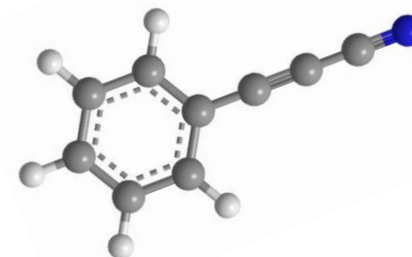


LOW RESOLUTION VIBRATIONAL AND PURE ROTATIONAL STUDIES OF CYANOPHENYLACETYLENE

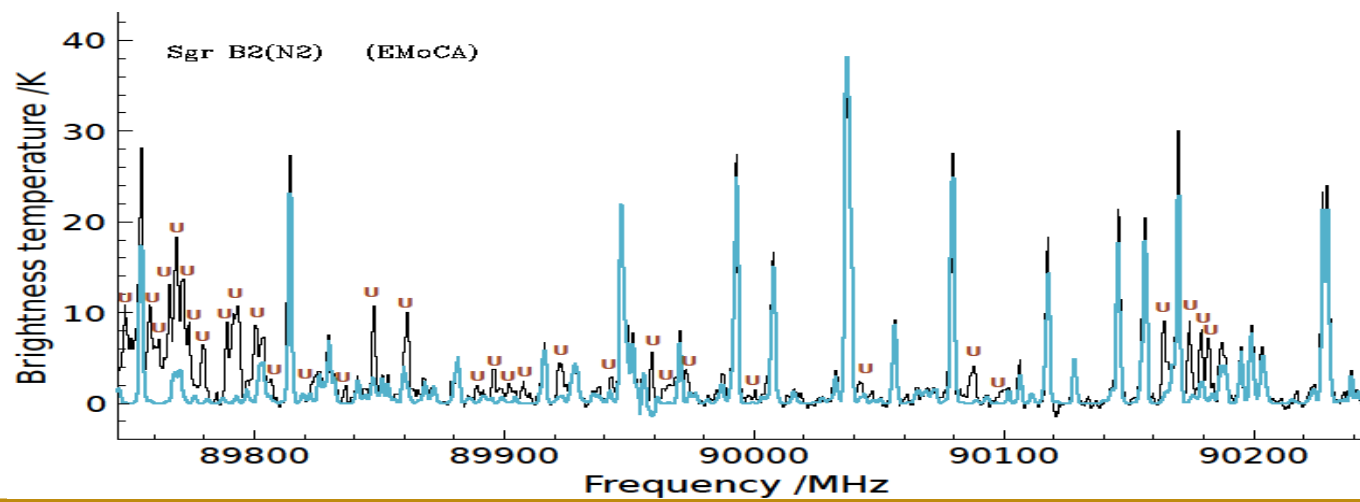
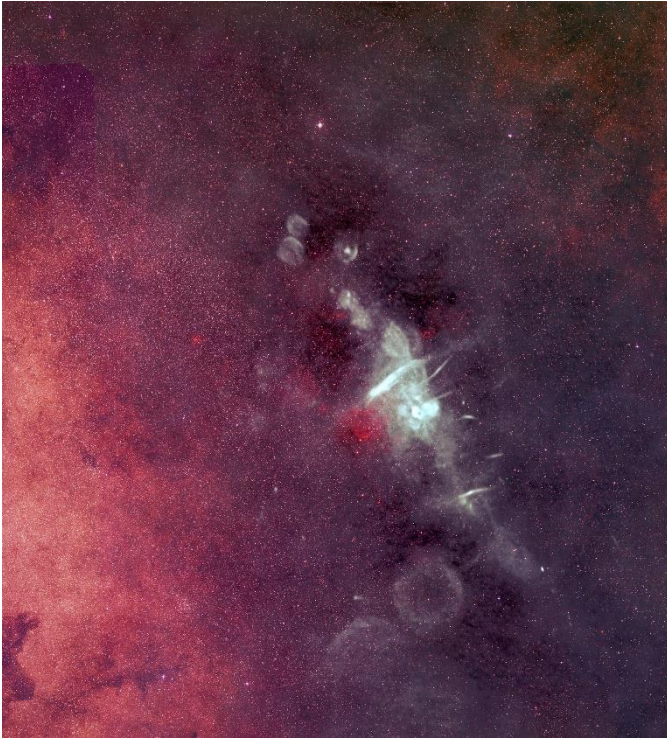
Zachary Buchanan, Olivia Chitarra,

Kelvin Lee, Mike McCarthy

Olivier Pirali, Marie-Aline Martin-Drumel



Studying molecules in space

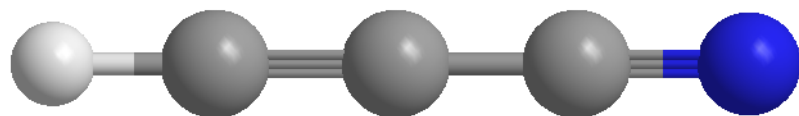


DETECTION OF INTERSTELLAR CYANOACETYLENE

B. E. TURNER

National Radio Astronomy Observatory,*
Green Bank, West Virginia

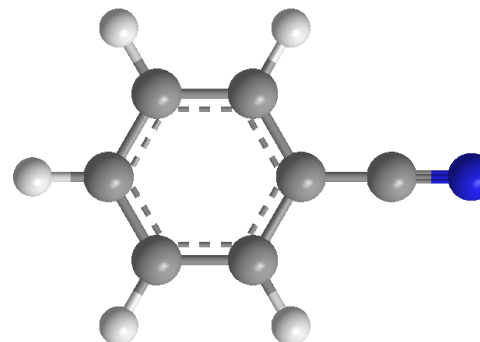
Received 1970 November 14



ASTROCHEMISTRY

Detection of the aromatic molecule benzonitrile (*c*-C₆H₅CN) in the interstellar medium

Brett A. McGuire,^{1,2*} Andrew M. Burkhardt,³ Sergei Kalenskii,⁴
Christopher N. Shingledecker,⁵ Anthony J. Remijan,¹
Eric Herbst,^{3,5} Michael C. McCarthy^{2,6}



