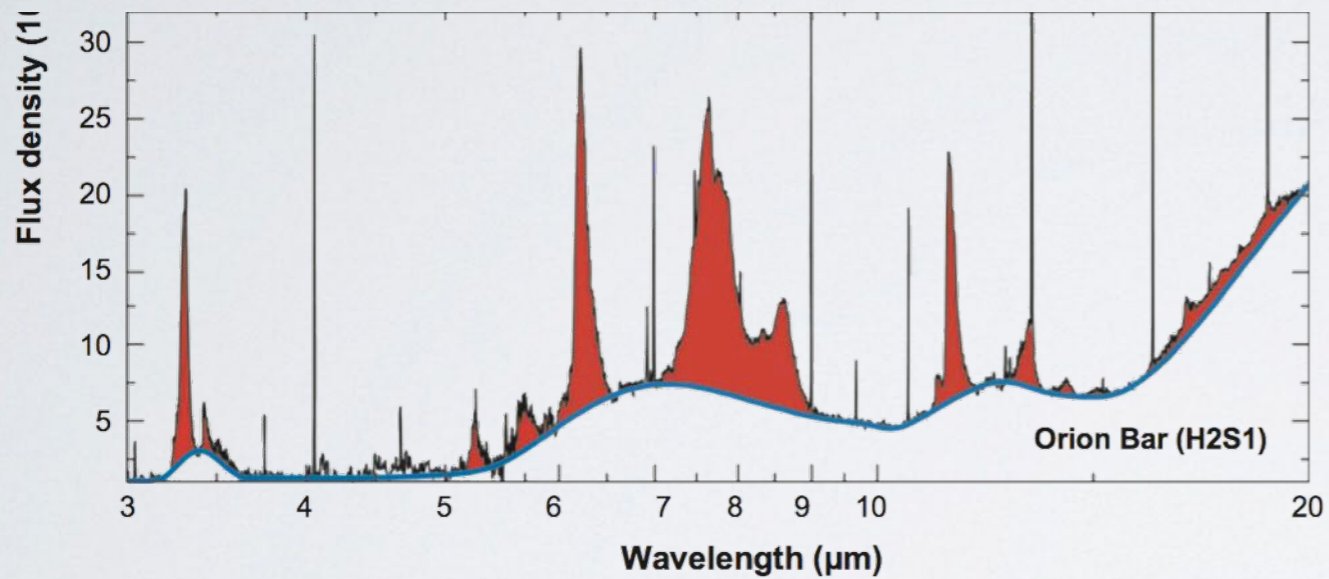
# Diffuse Interstellar Bands 1920s



- ✓ Individual Carrier
- ✗ General Composition



# Unidentified Infrared Bands 1980s



- ✗ Individual Carrier
- ✓ General Composition

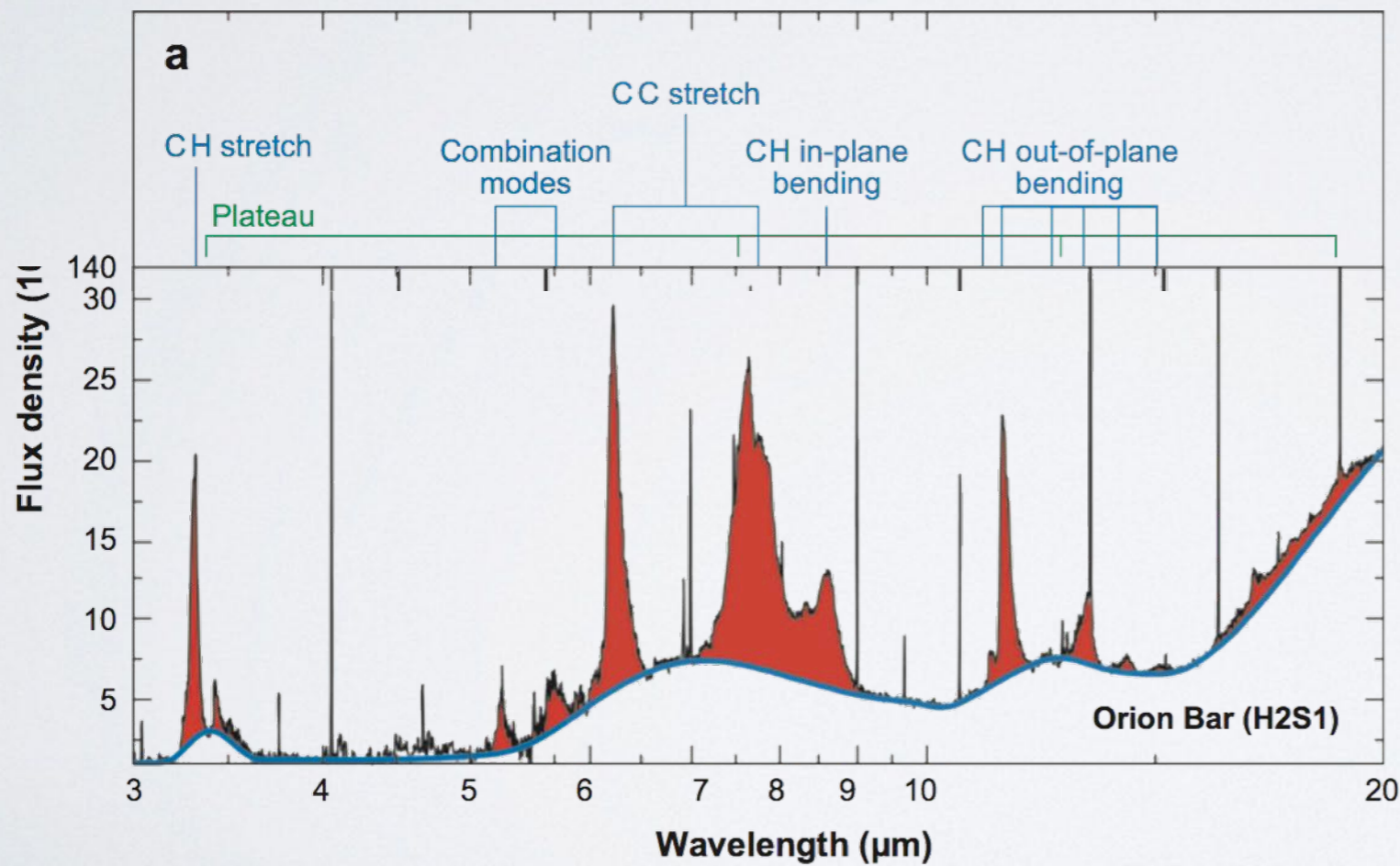
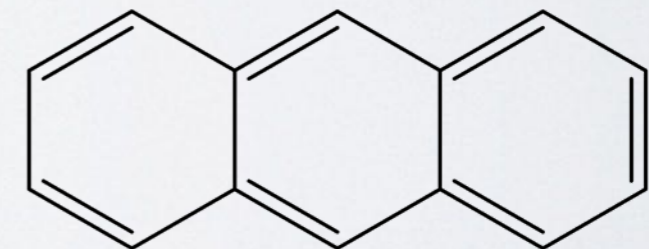
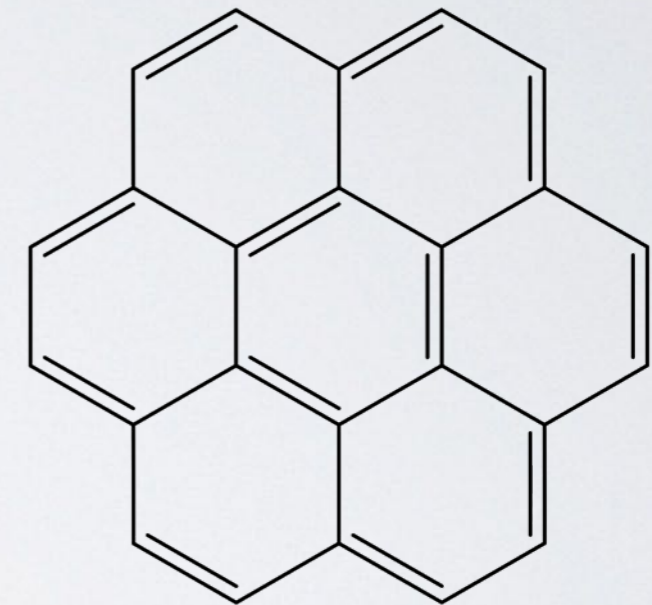
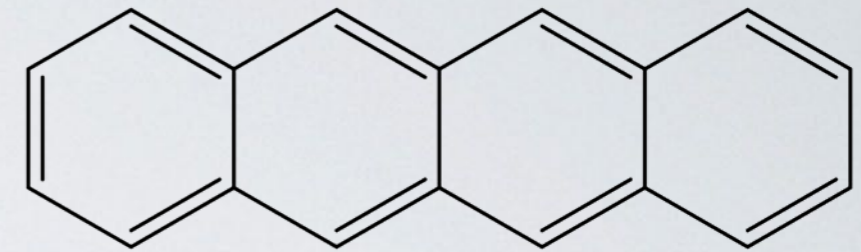
# Diffuse Interstellar Bands 1920s



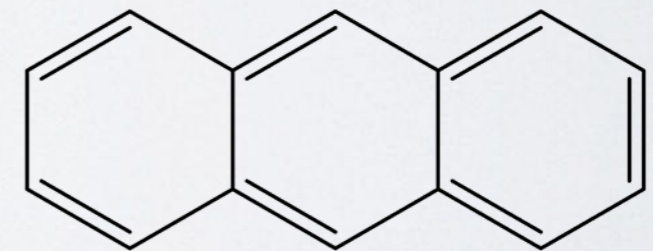
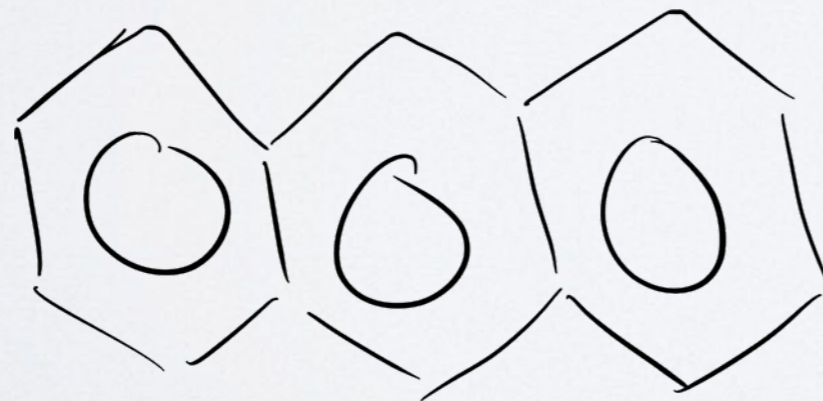
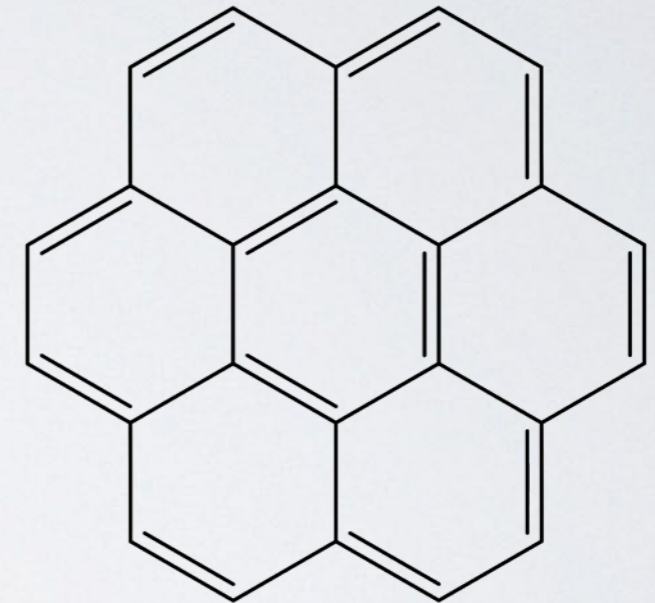
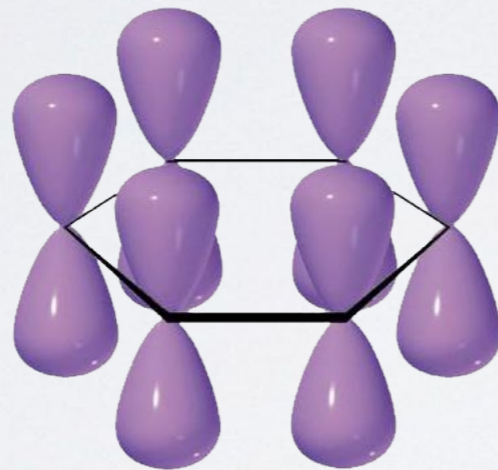
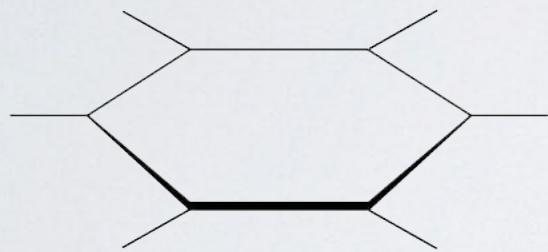
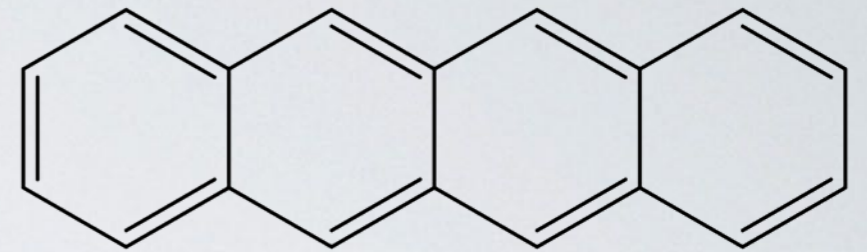
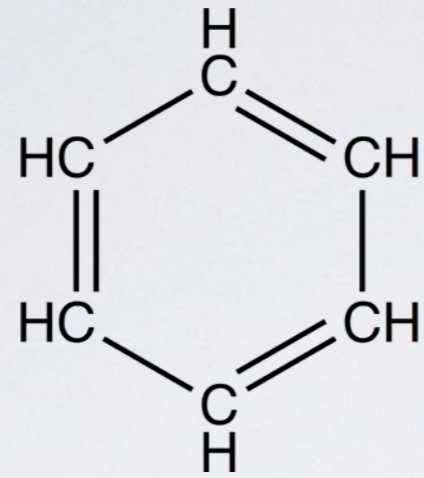
- ✓ Individual Carrier
- ✗ General Composition



# Polycyclic Aromatic Hydrocarbons (PAHs)

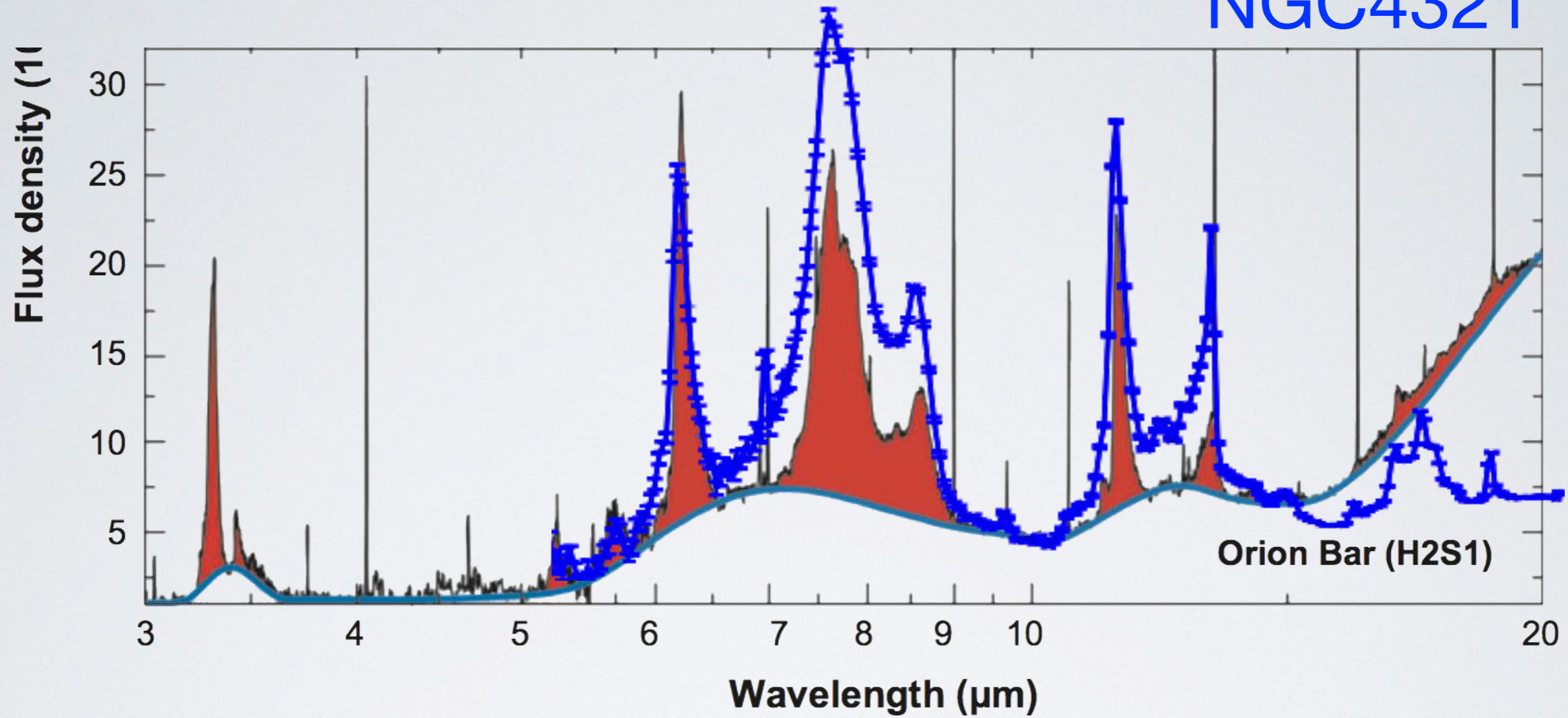




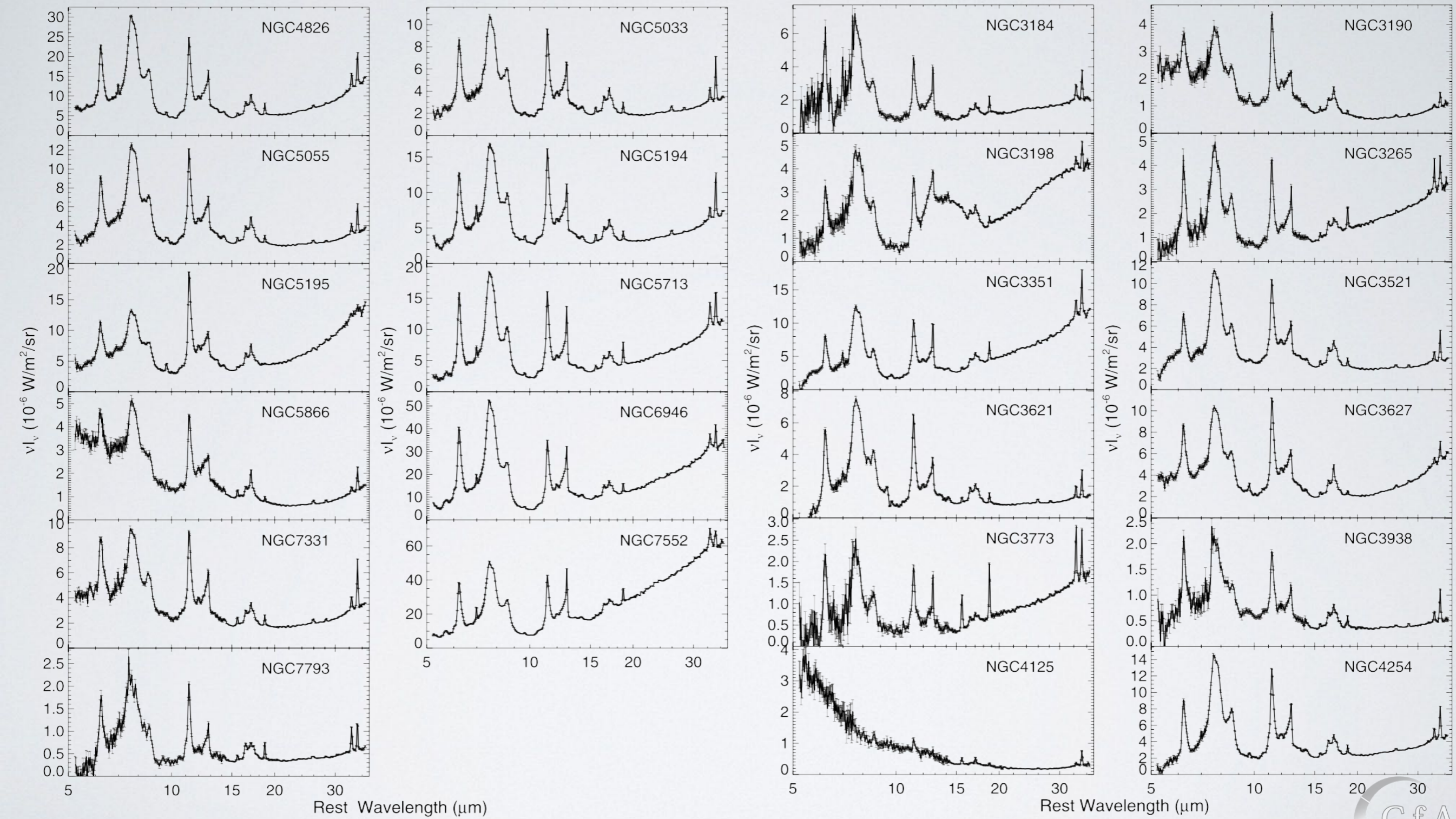




# NGC4321

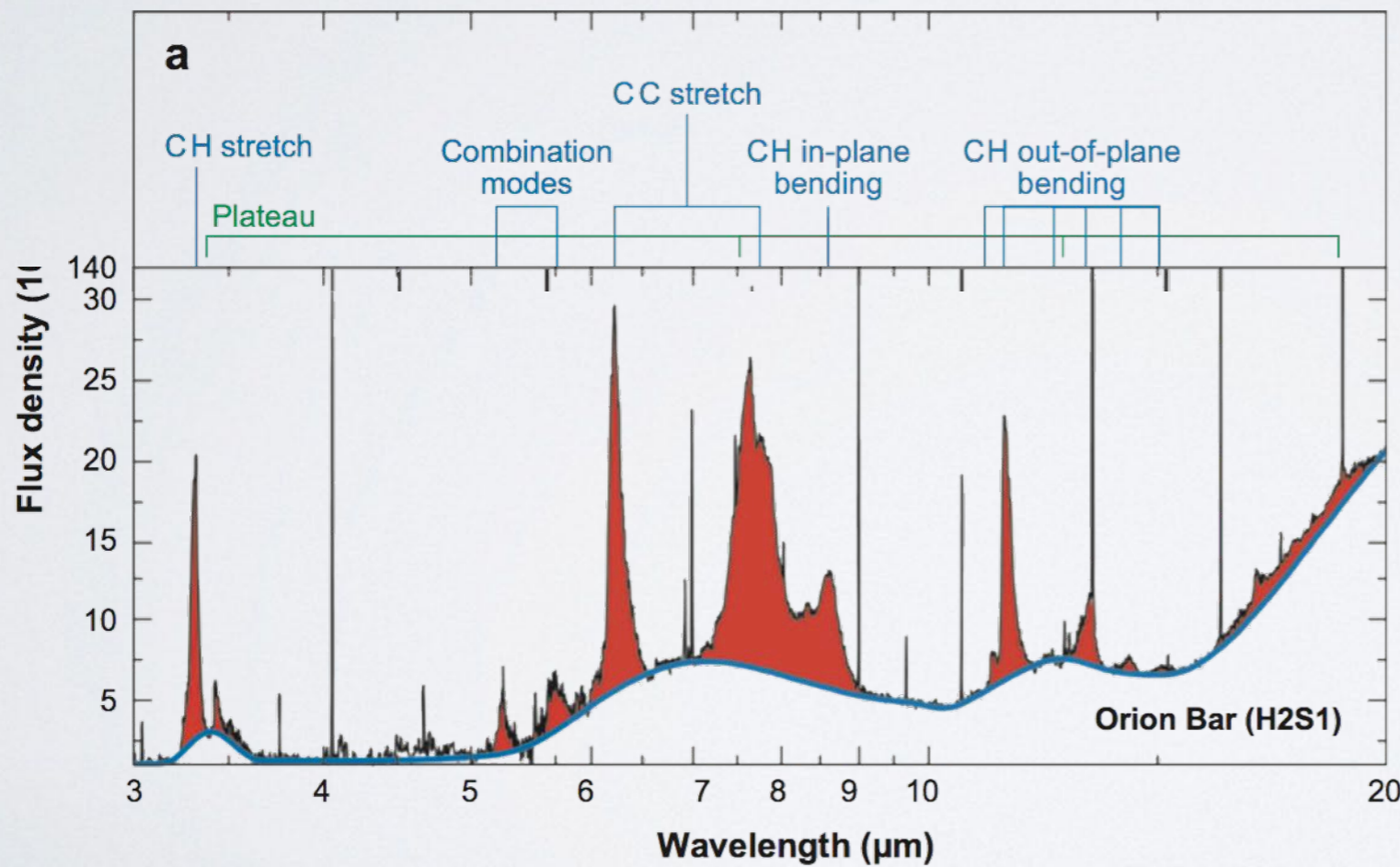
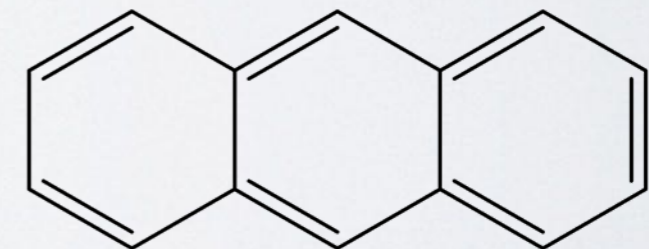
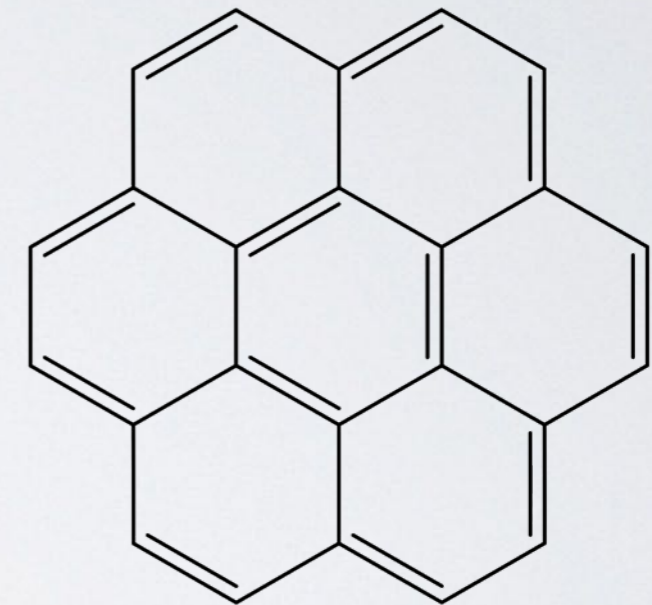
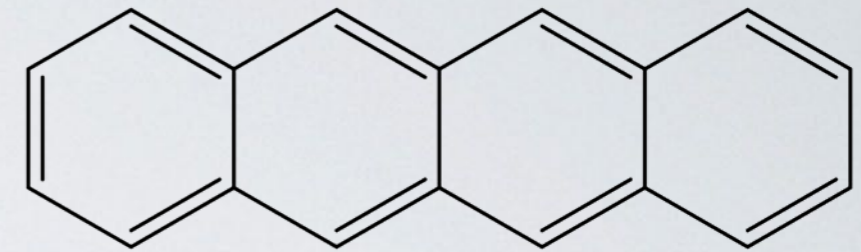




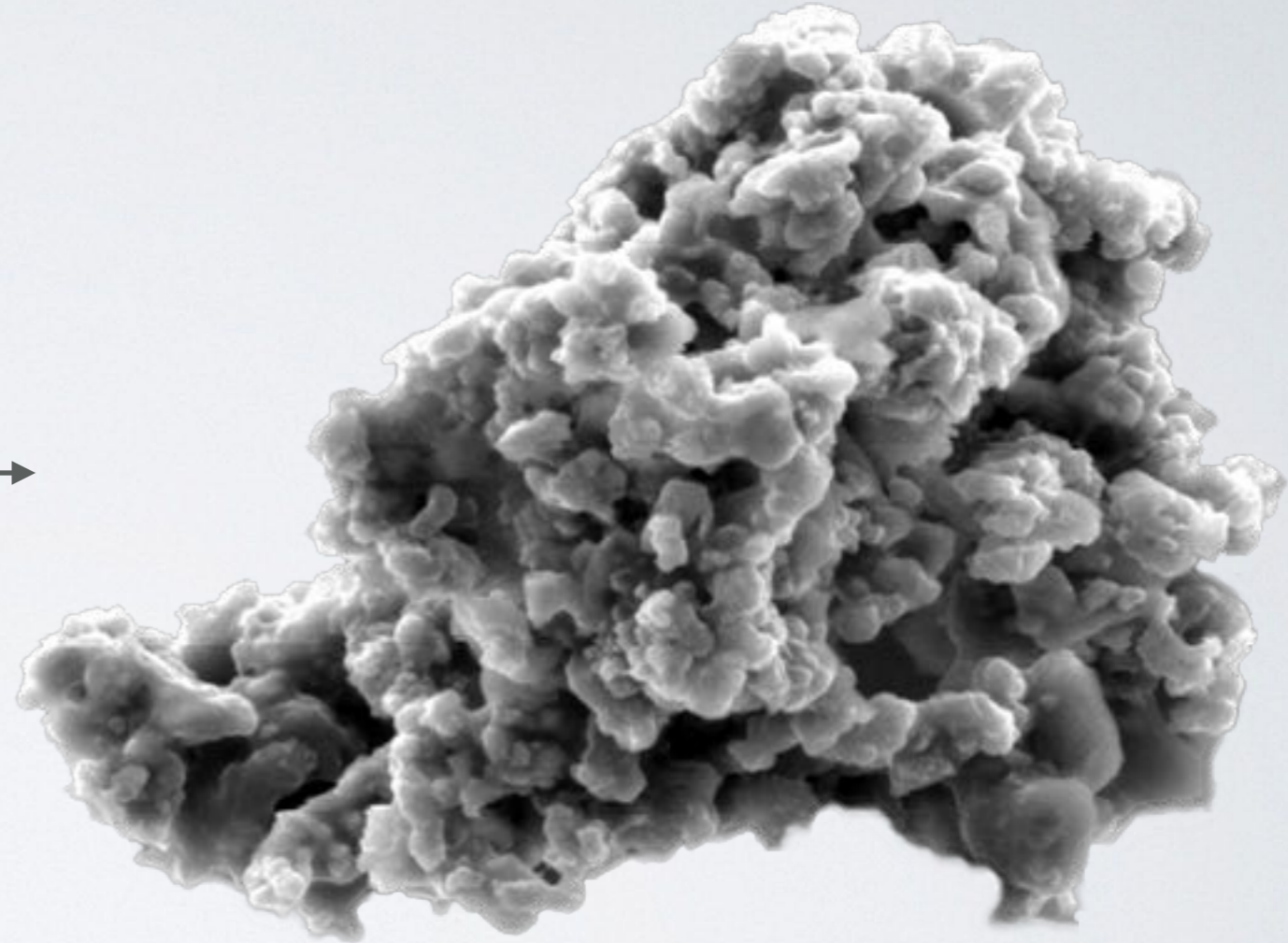
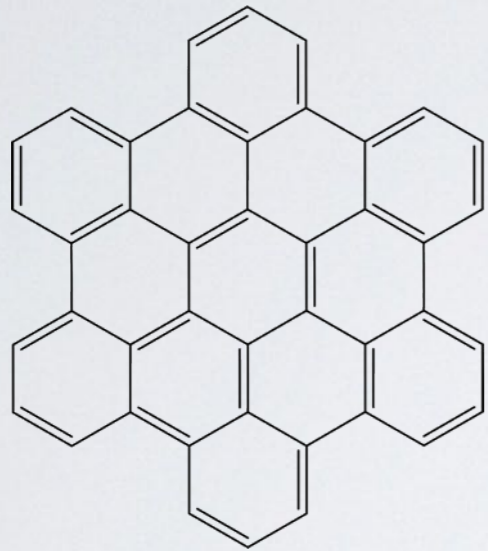




~10% of carbon in  
the Universe locked  
up in PAHs

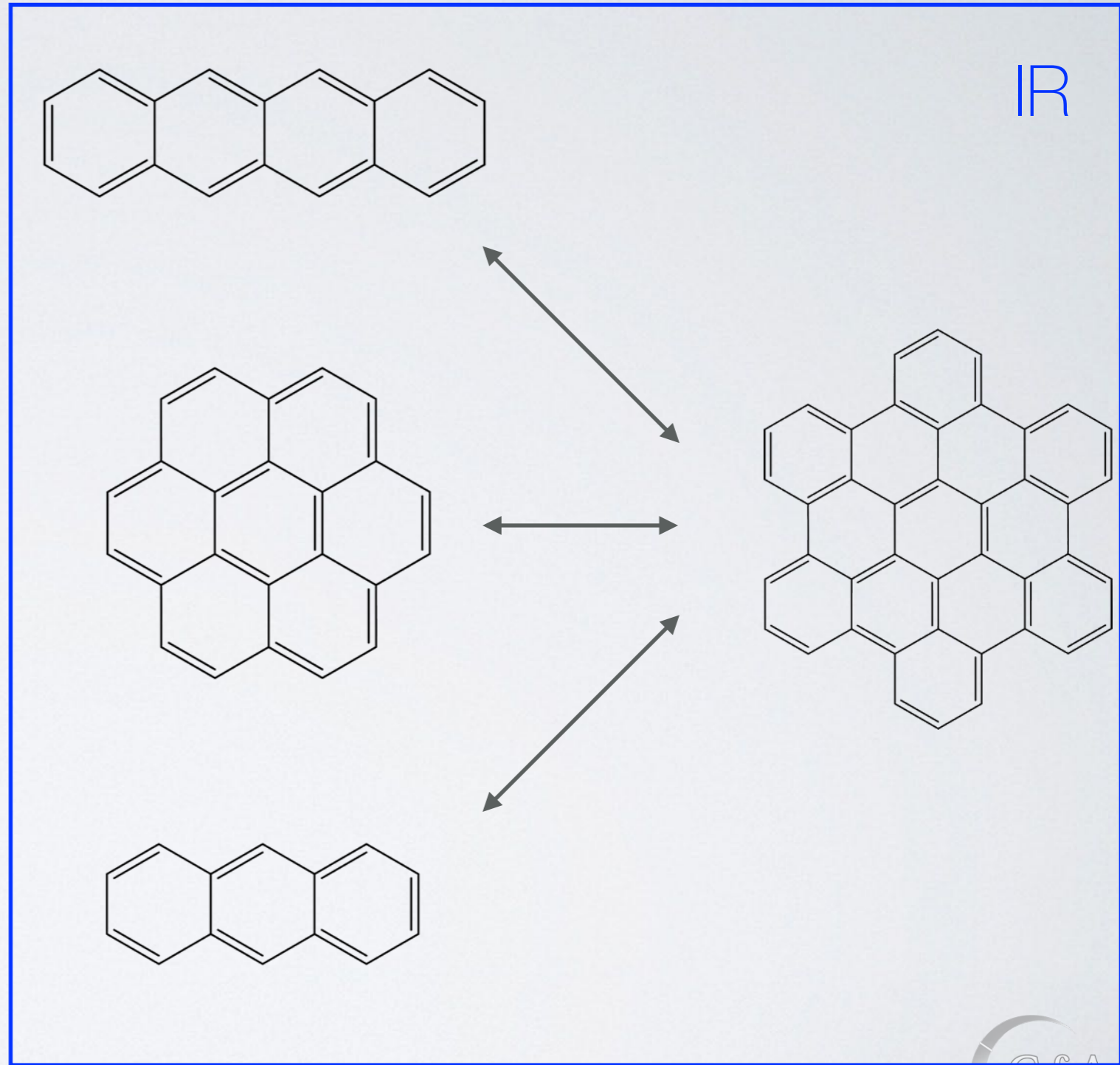
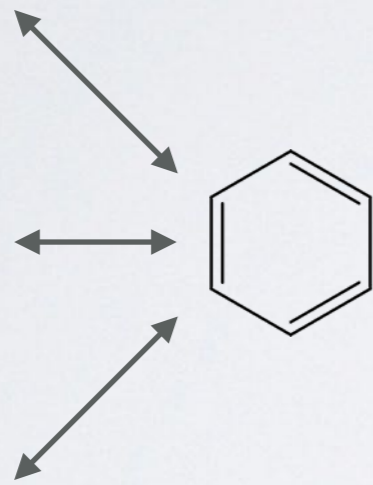
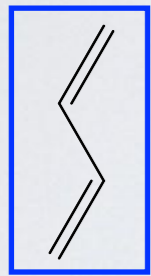
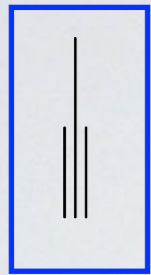




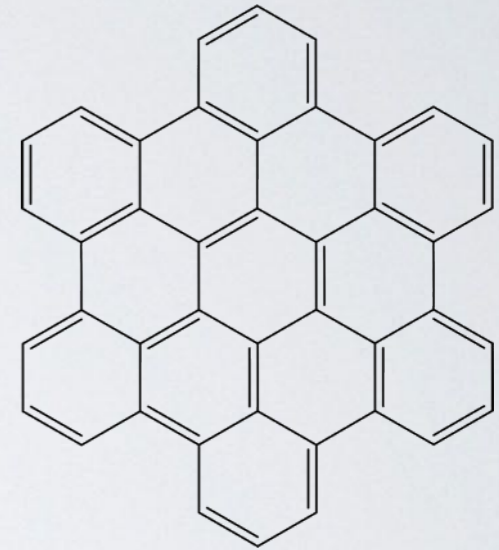




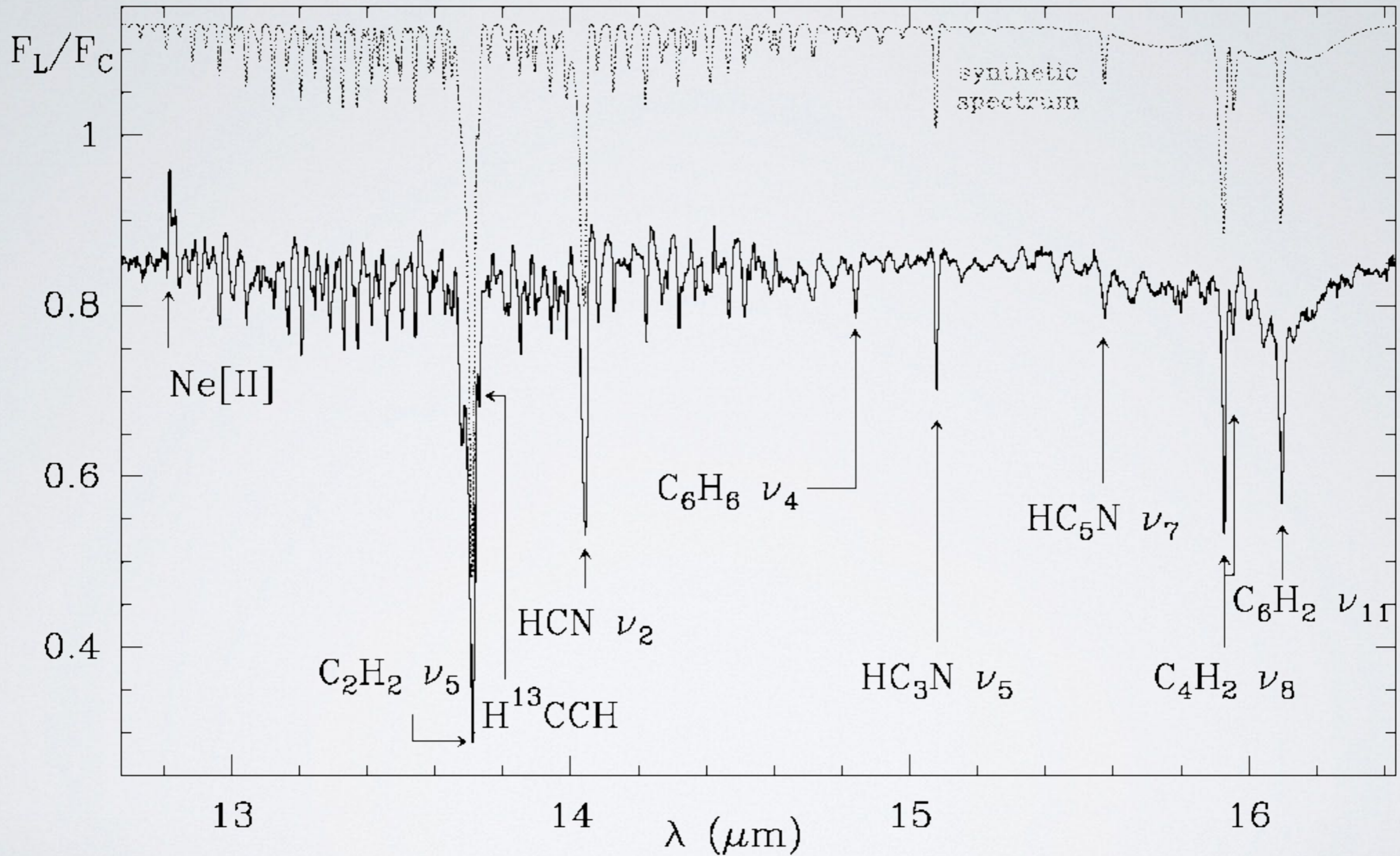
Radio  
IR



IR









$$T_A \propto \frac{N \mu^2}{r^3 \sqrt{T^3 m^3}}$$



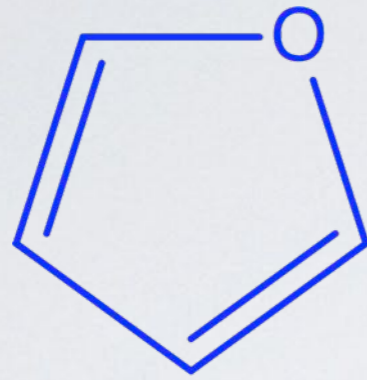
Factor	Reduces $T_A$ ?	PAHs?
Low $N_T$	✓	✓
Low Dipole	✓	✓
Hot	✓	✓
Big	✓	✓

$$T_A \propto \frac{N\mu^2}{r^3\sqrt{T^3m^3}}$$

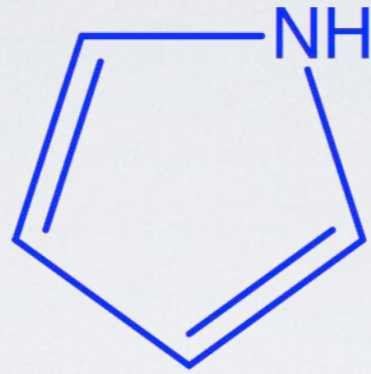


Factor	Reduces $T_A$ ?	PAHs?
Low $N_T$	✓	✓
Low Dipole	Huge Dipole	
Hot	Cold	
Big	Small (relatively speaking)	