Potential for cyanophenylacetylene in space

DETECTION OF INTERSTELLAR CYANOACETYLENE

B. E. TURNER

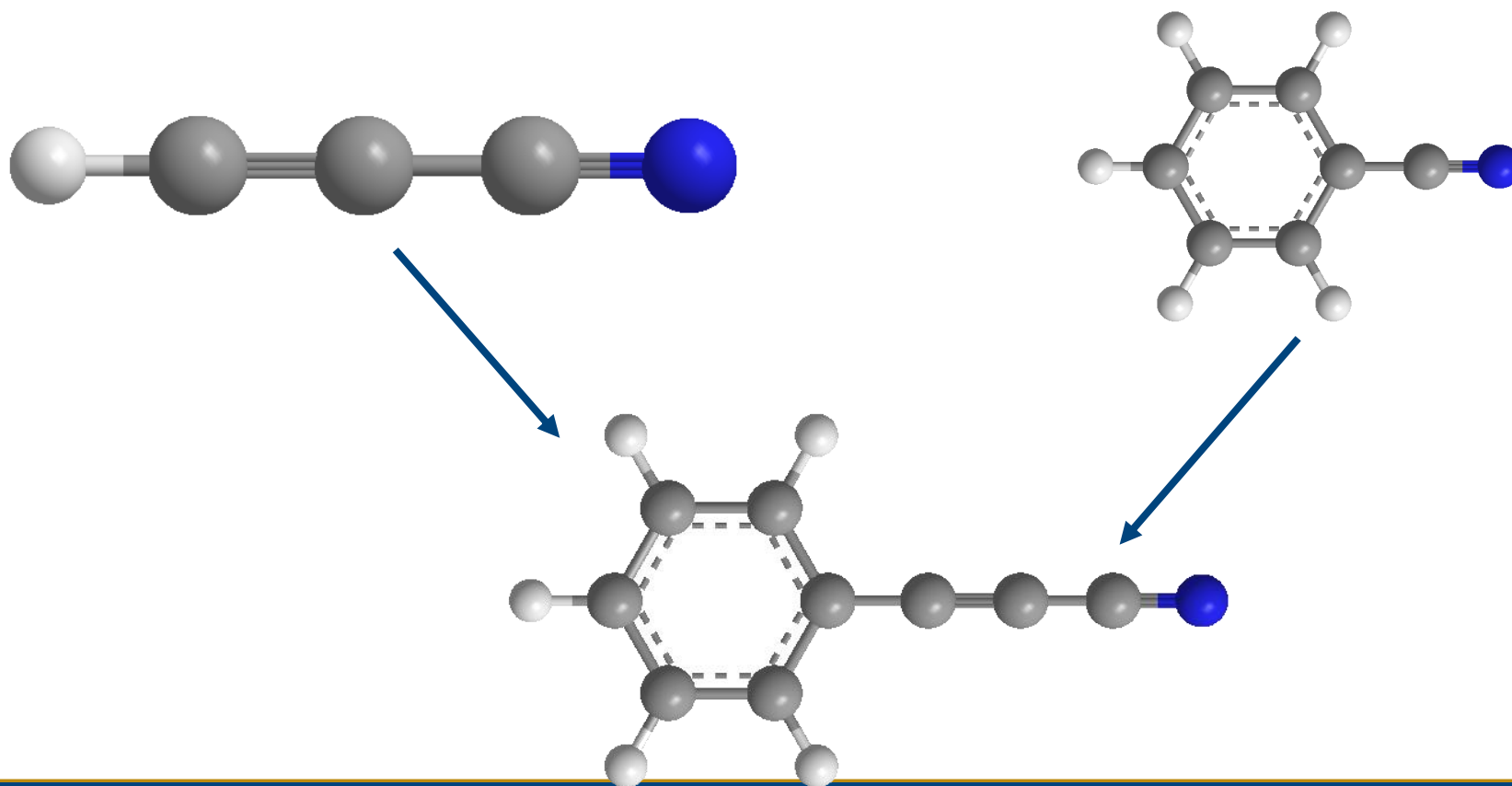
National Radio Astronomy Observatory,*
Green Bank, West Virginia

Received 1970 November 14

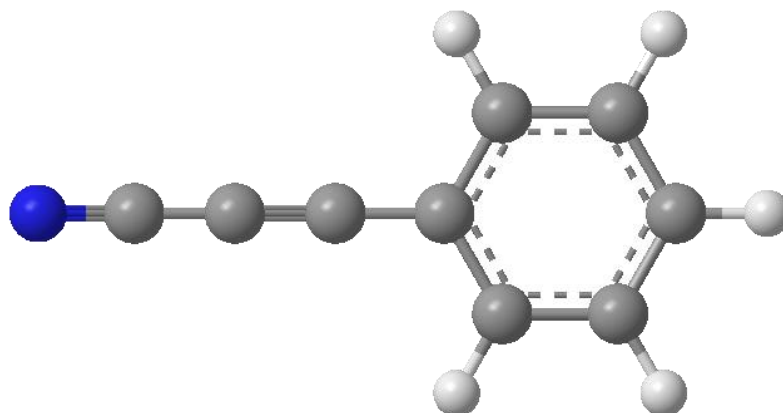
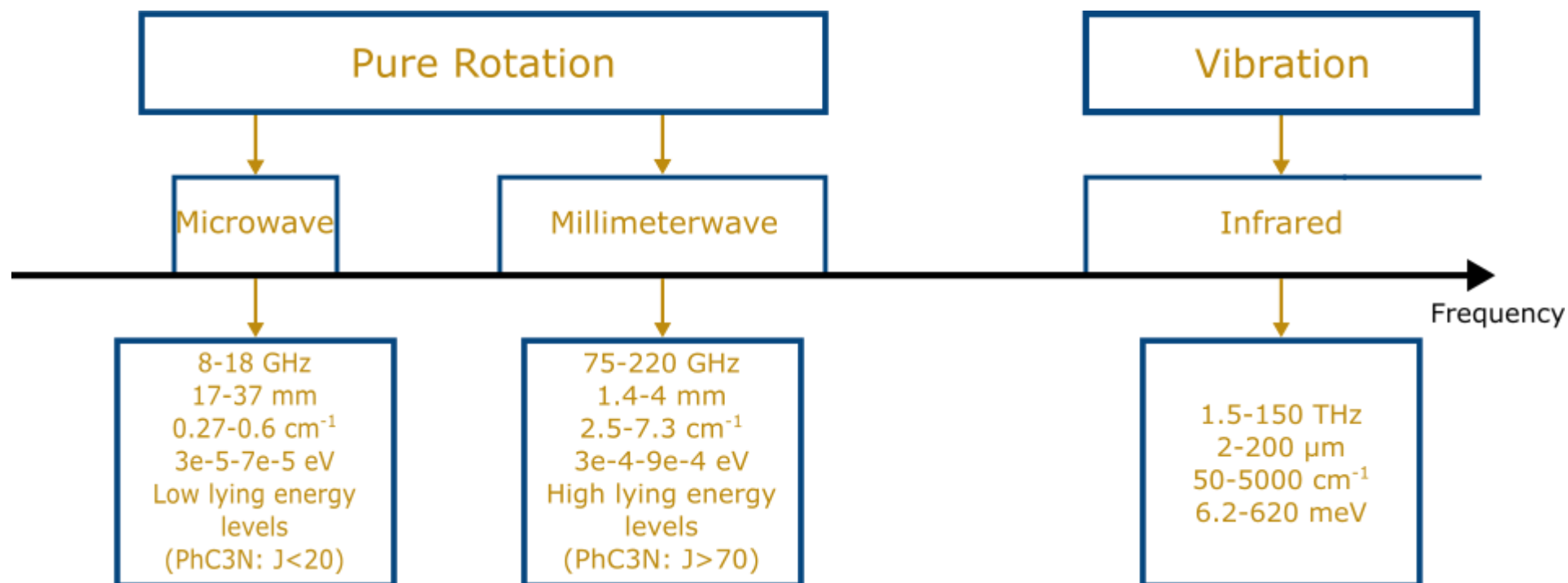
ASTROCHEMISTRY