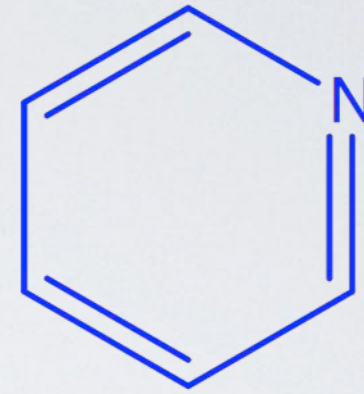




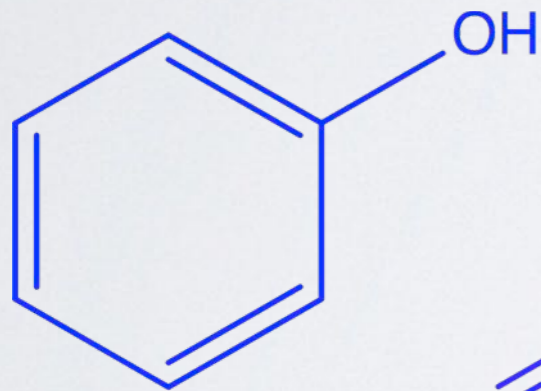
furan



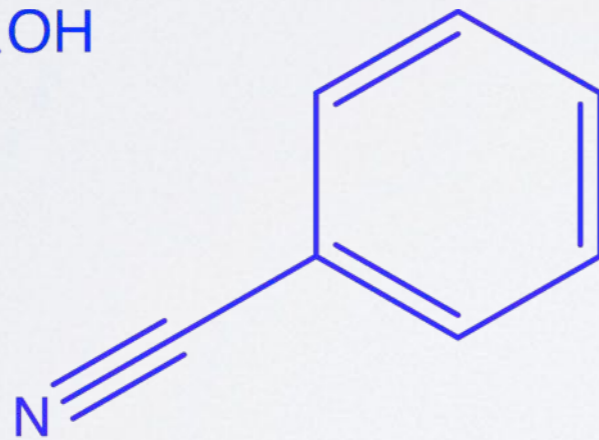
pyrrole



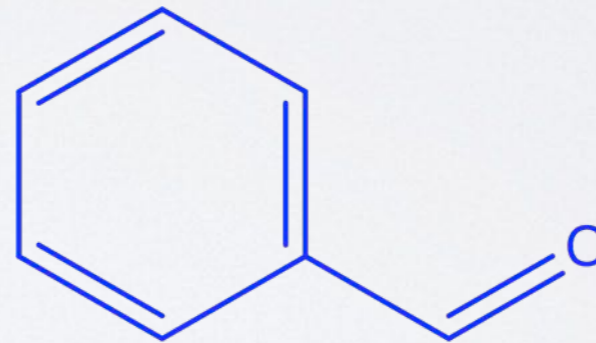
pyridine



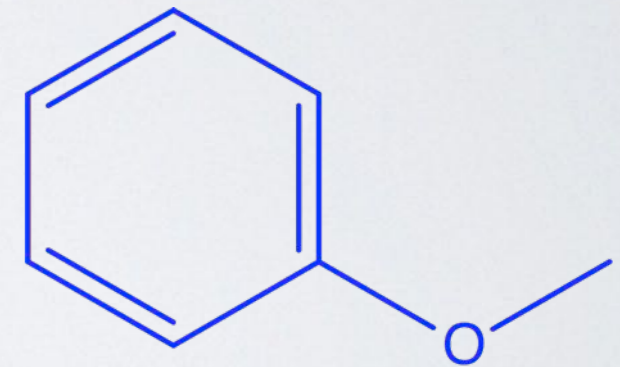
phenol



benzonitrile



benzaldehyde



anisole



# Taurus Molecular Cloud 1 (TMC-1)



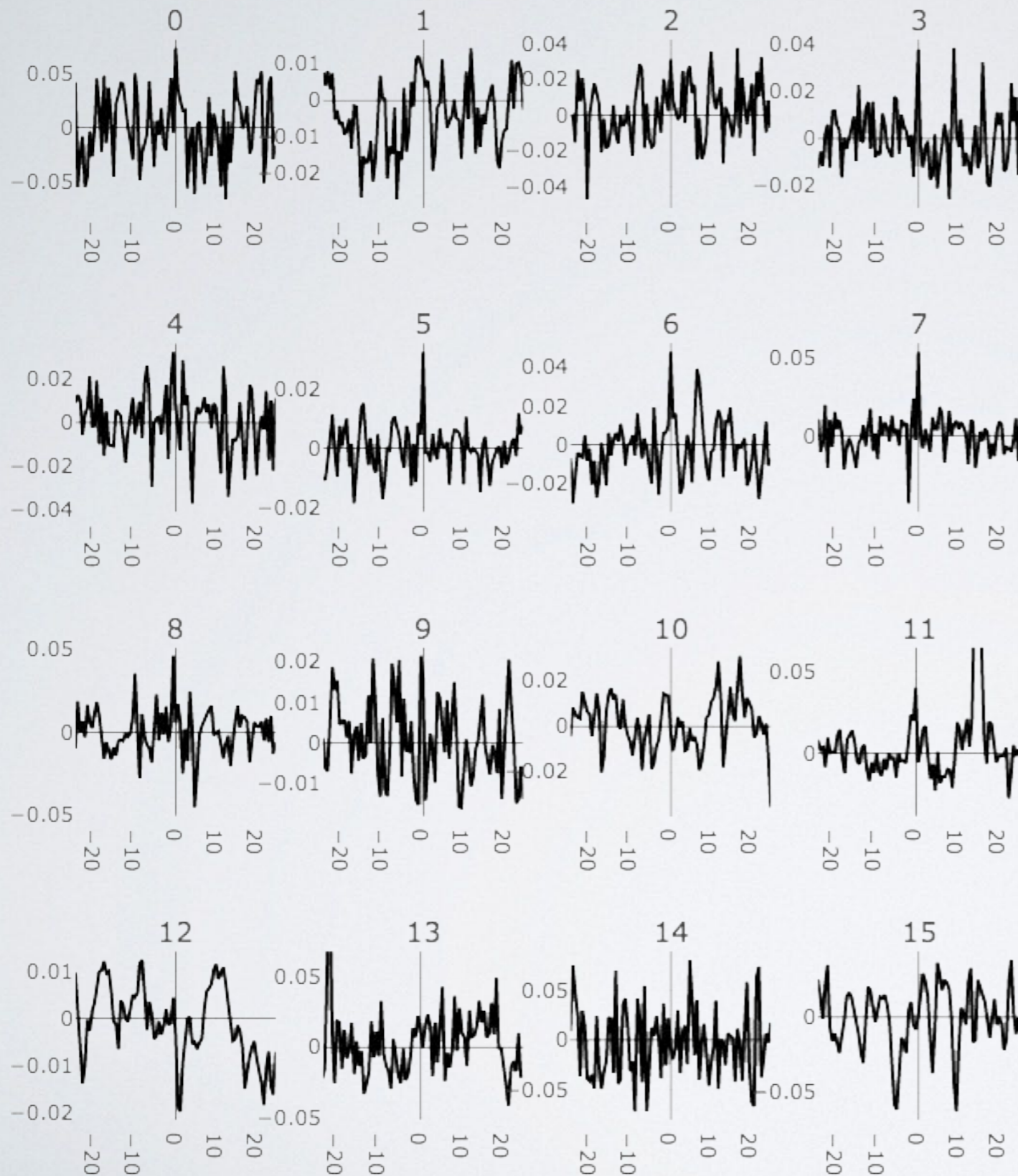
Cold:  $T_k \sim 10$  K

Dense(ish):  $n_H \sim 10^4$  cm<sup>-3</sup>

Narrow Lines:  $\sim 0.3$  km s<sup>-1</sup>

Favorable Chemistry



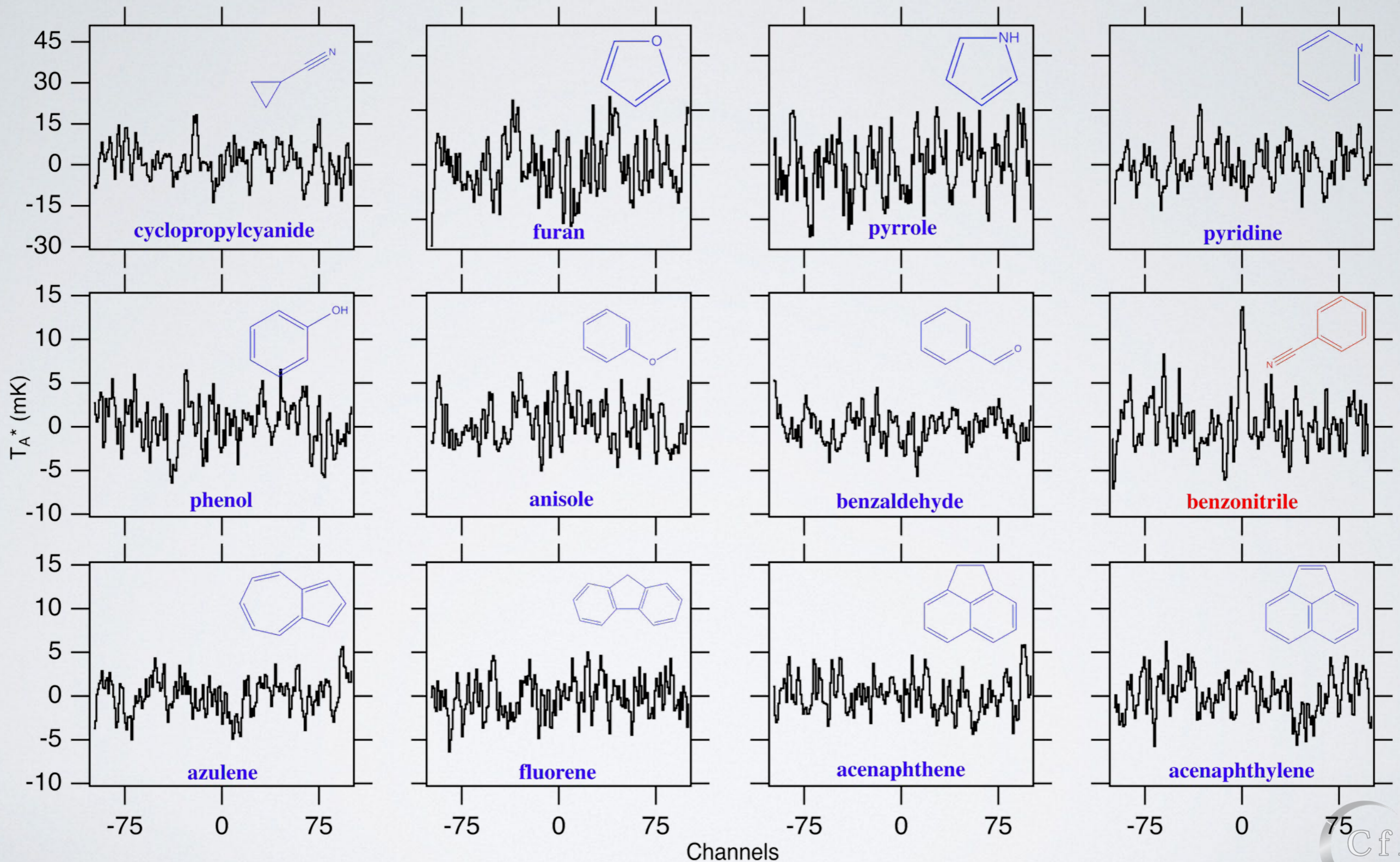


## A 8.8–50 GHz Complete Spectral Line Survey toward TMC-1 I. Survey Data

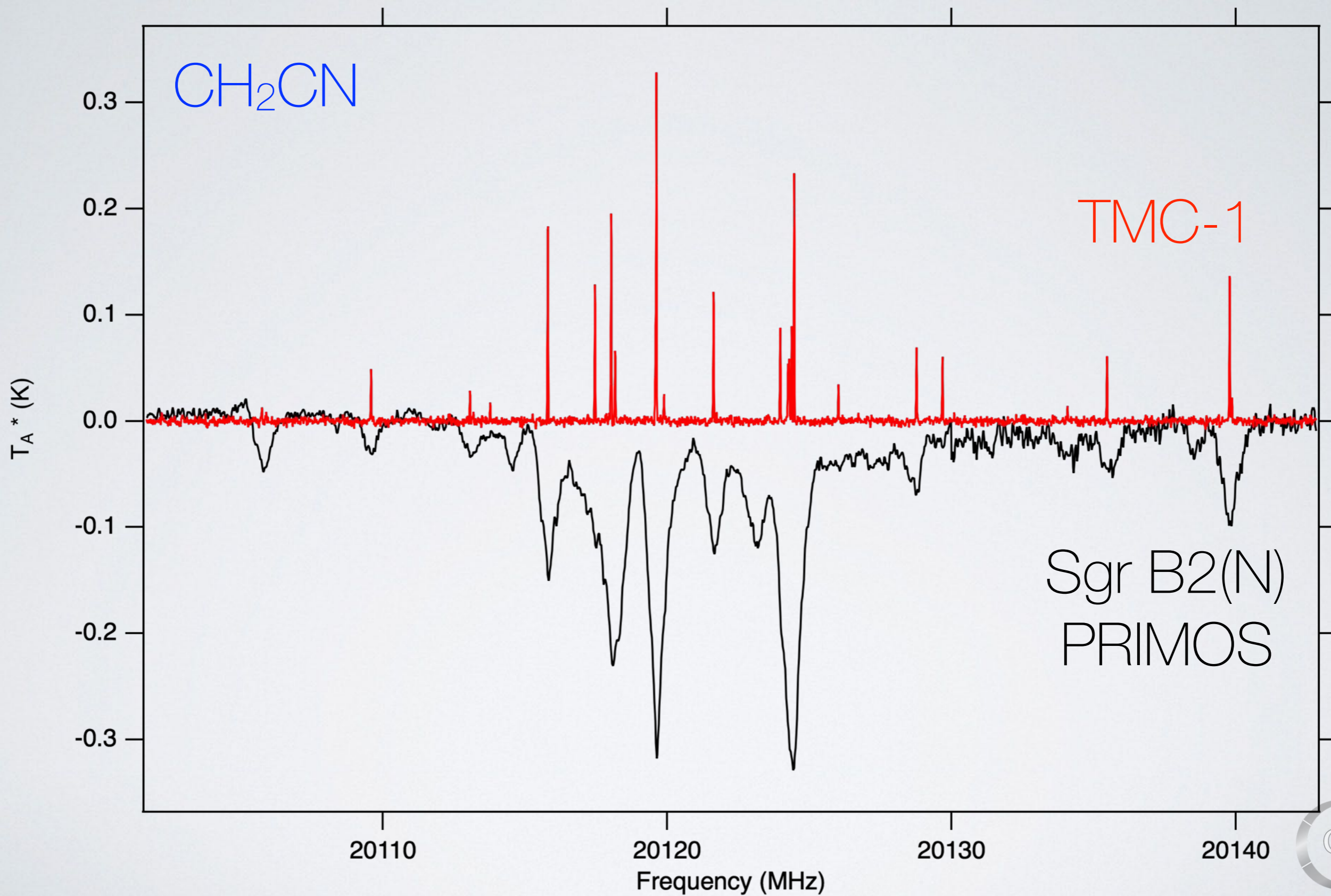
Norio KAIFU,<sup>1</sup> Masatoshi OHISHI,<sup>2</sup> Kentarou KAWAGUCHI,<sup>3</sup> Shuji SAITO,<sup>4</sup>  
Satoshi YAMAMOTO,<sup>5</sup> Takeshi MIYAJI,<sup>6</sup> Keisuke MIYAZAWA,<sup>6</sup>  
Shin-ichi ISHIKAWA,<sup>6</sup> Chiaki NOUMARU,<sup>1</sup> Sumiko HARASAWA,<sup>7</sup> Michiko OKUDA,<sup>1</sup>  
and  
Hiroko SUZUKI<sup>6,8</sup>