Detection of the aromatic molecule benzonitrile ($c\text{-C}_6\text{H}_5\text{CN}$) in the interstellar medium

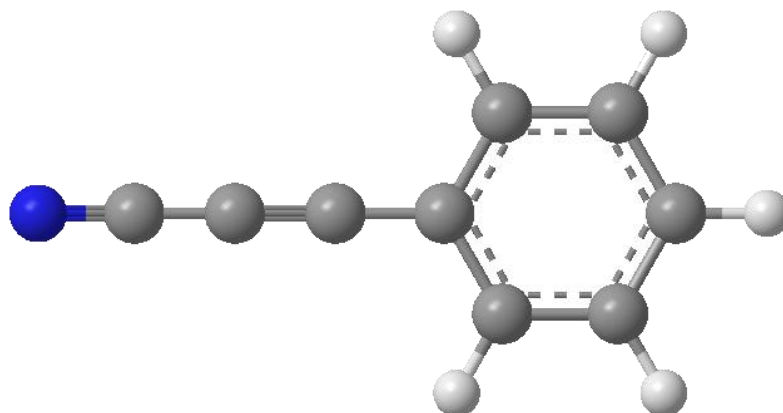
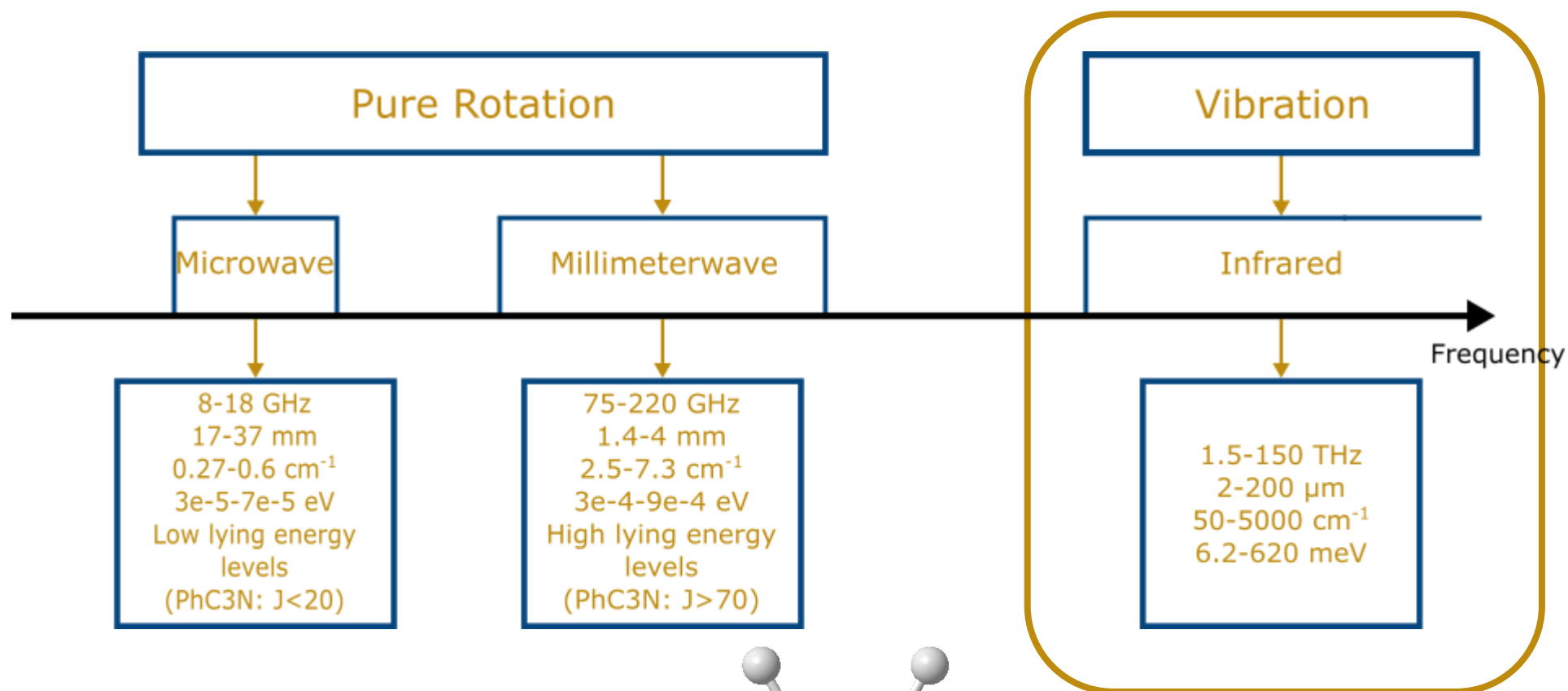
Brett A. McGuire,^{1,2*} Andrew M. Burkhardt,³ Sergei Kalenskii,⁴
Christopher N. Shingledecker,⁵ Anthony J. Remijan,¹
Eric Herbst,^{3,5} Michael C. McCarthy^{2,6}



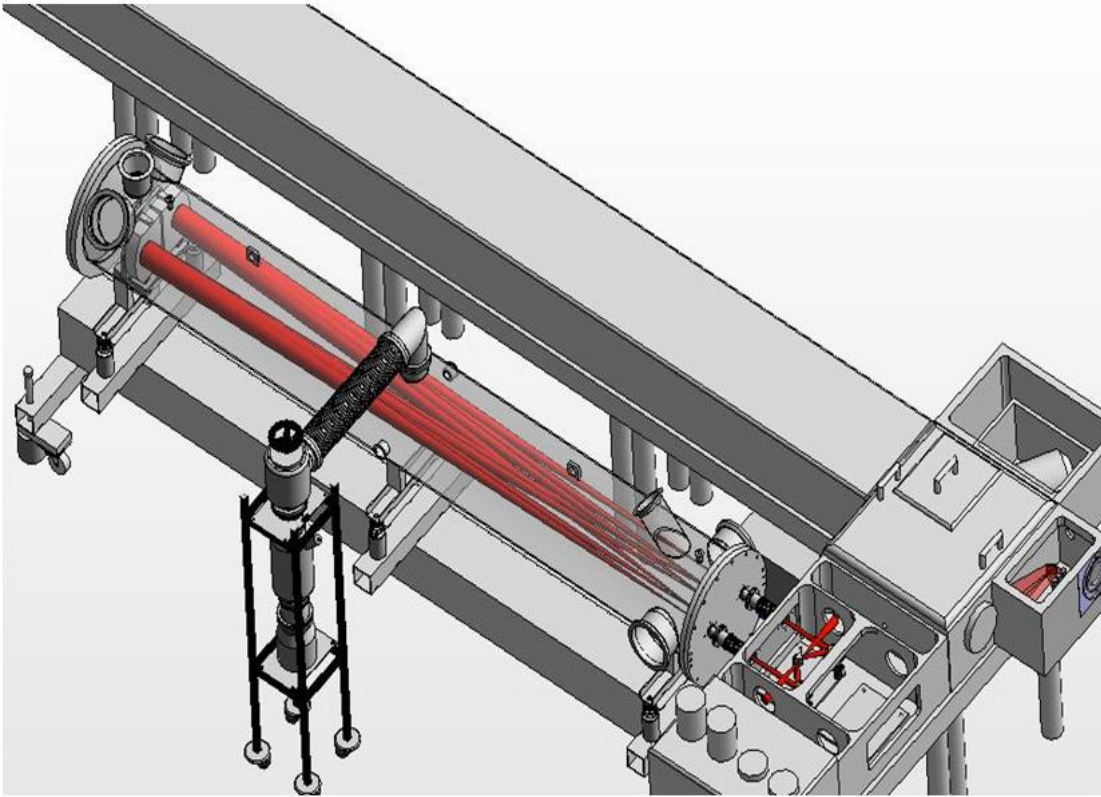
Outline



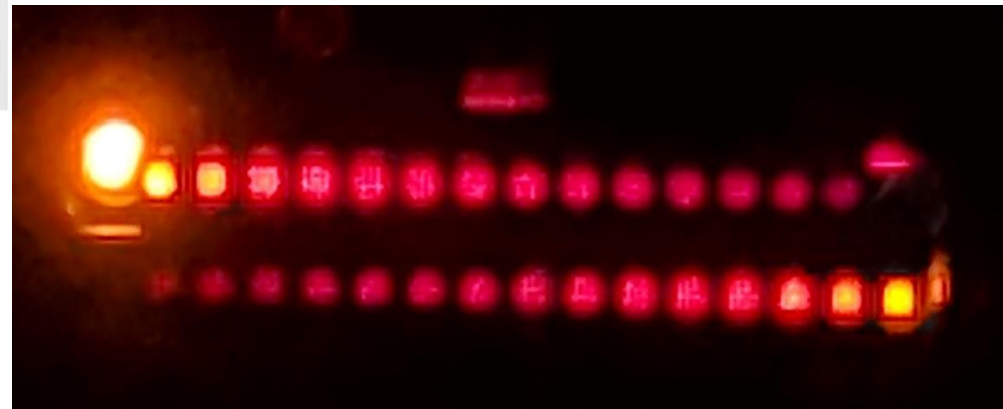
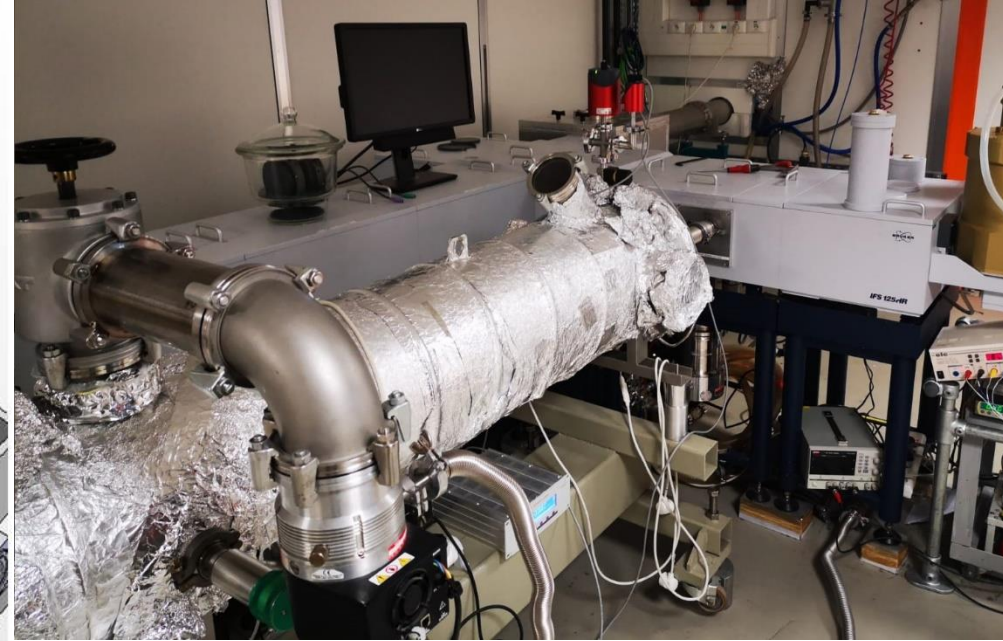
Outline