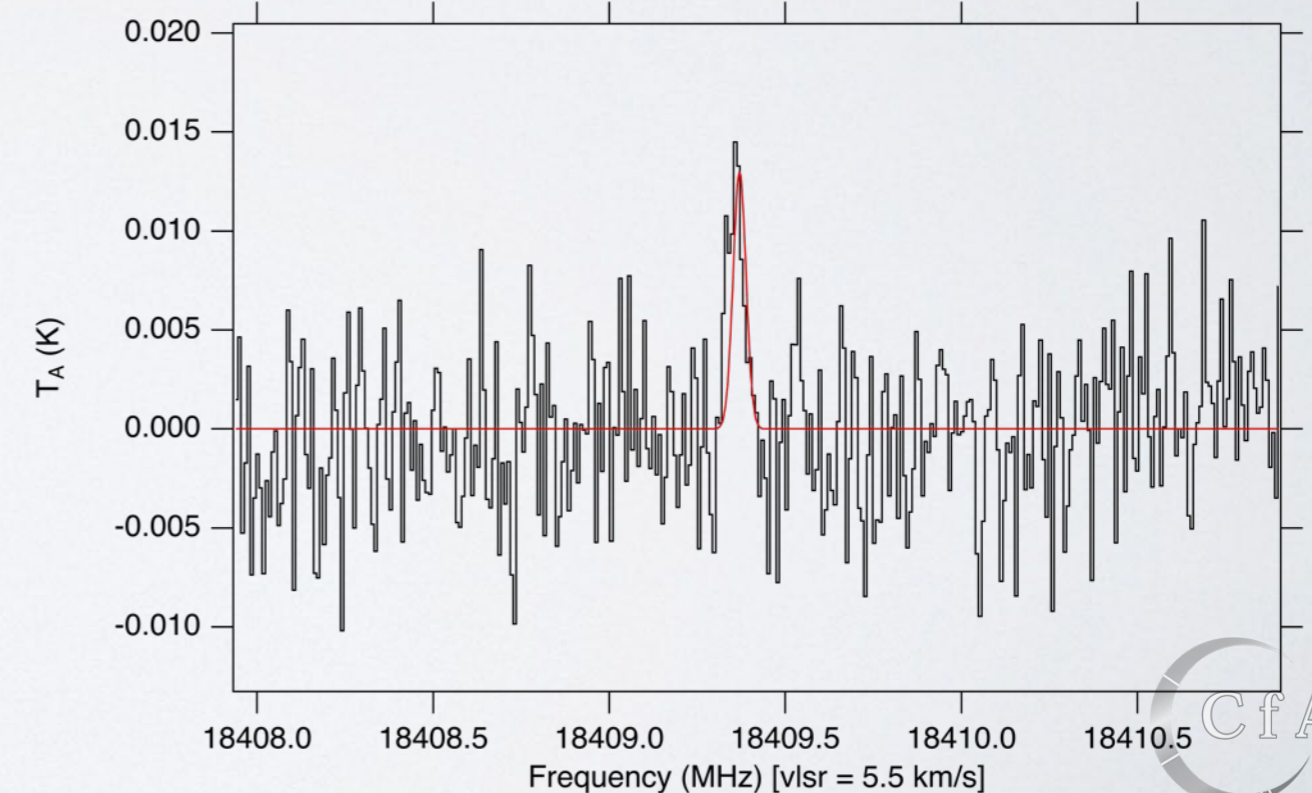
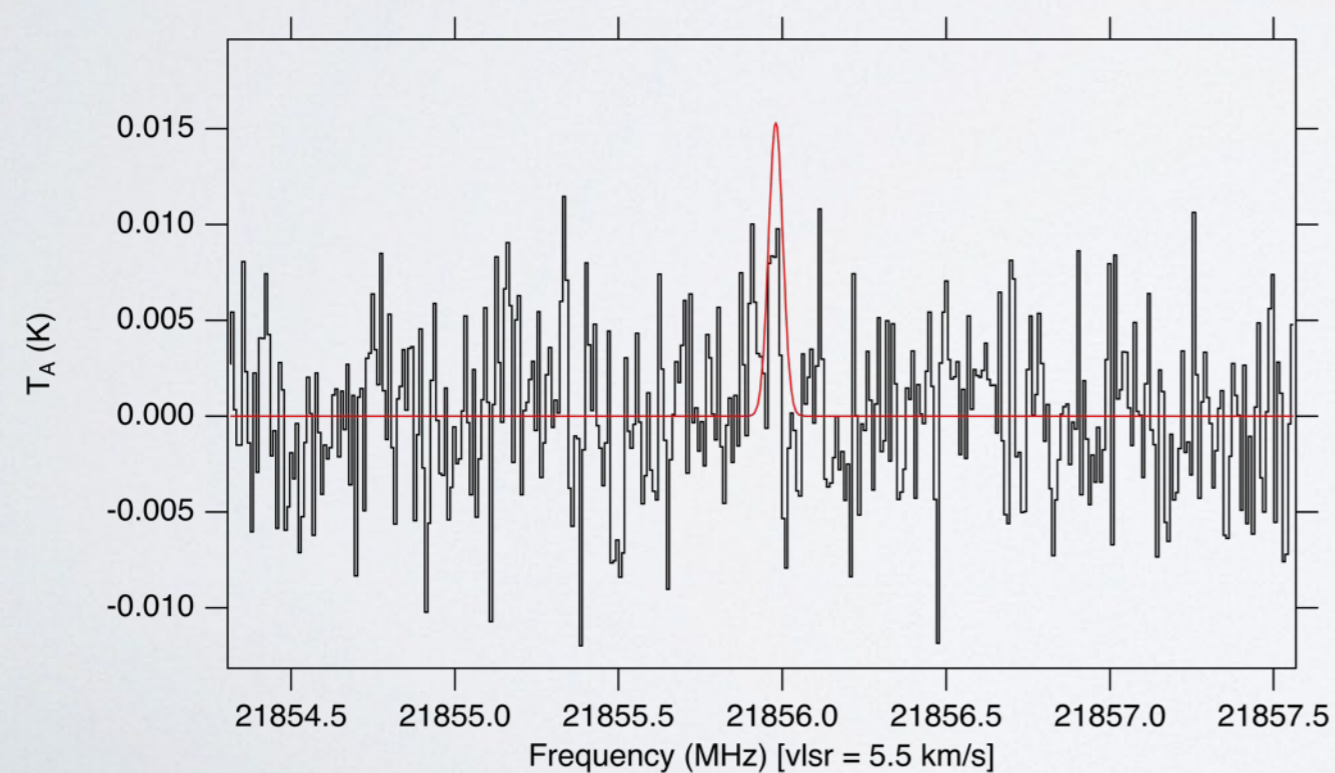
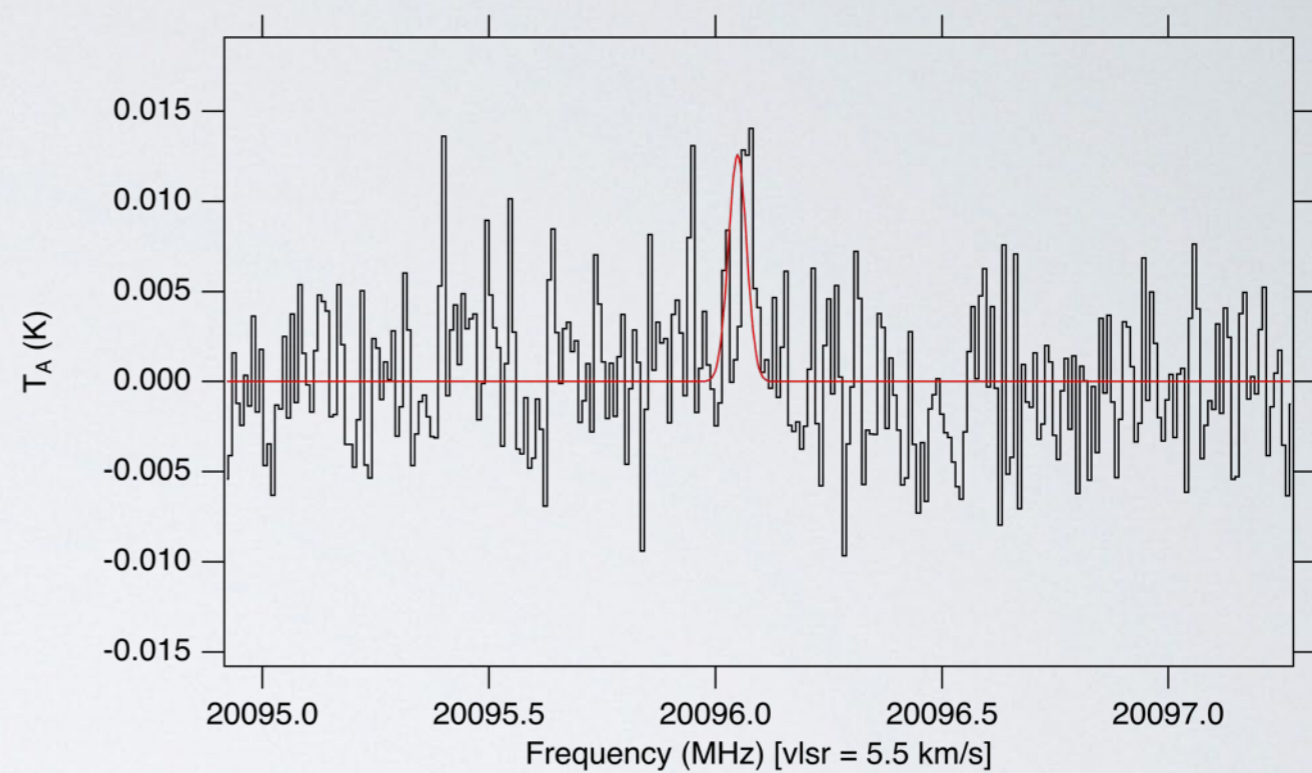
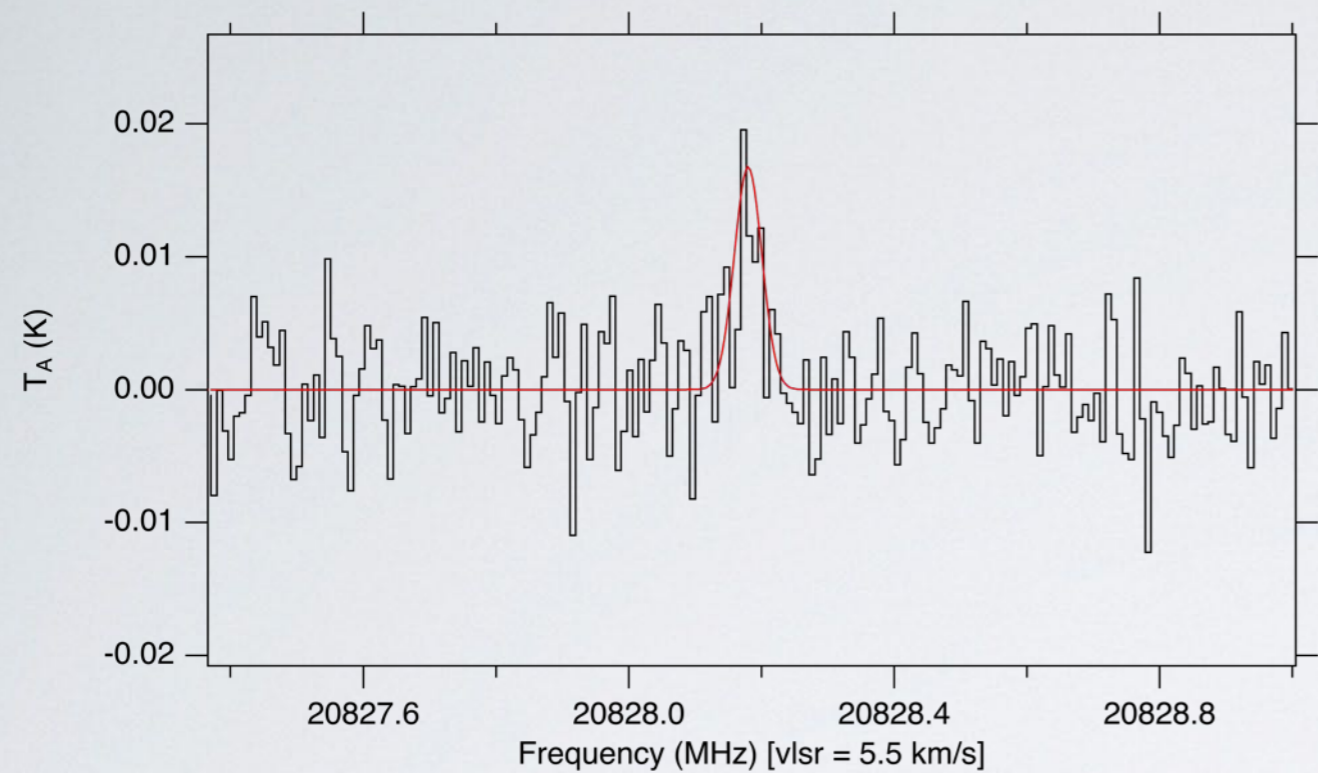




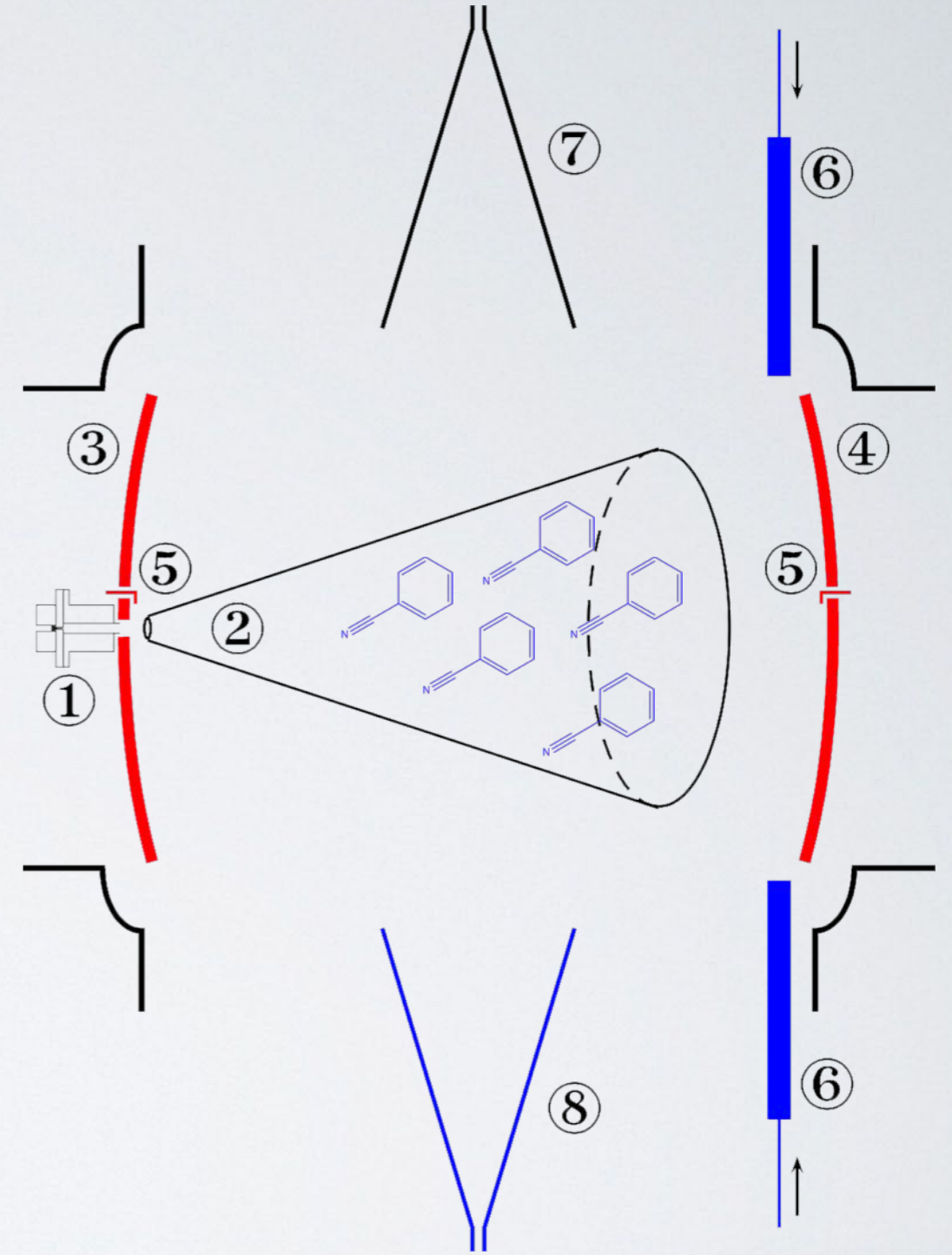
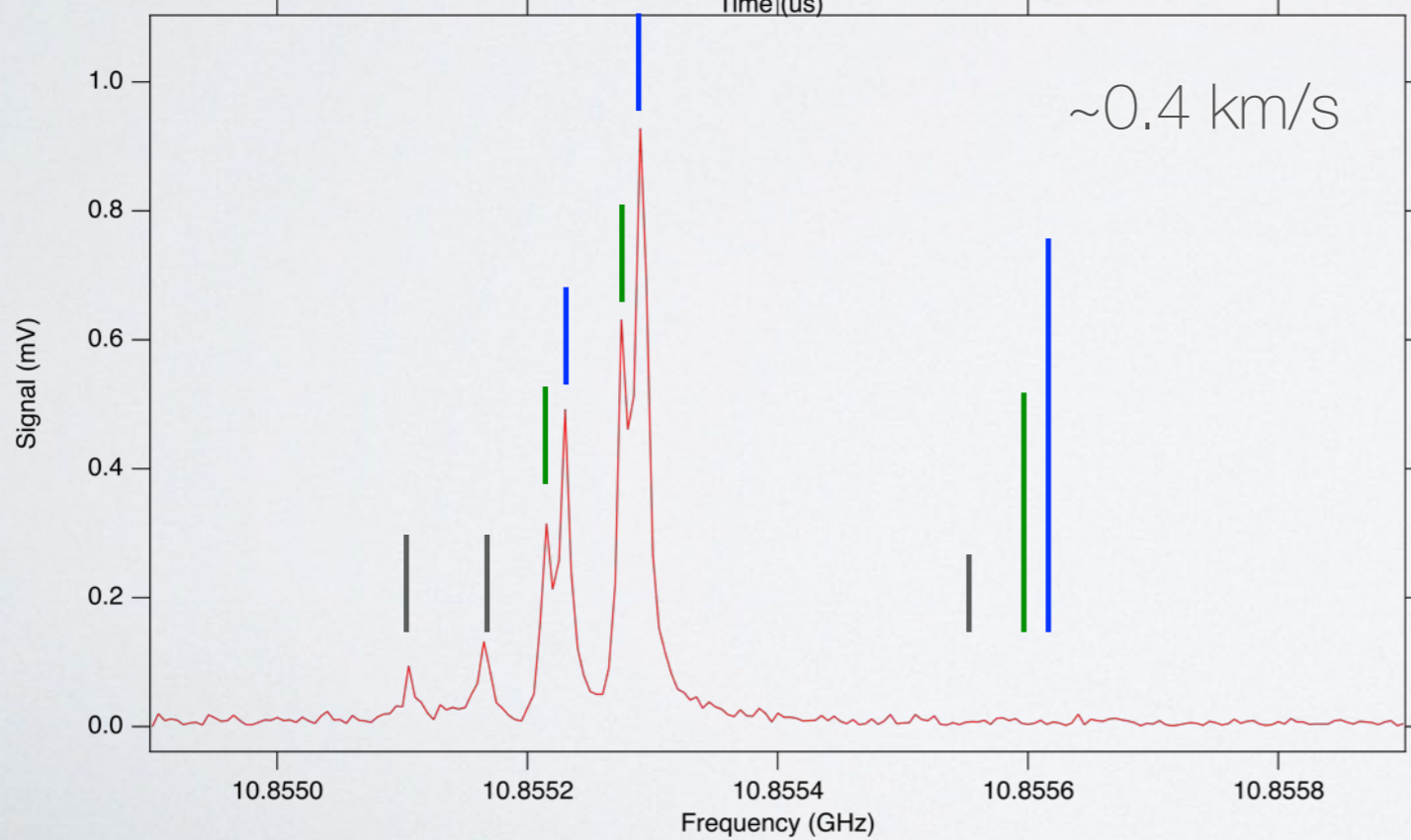
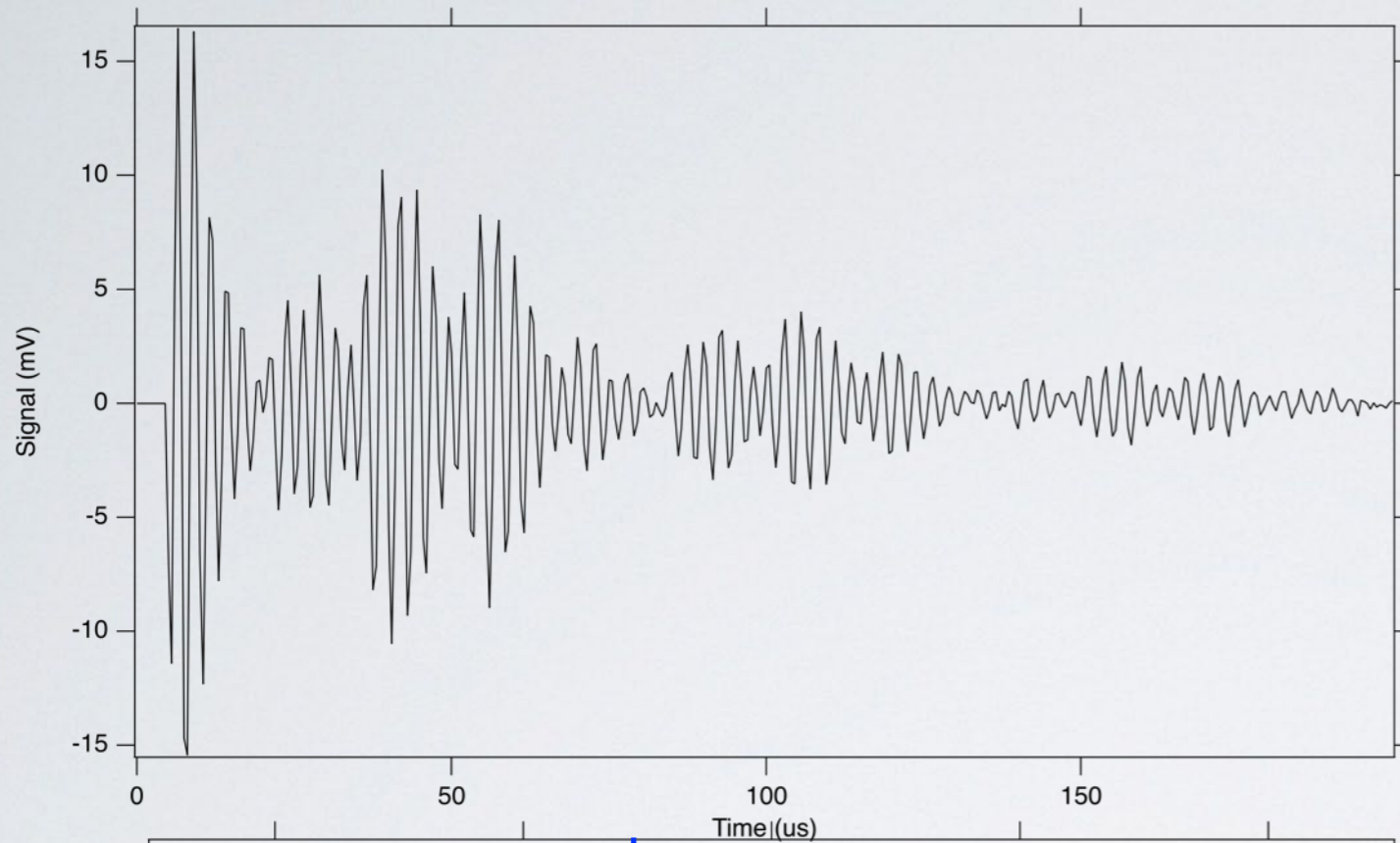






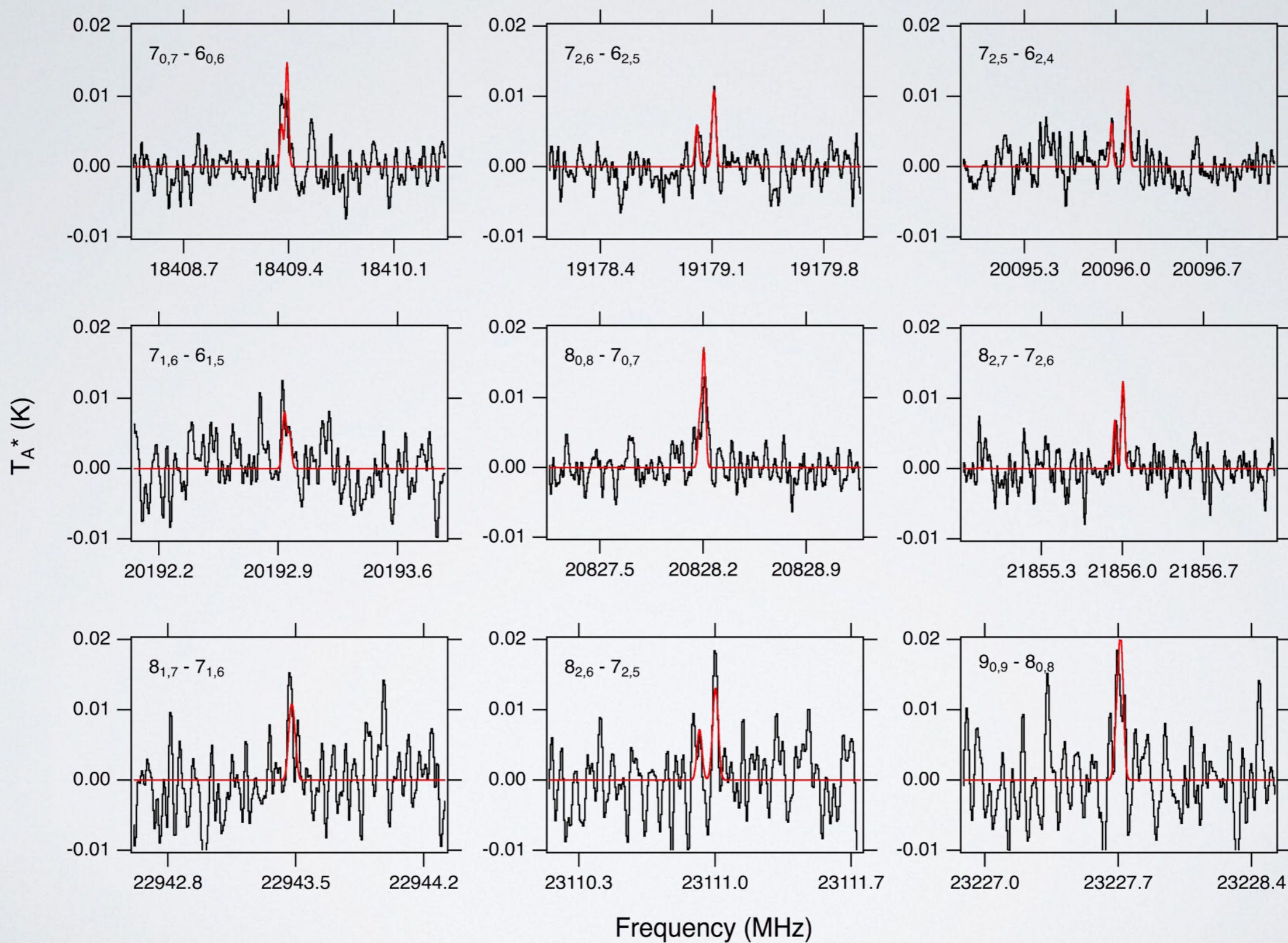




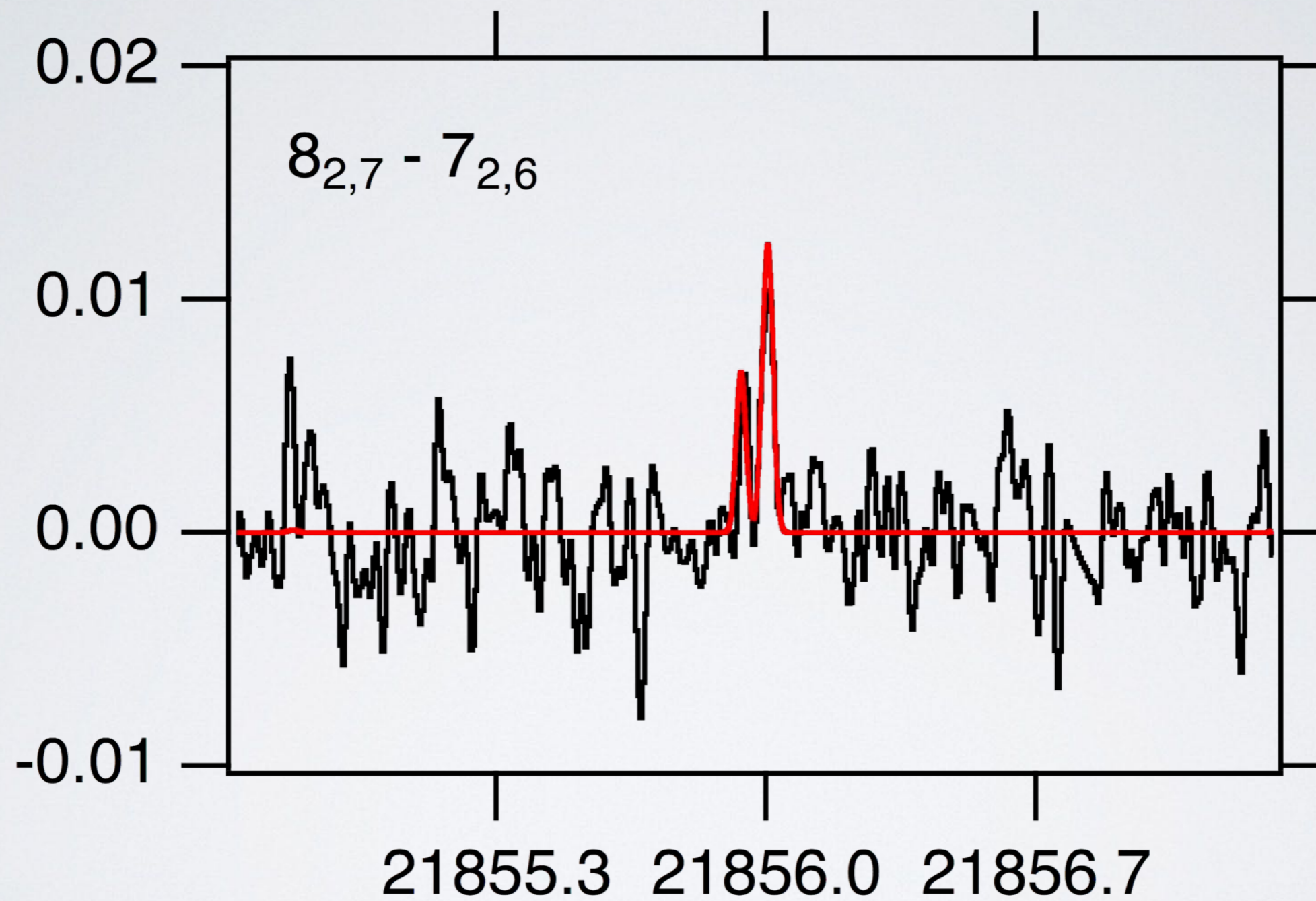


5 - 40 GHz

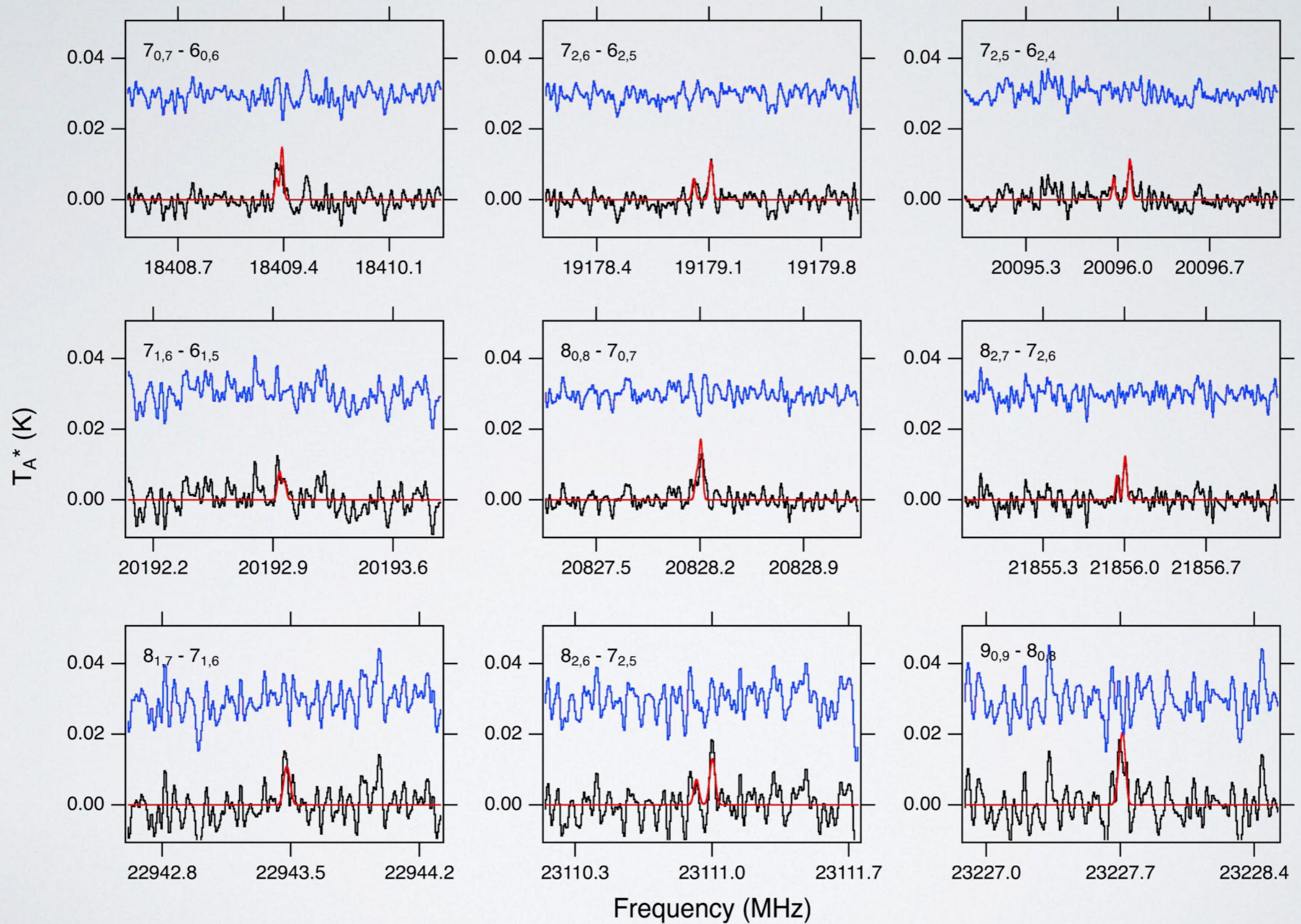




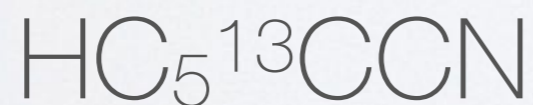
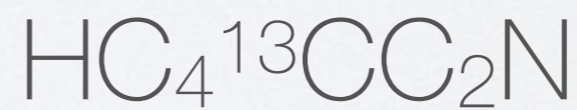
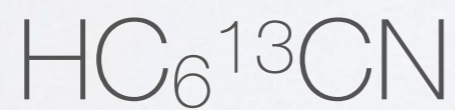
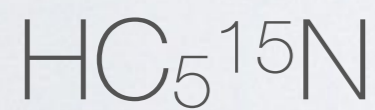
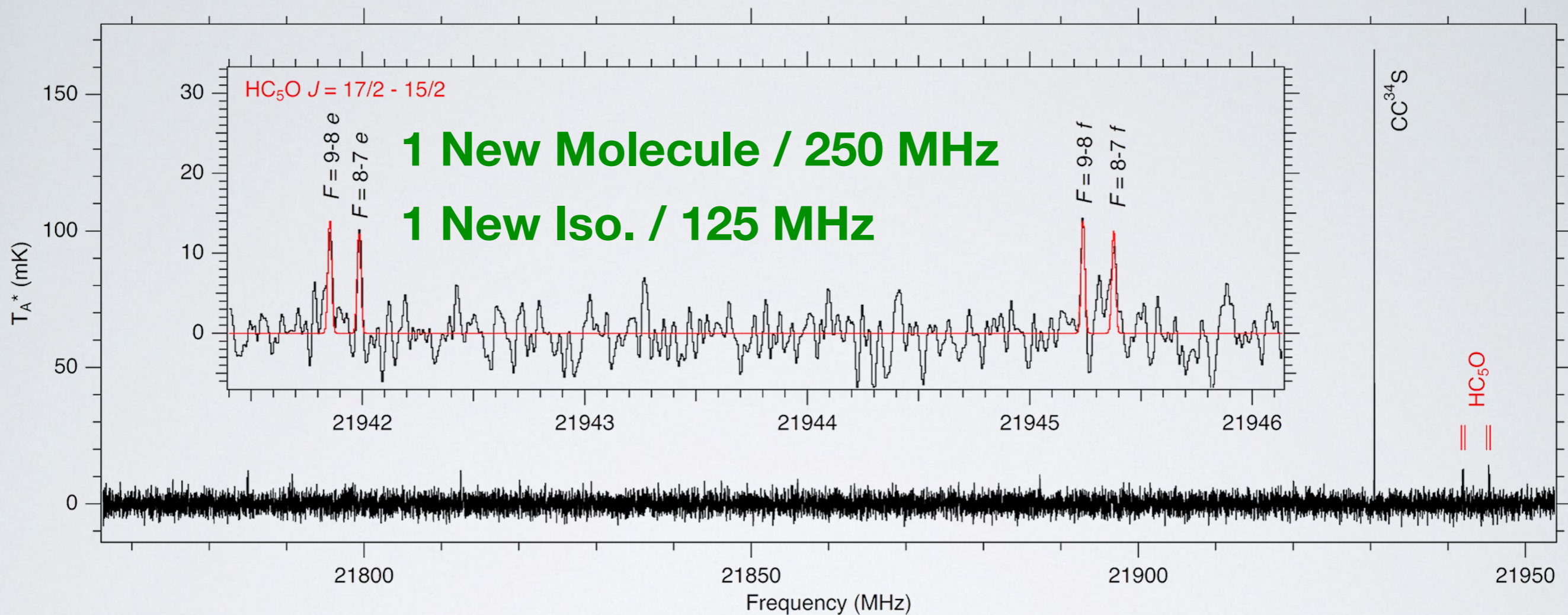






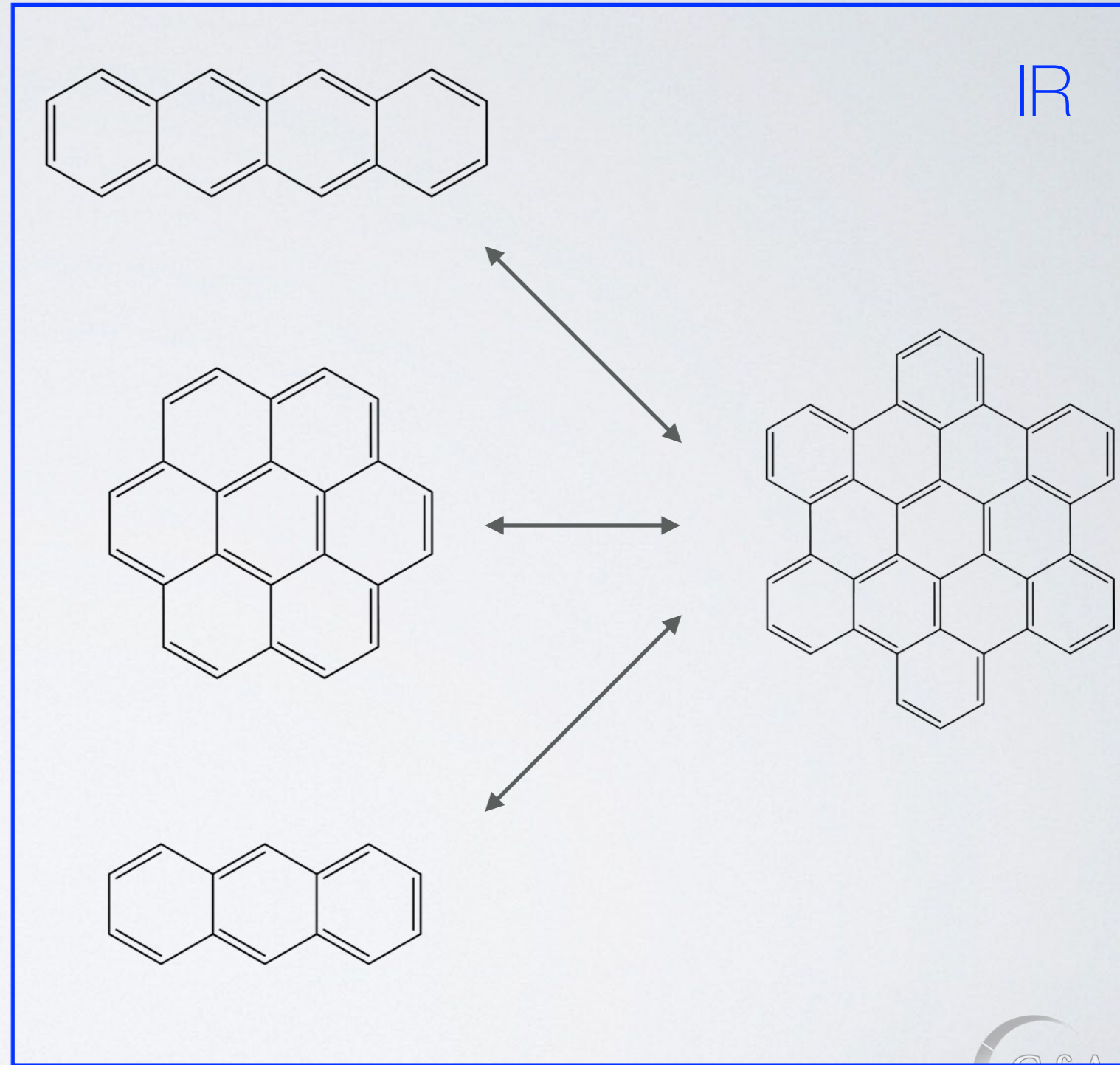
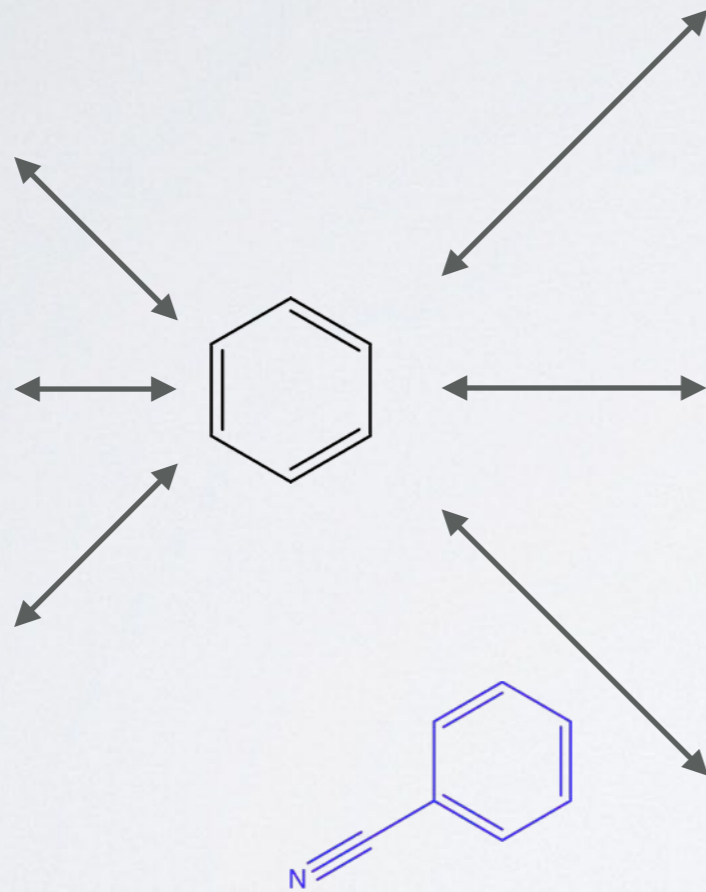
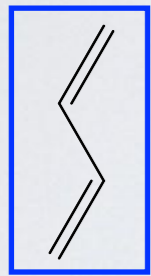
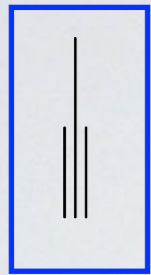