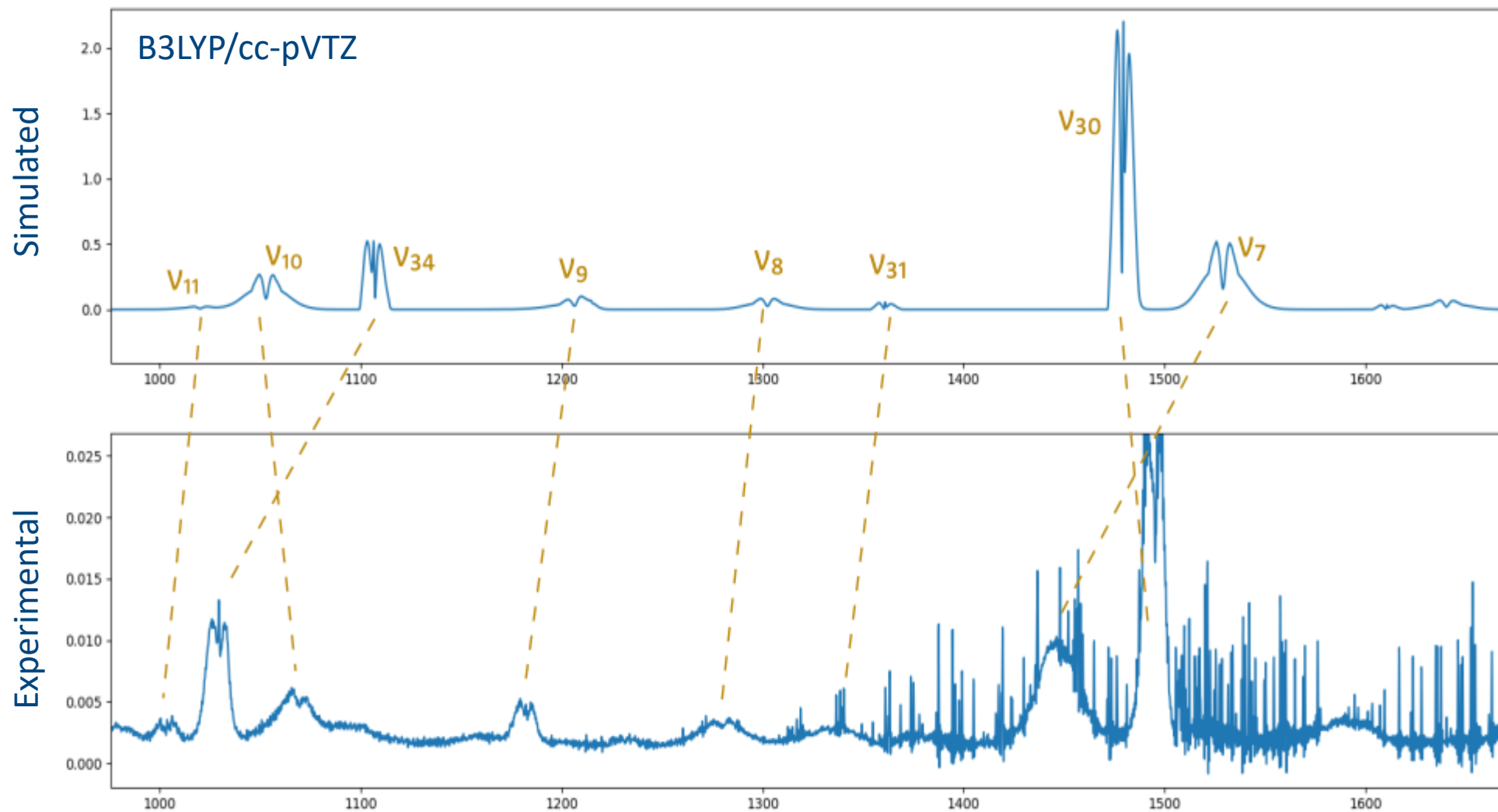
Vibrational spectroscopy experiments



- Room temperature
- 150 m path length
- 1 μ bar pressure

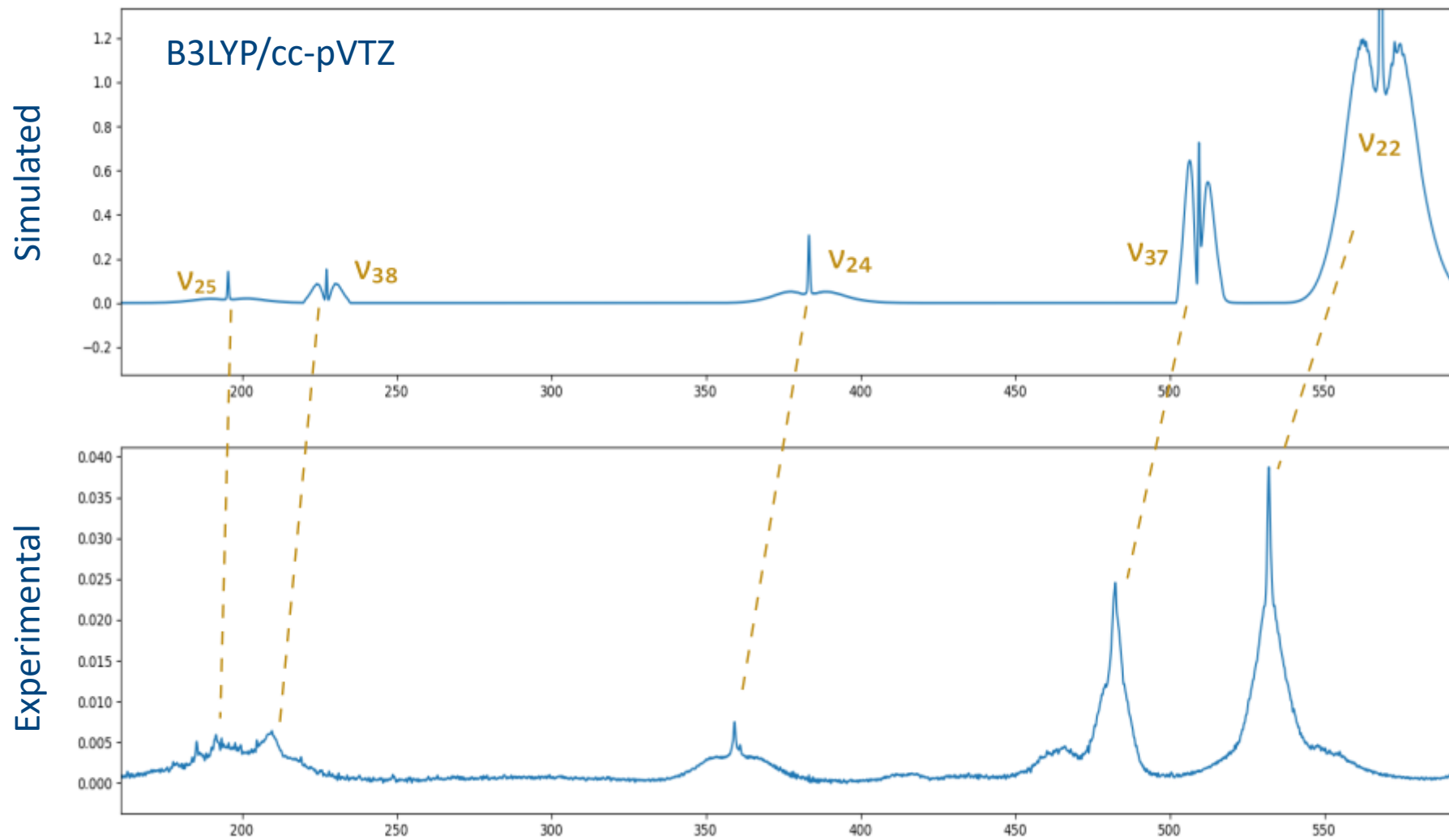