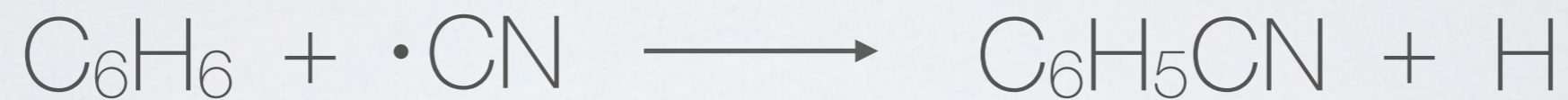


Radio  
IR

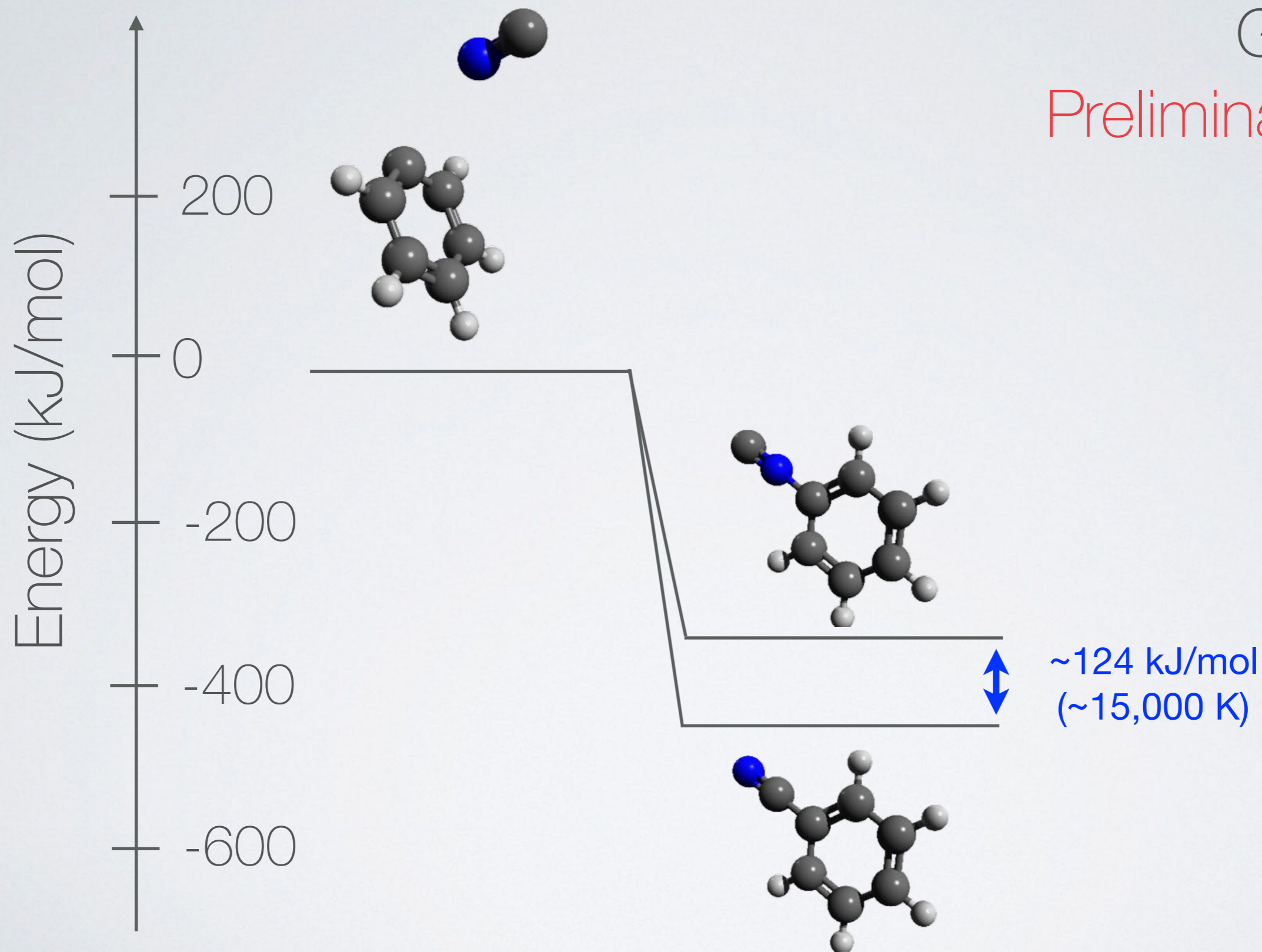


IR



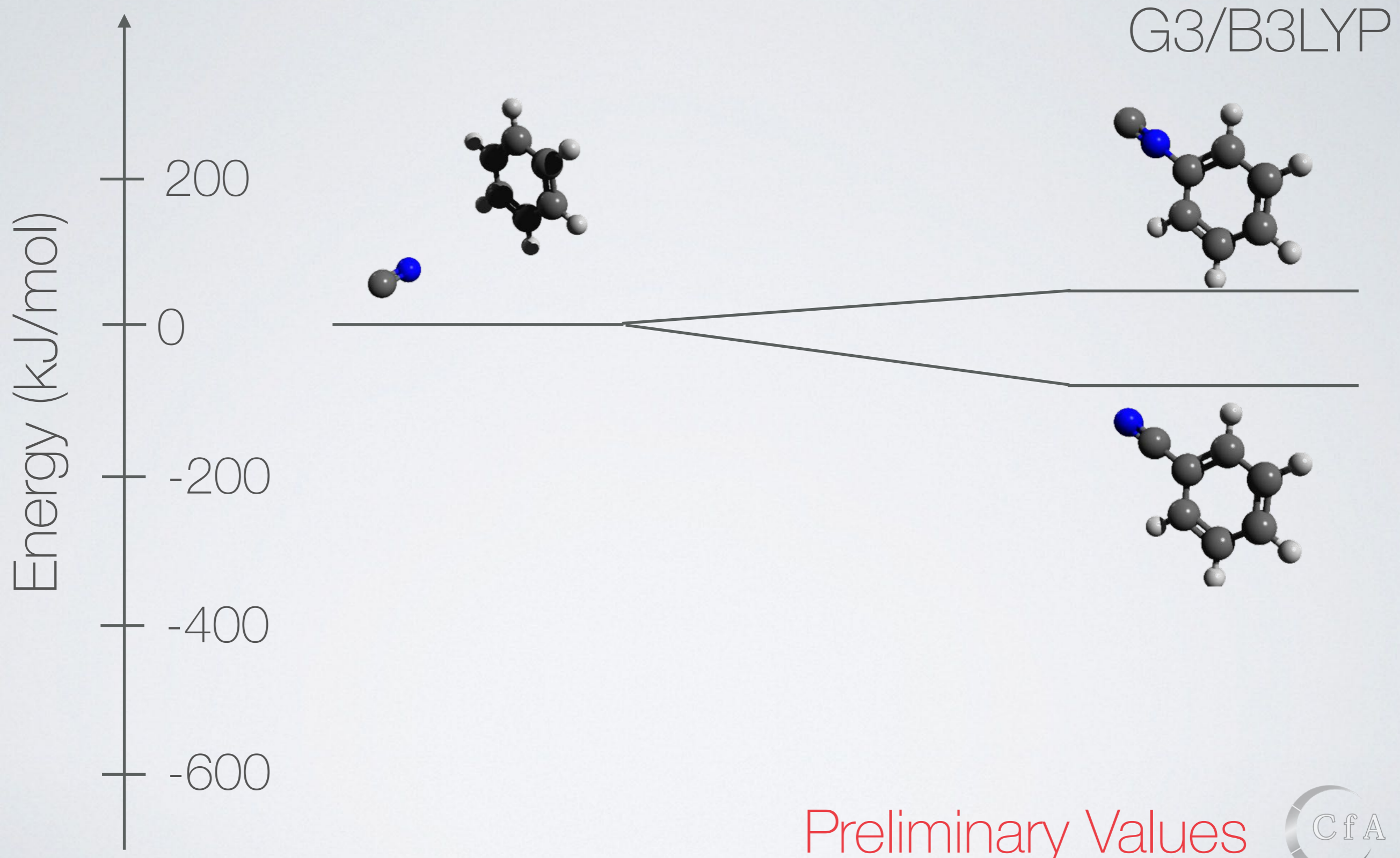






G3/B3LYP  
Preliminary Values











# Two Spectroscopic Tools

## *Cavity-Enhanced Fourier-Transform Microwave Spectroscopy*

Narrowband (~1 MHz)

High Sensitivity

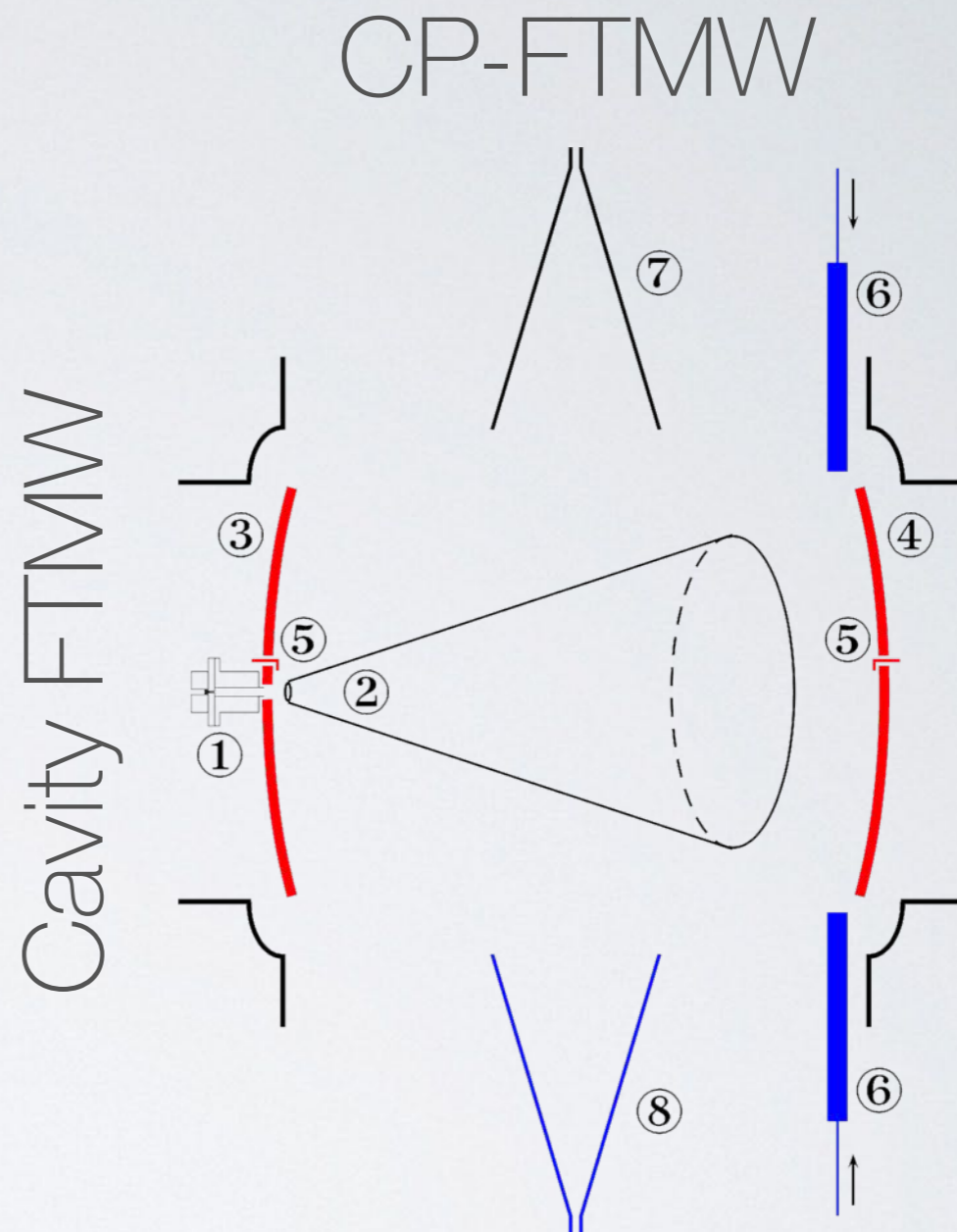
High Speed

## *Chirped-Pulse Fourier-Transform Microwave Spectroscopy*

Broadband (~10 GHz)

Modest Sensitivity

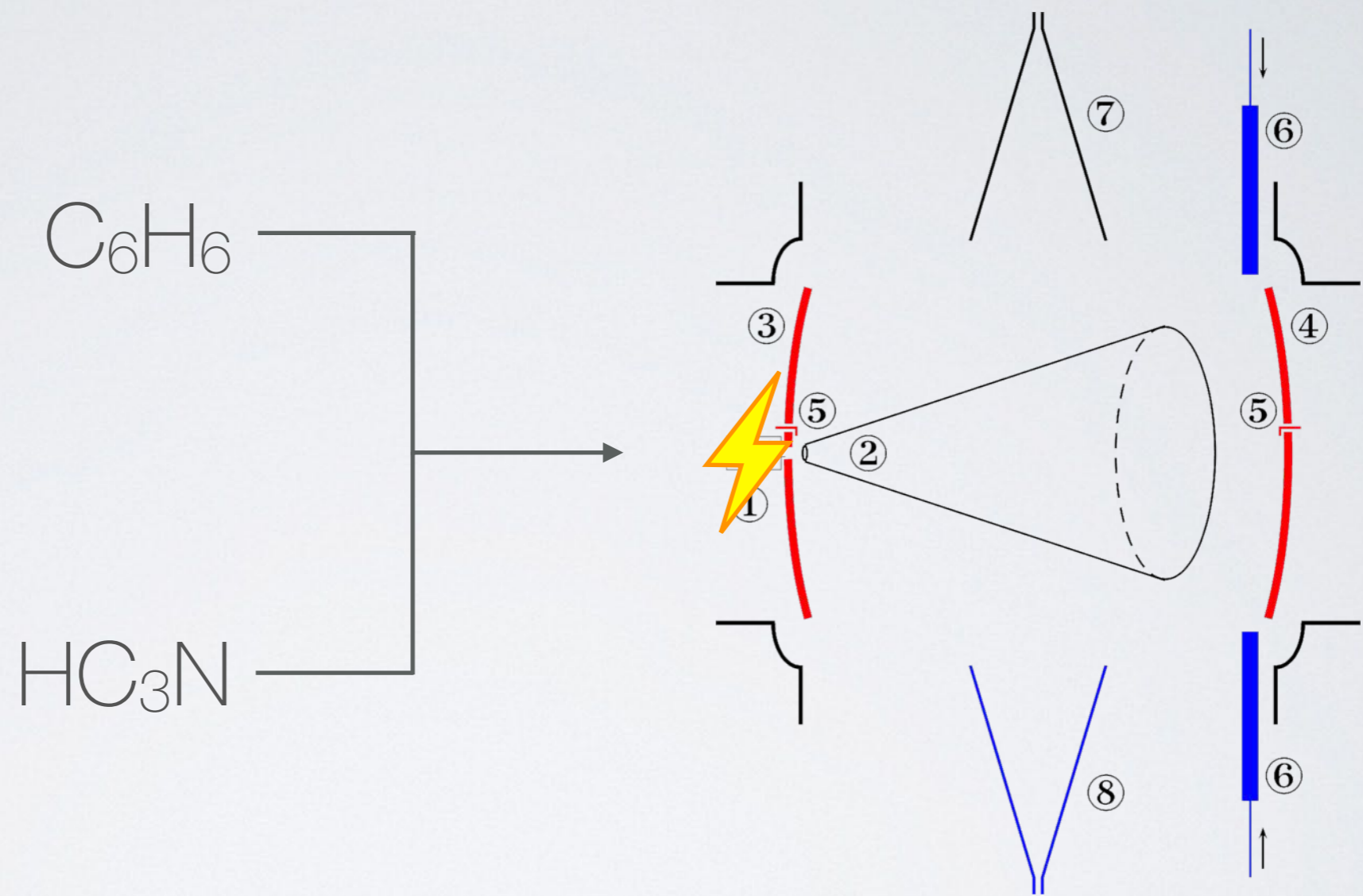
Modest Speed



8 - 18 GHz

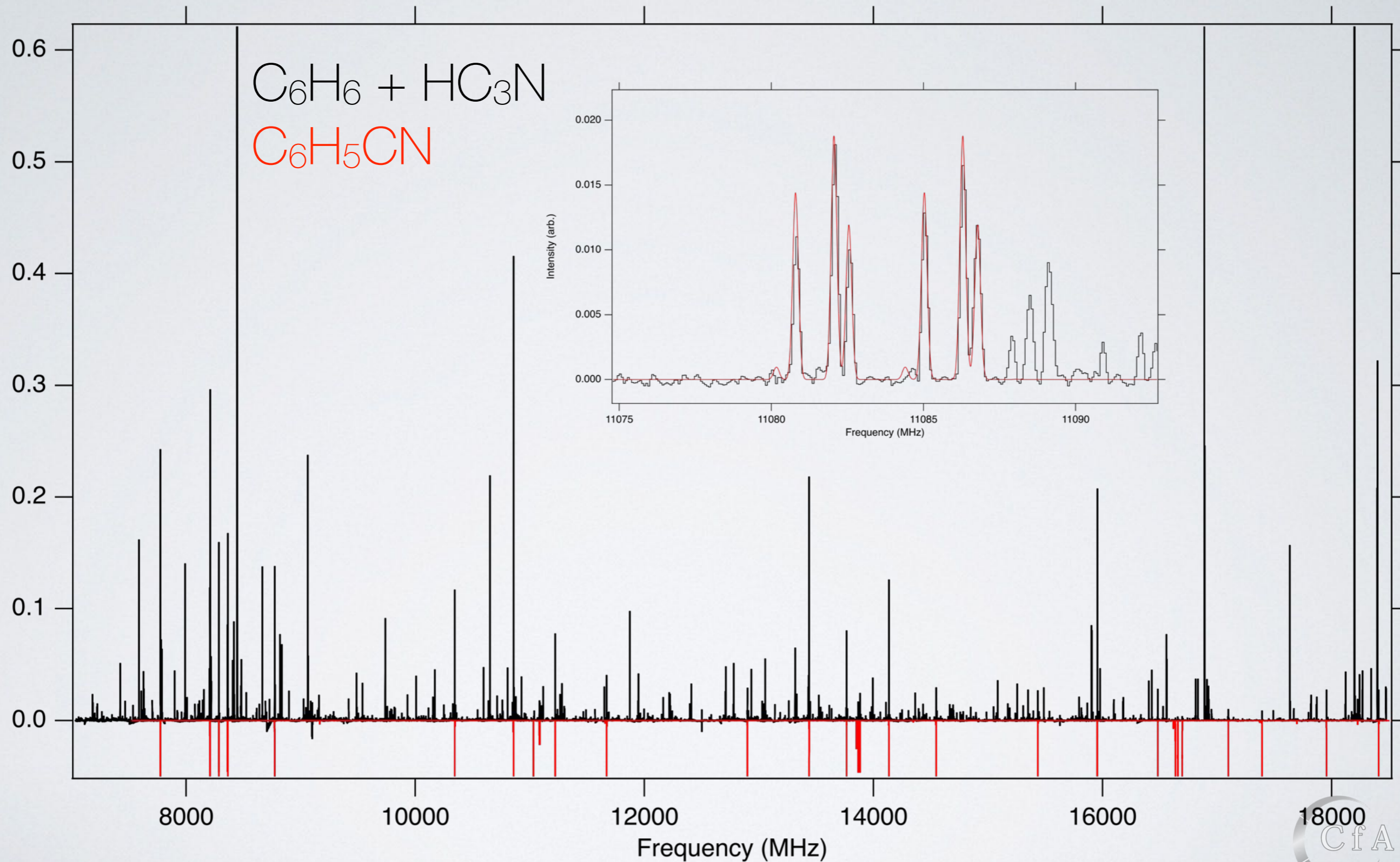


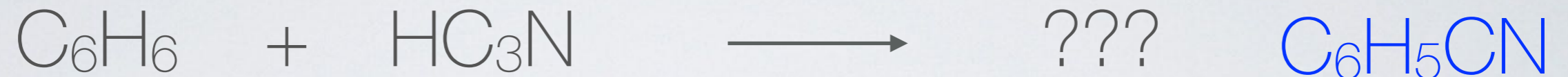
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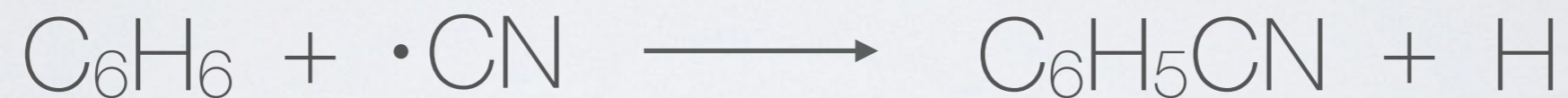
8 - 18 GHz