Comparing simulation with experimental

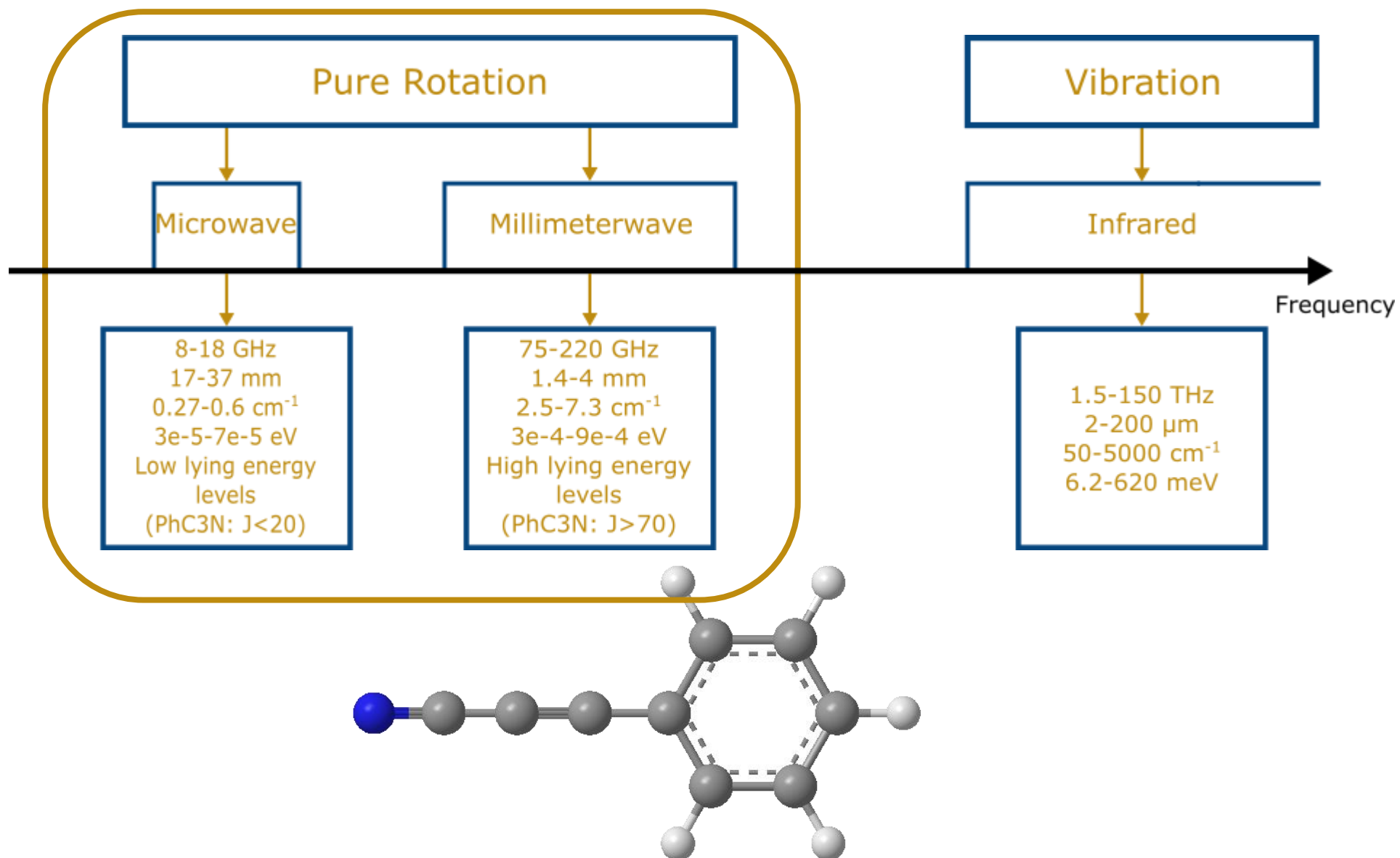


0.5 cm^{-1} resolution, band center accuracy $\approx 1 \text{ cm}^{-1}$

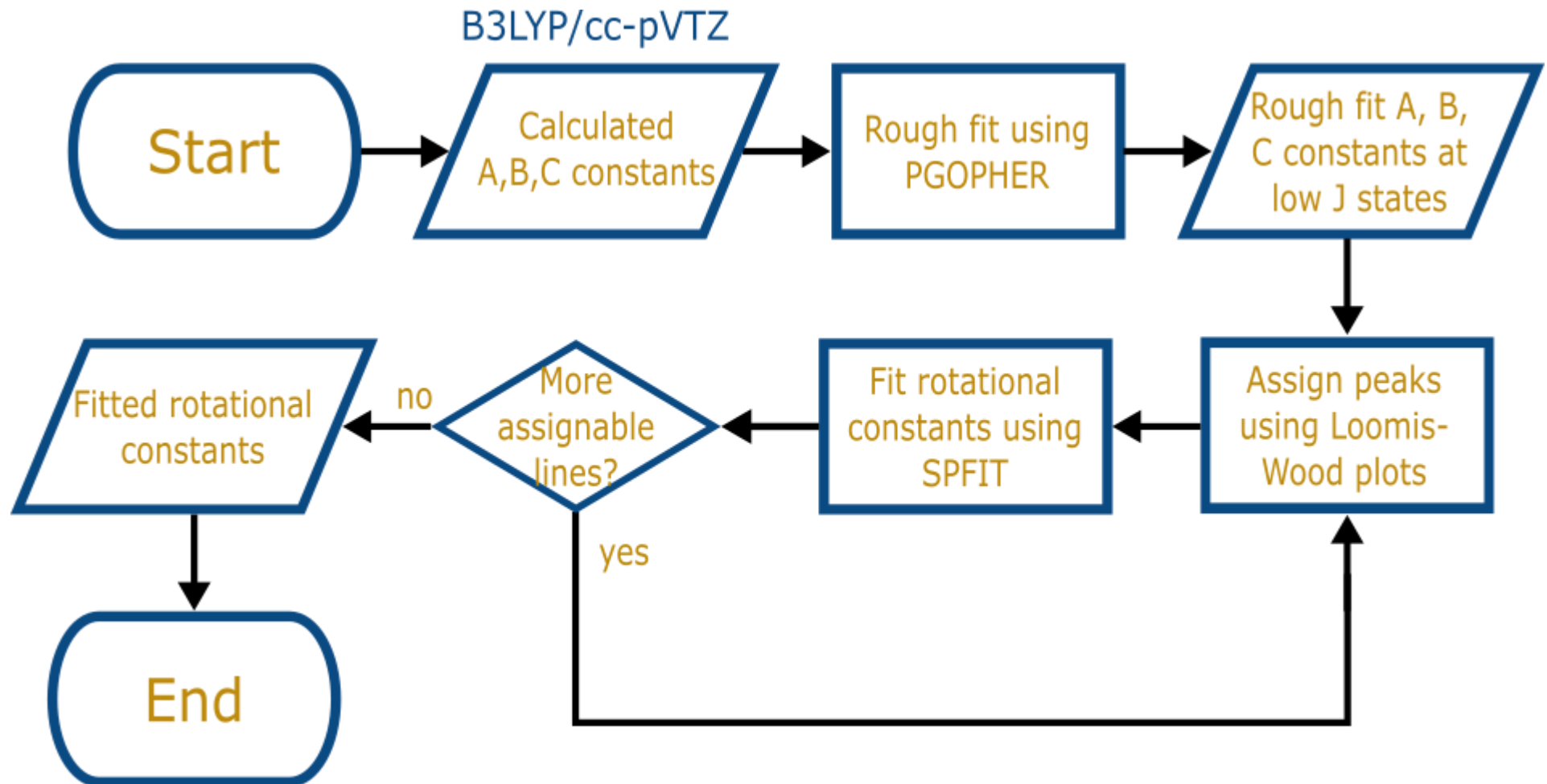