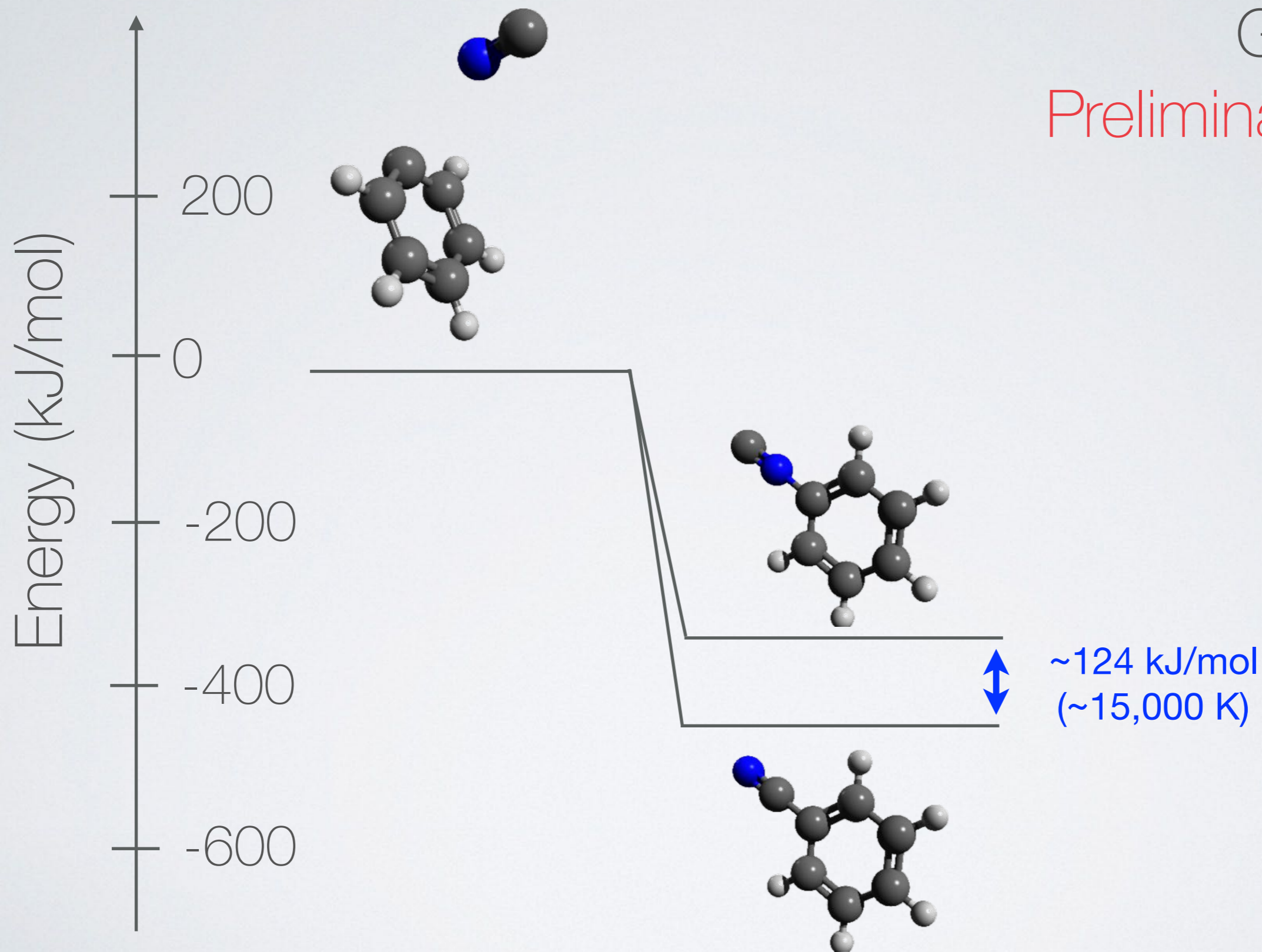






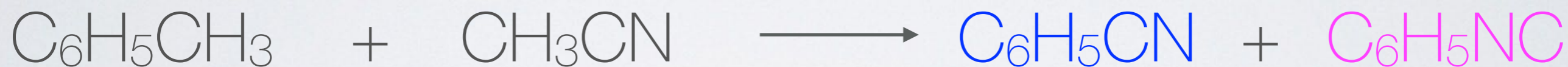
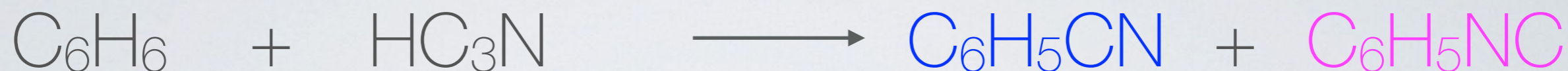






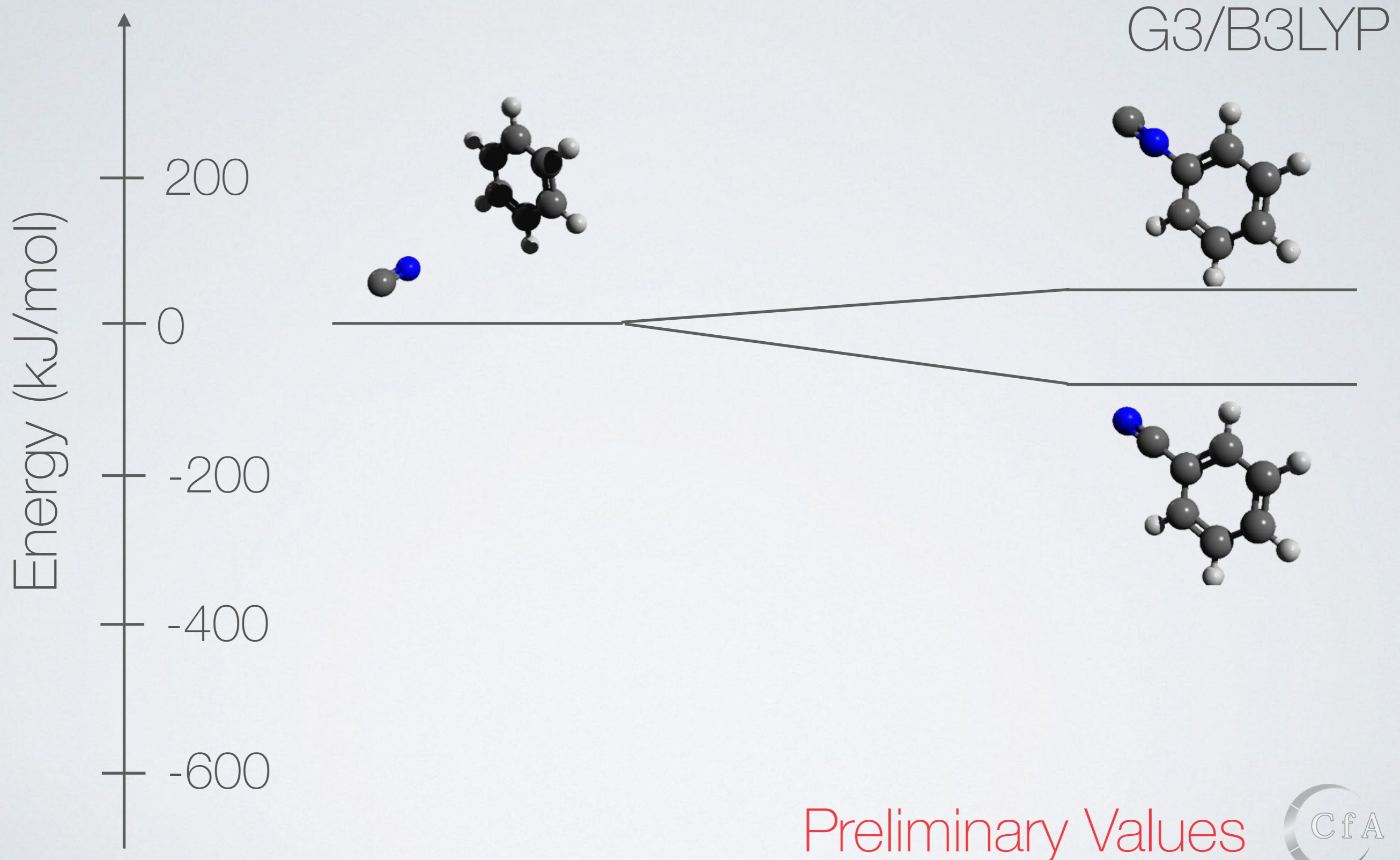
G3/B3LYP  
Preliminary Values





>1000 : 1

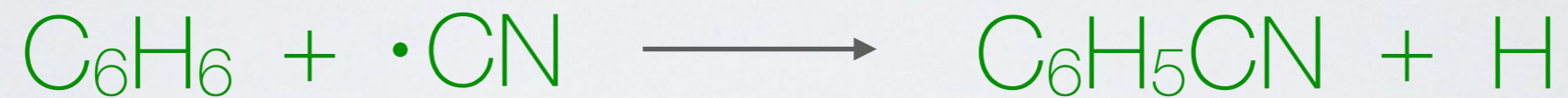
There must be a kinetic barrier to forming  $\text{C}_6\text{H}_5\text{NC}$  vs  $\text{C}_6\text{H}_5\text{CN}$



Preliminary Values







THE ASTROPHYSICAL JOURNAL SUPPLEMENT SERIES, 217:20 (7pp), 2015 April

[doi:10.1088/0067-0049/217/2/20](https://doi.org/10.1088/0067-0049/217/2/20)

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## THE 2014 KIDA NETWORK FOR INTERSTELLAR CHEMISTRY

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S. D. LE PICARD<sup>17</sup>, G. NYMAN<sup>18</sup>, M. RUAUD<sup>1,2</sup>, S. SCHLEMMER<sup>19</sup>, I. R. SIMS<sup>17</sup>, D. TALBI<sup>20</sup>, J. TENNYSON<sup>21</sup>, AND R. WESTER<sup>22</sup>

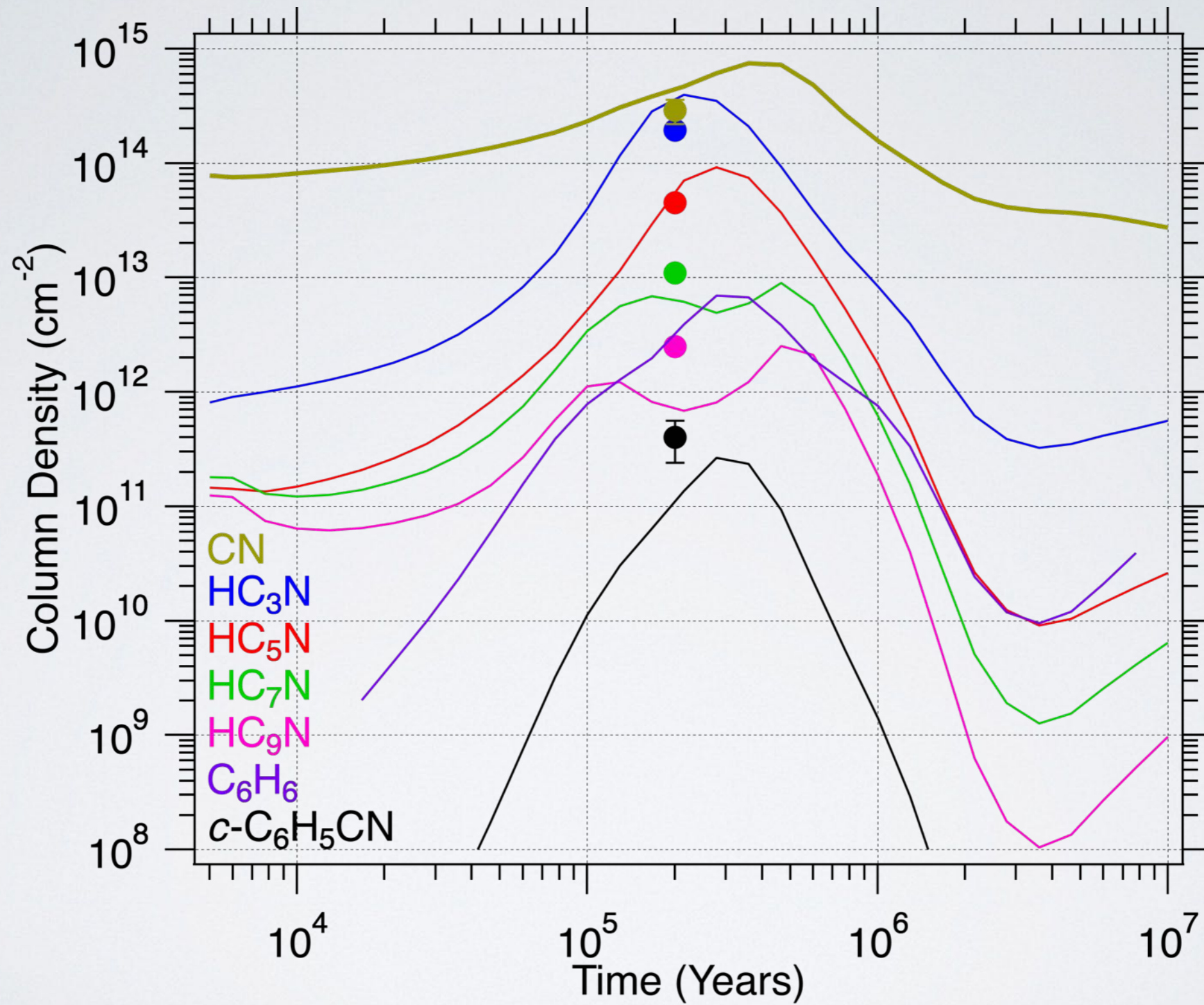
MNRAS **459**, 3756–3767 (2016)[doi:10.1093/mnras/stw887](https://doi.org/10.1093/mnras/stw887)

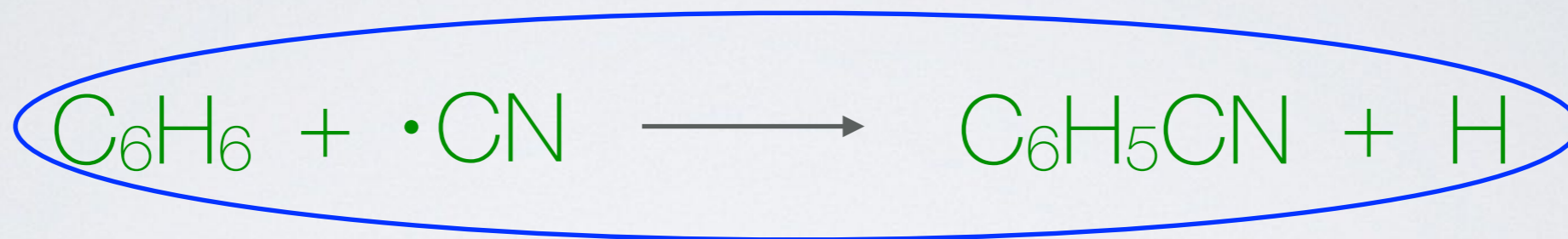
Advance Access publication 2016 April 15

## Gas and grain chemical composition in cold cores as predicted by the Nautilus three-phase model

Maxime Ruaud,<sup>1,2</sup>★ Valentine Wakelam<sup>1,2</sup> and Franck Hersant<sup>1,2</sup>

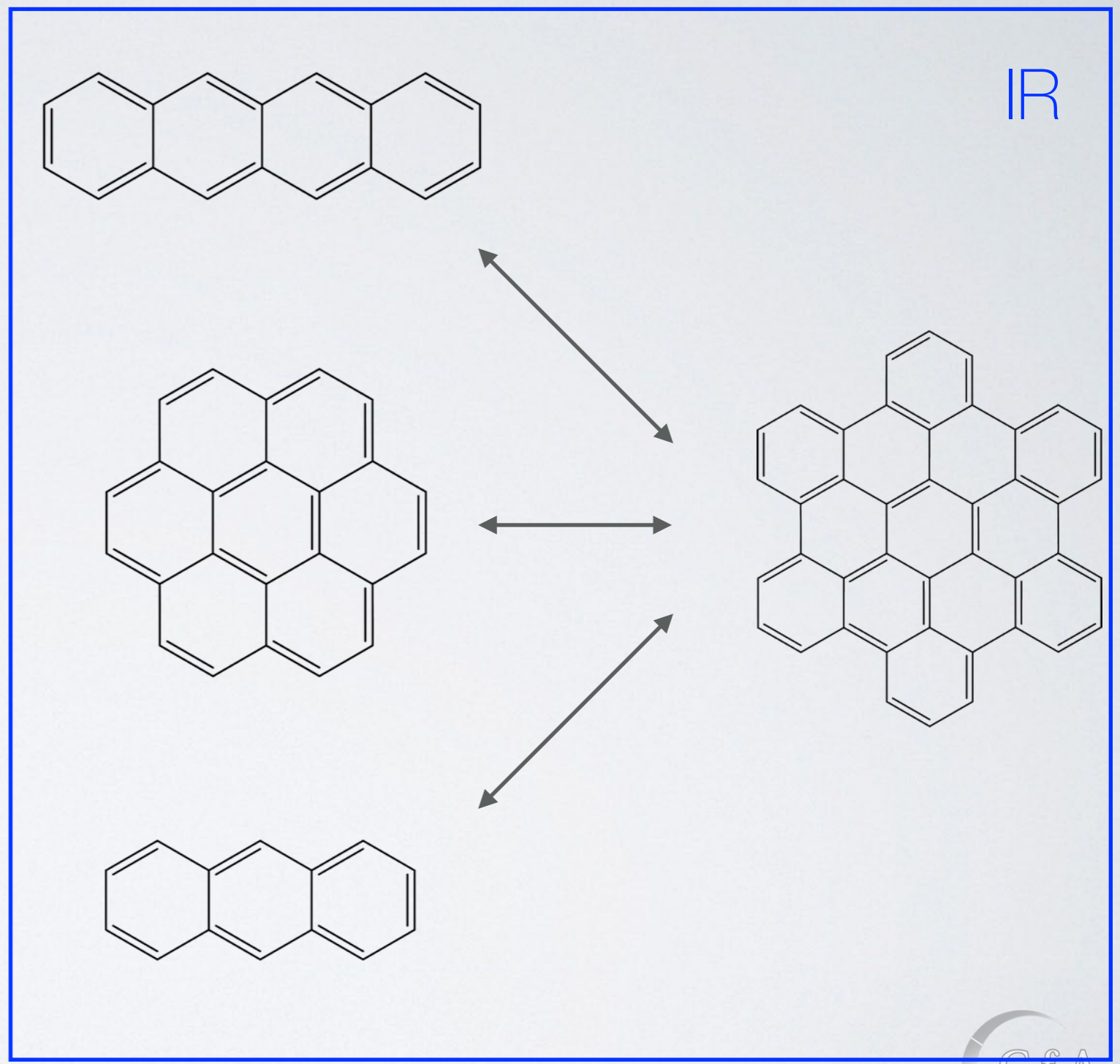
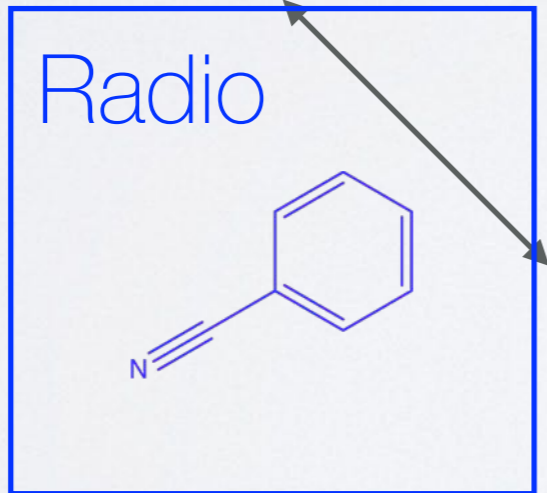
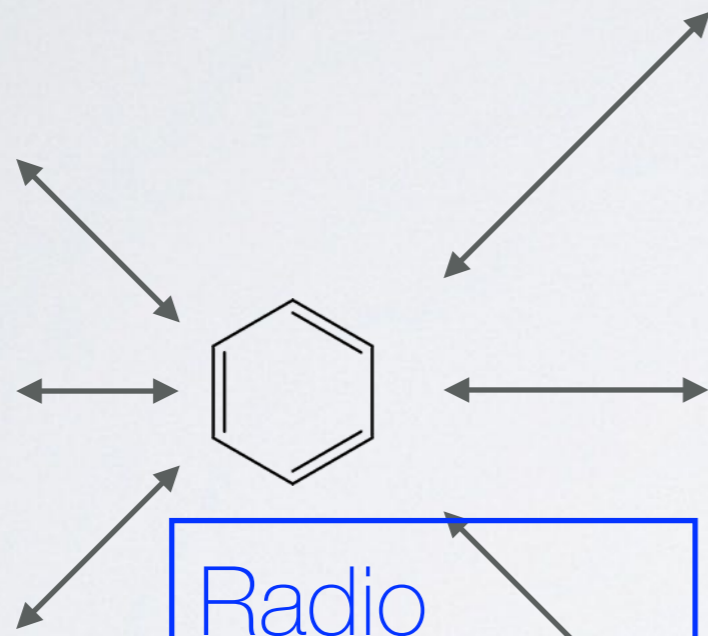
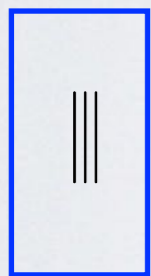
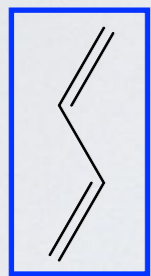
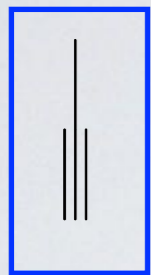