Comparing simulation with experimental



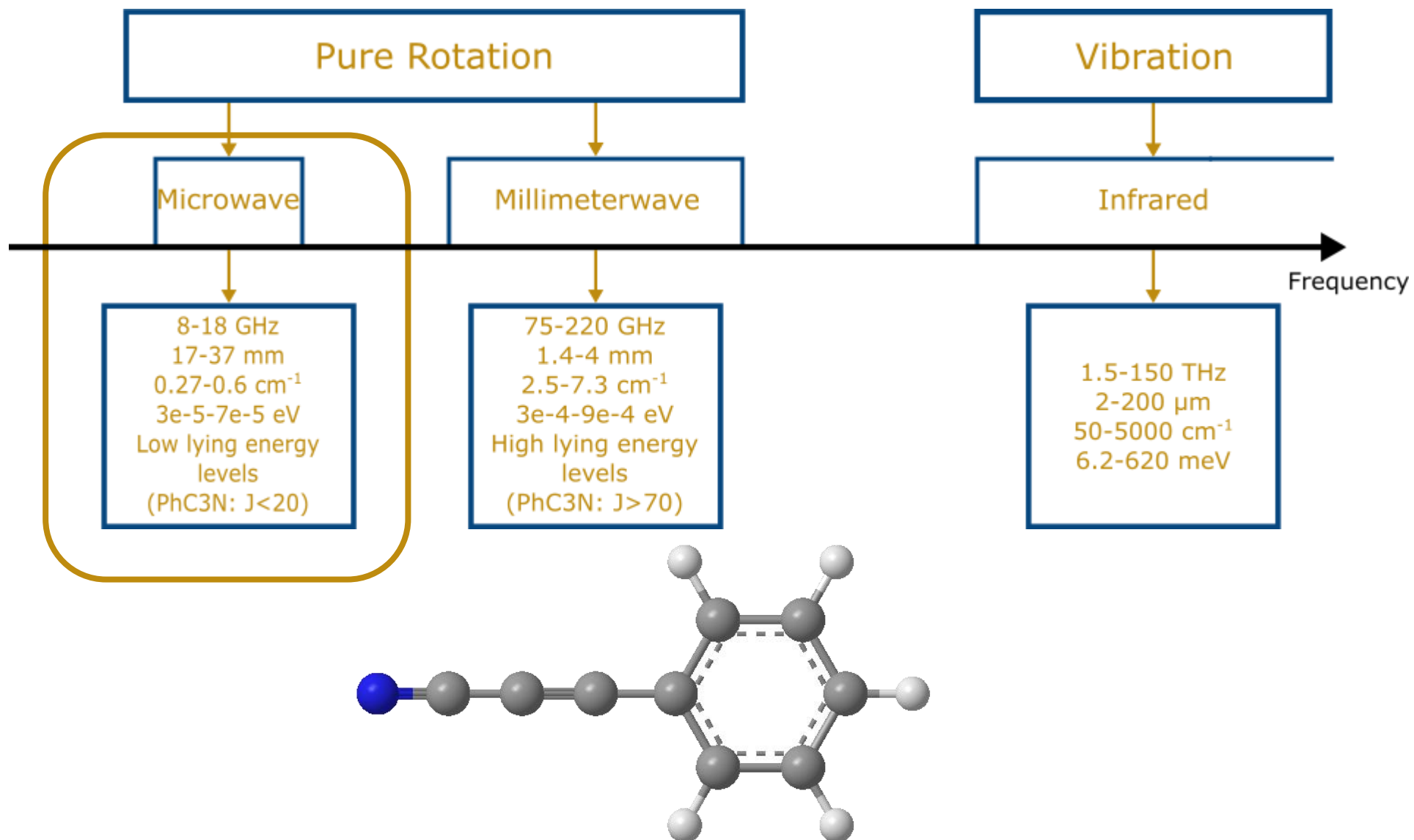
Outline



Assignment process for rotational spectra

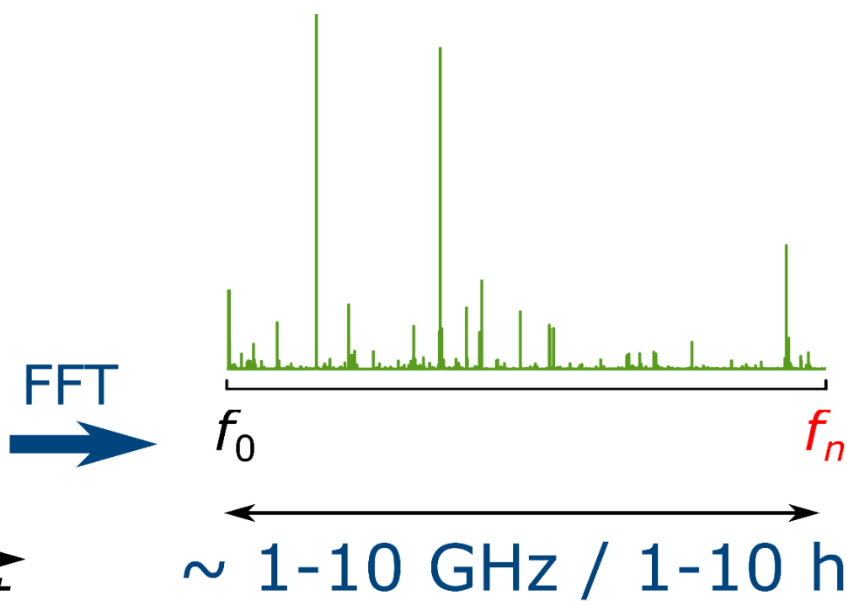