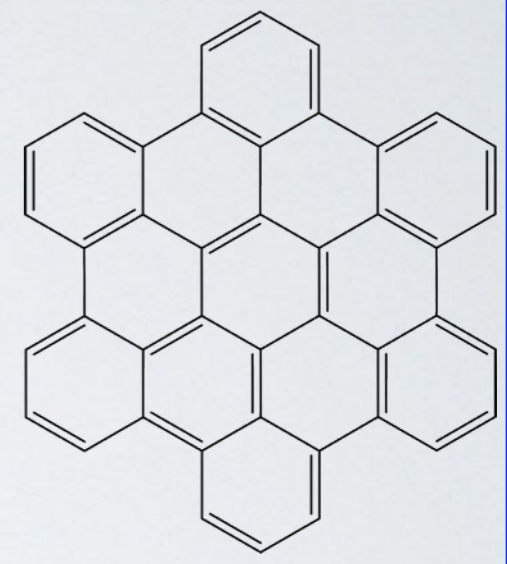


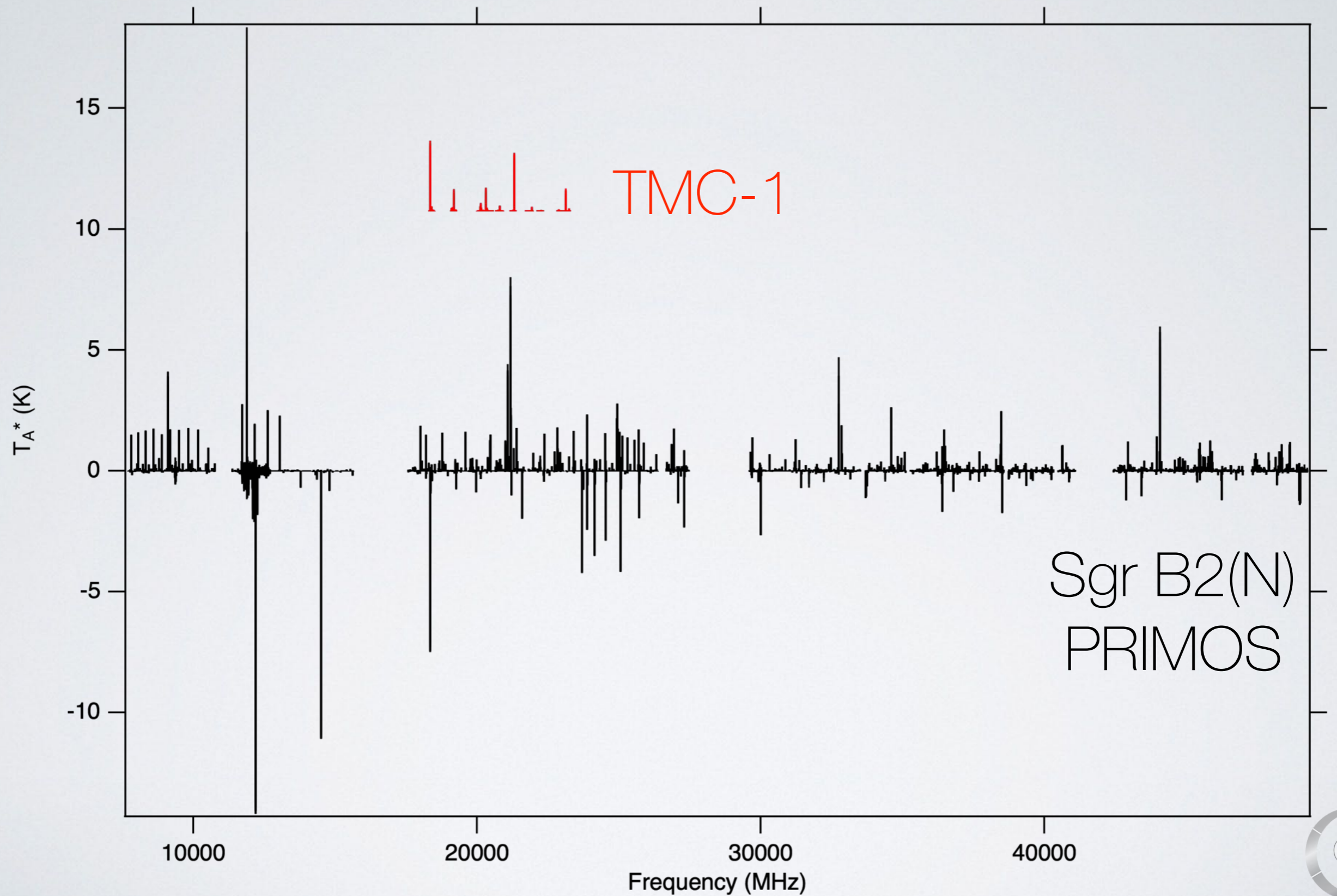


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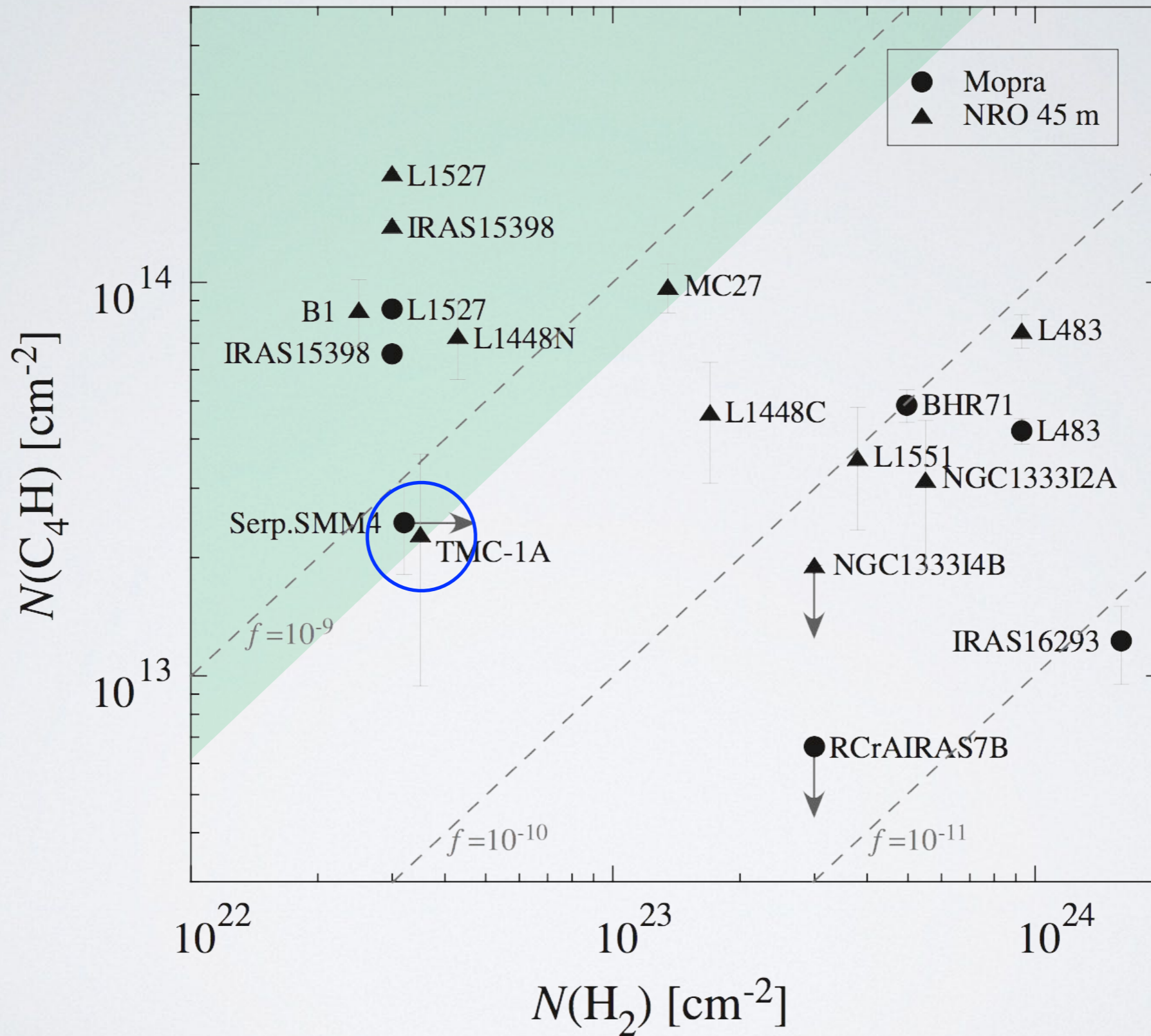


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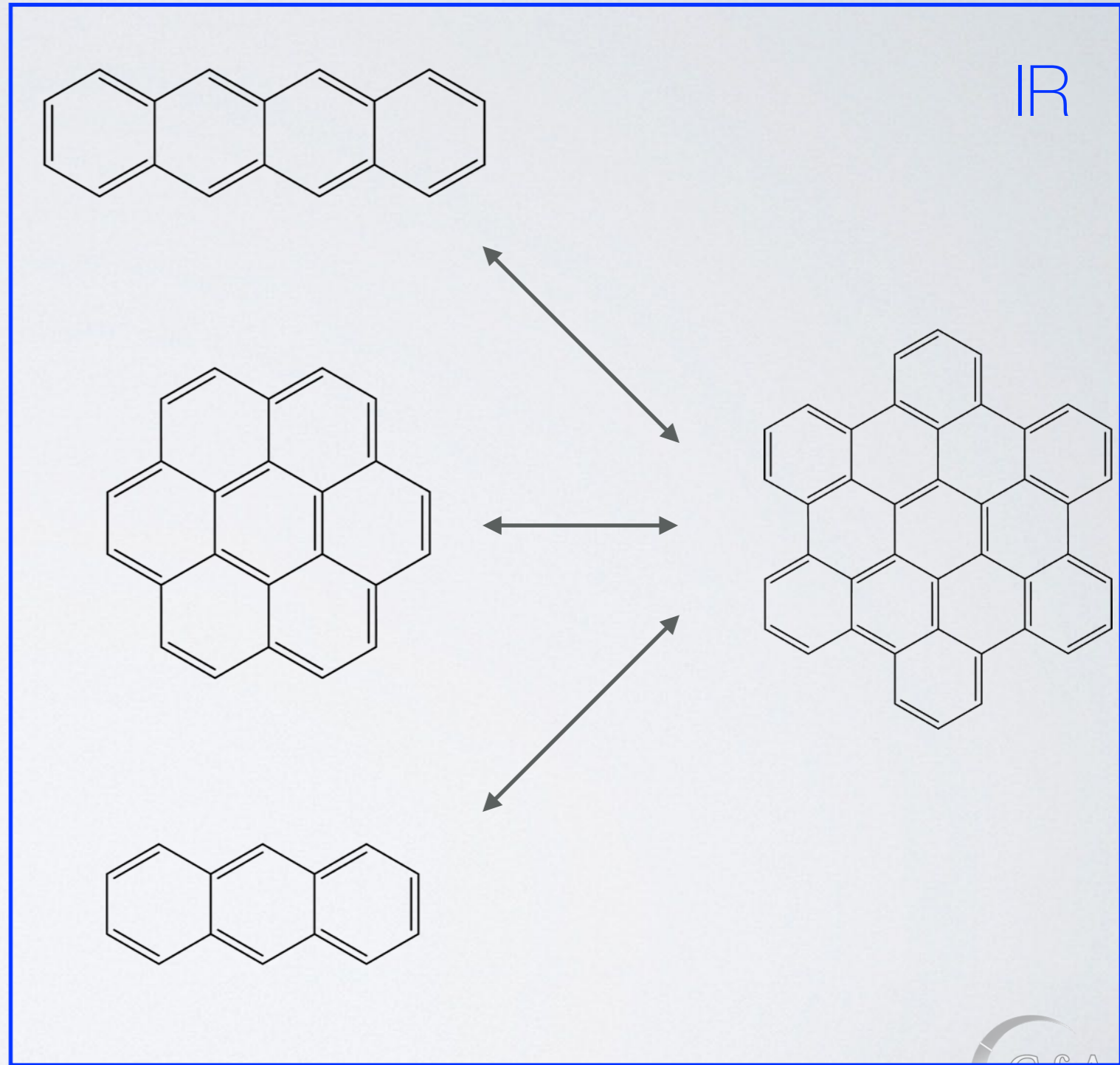
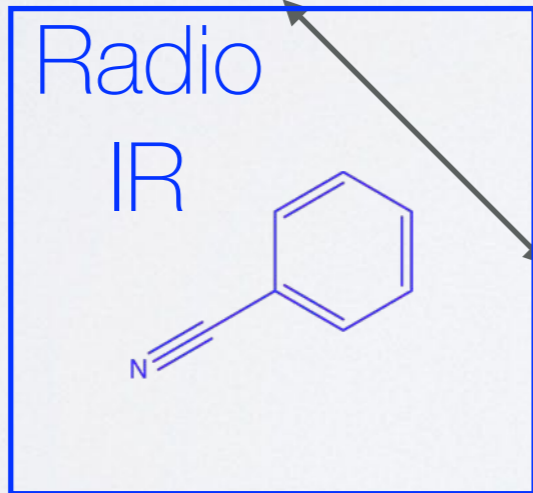
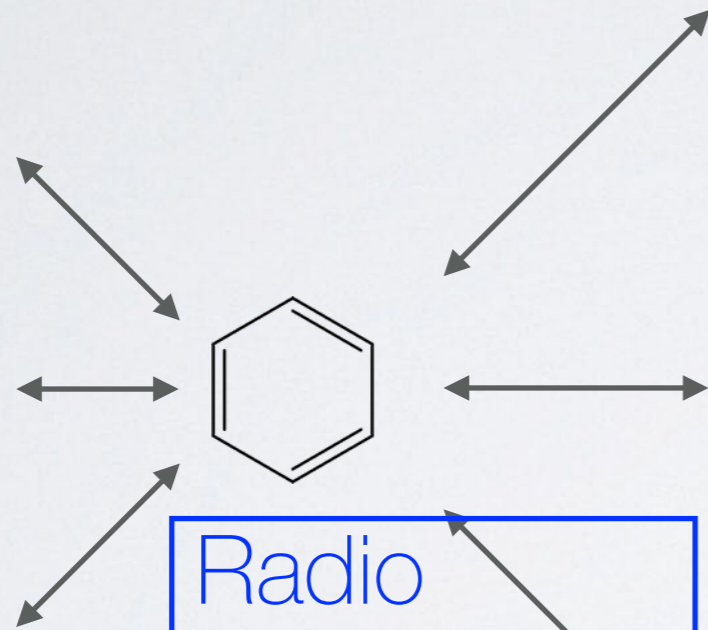
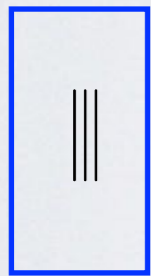
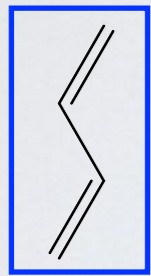
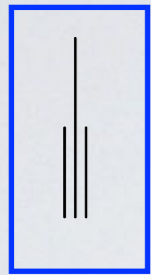






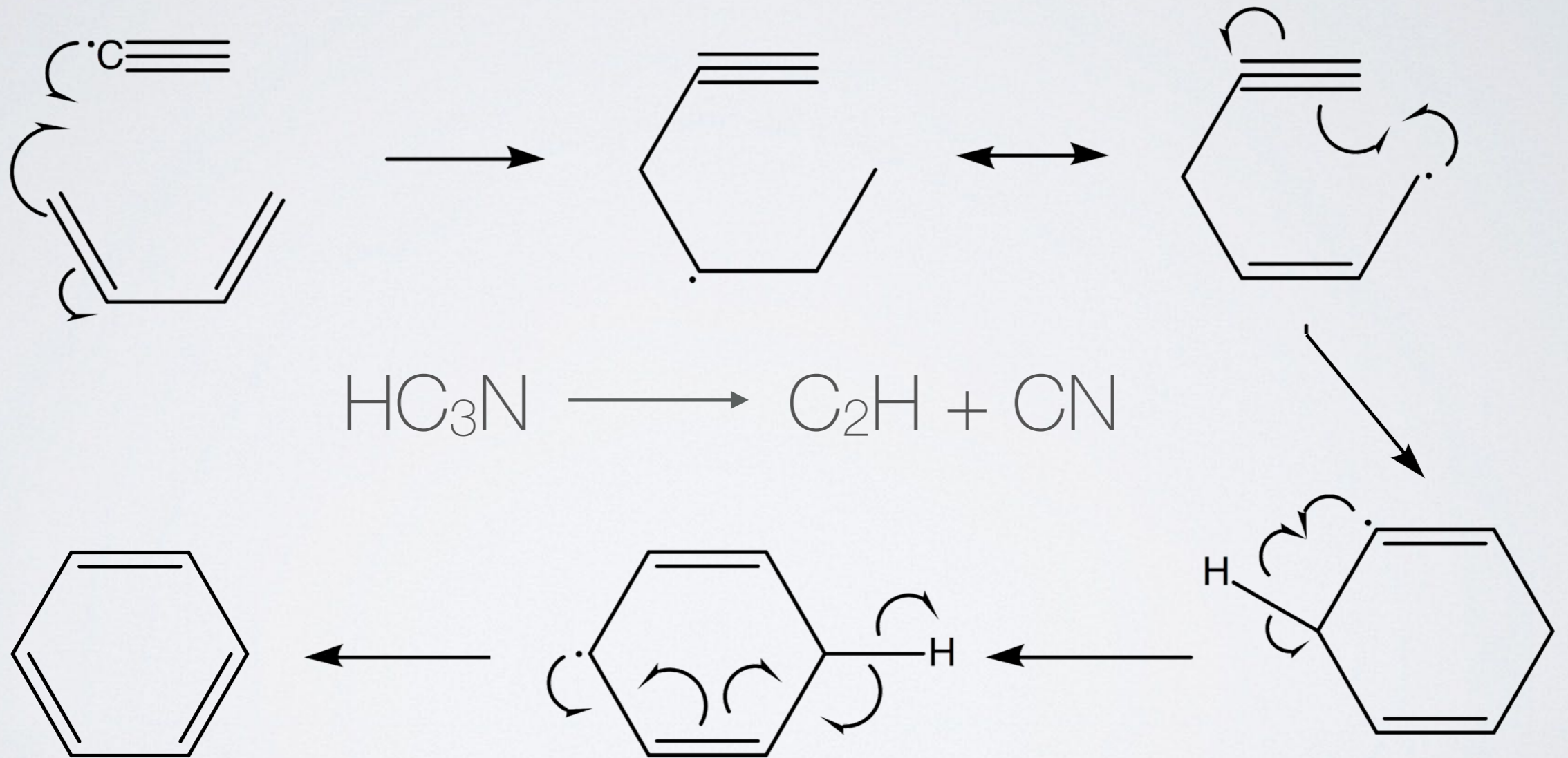


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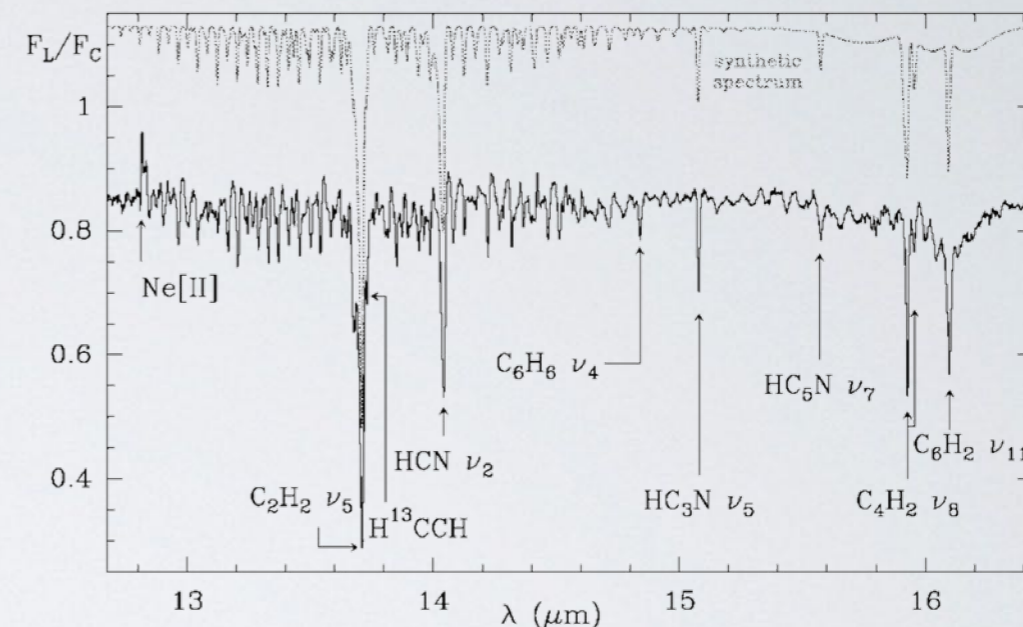


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## Vibrational spectra of benzene derivatives—XVII. Benzonitrile and substituted benzonitriles

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