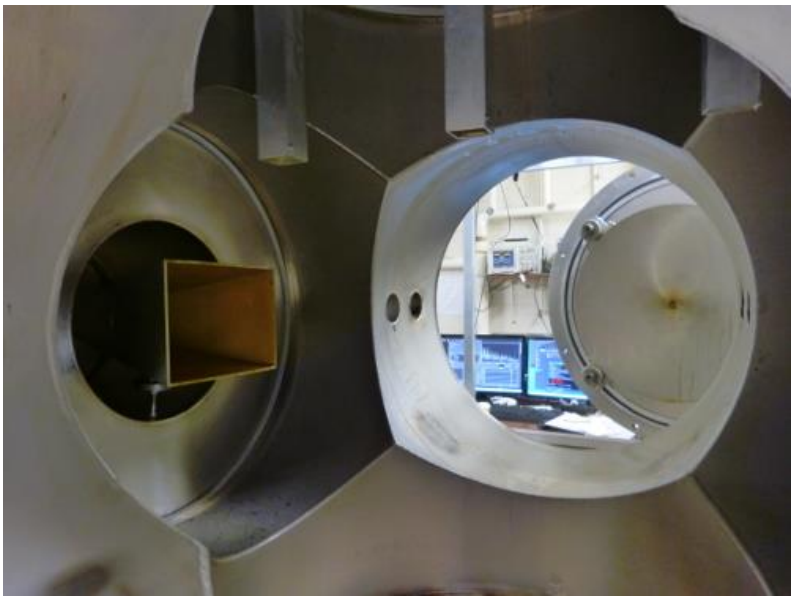
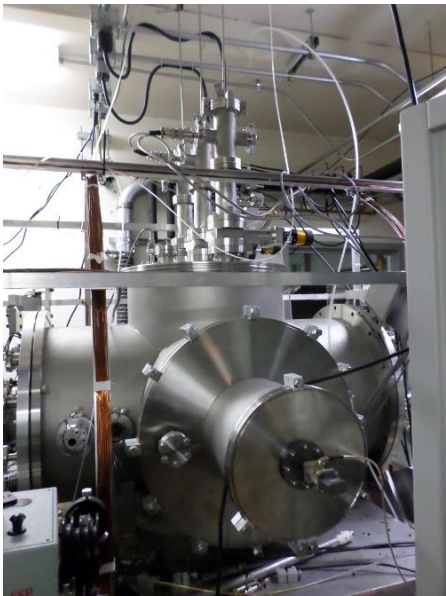
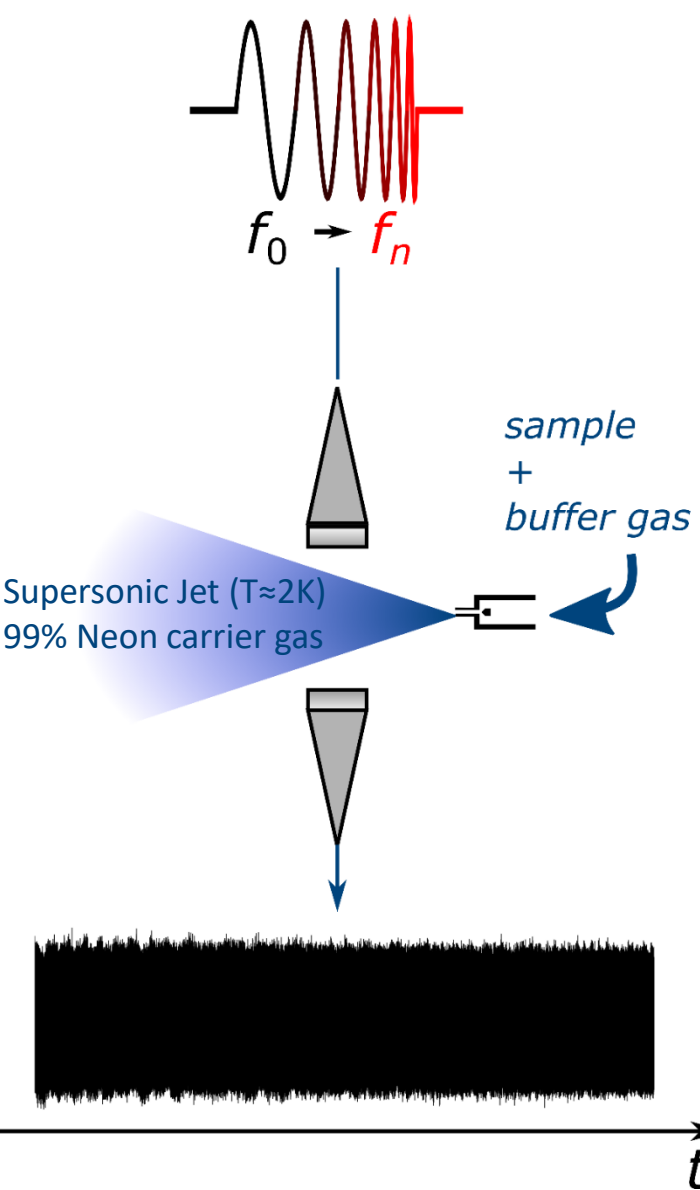


Outline



8-18 GHz experimental setup

Chirped-pulse

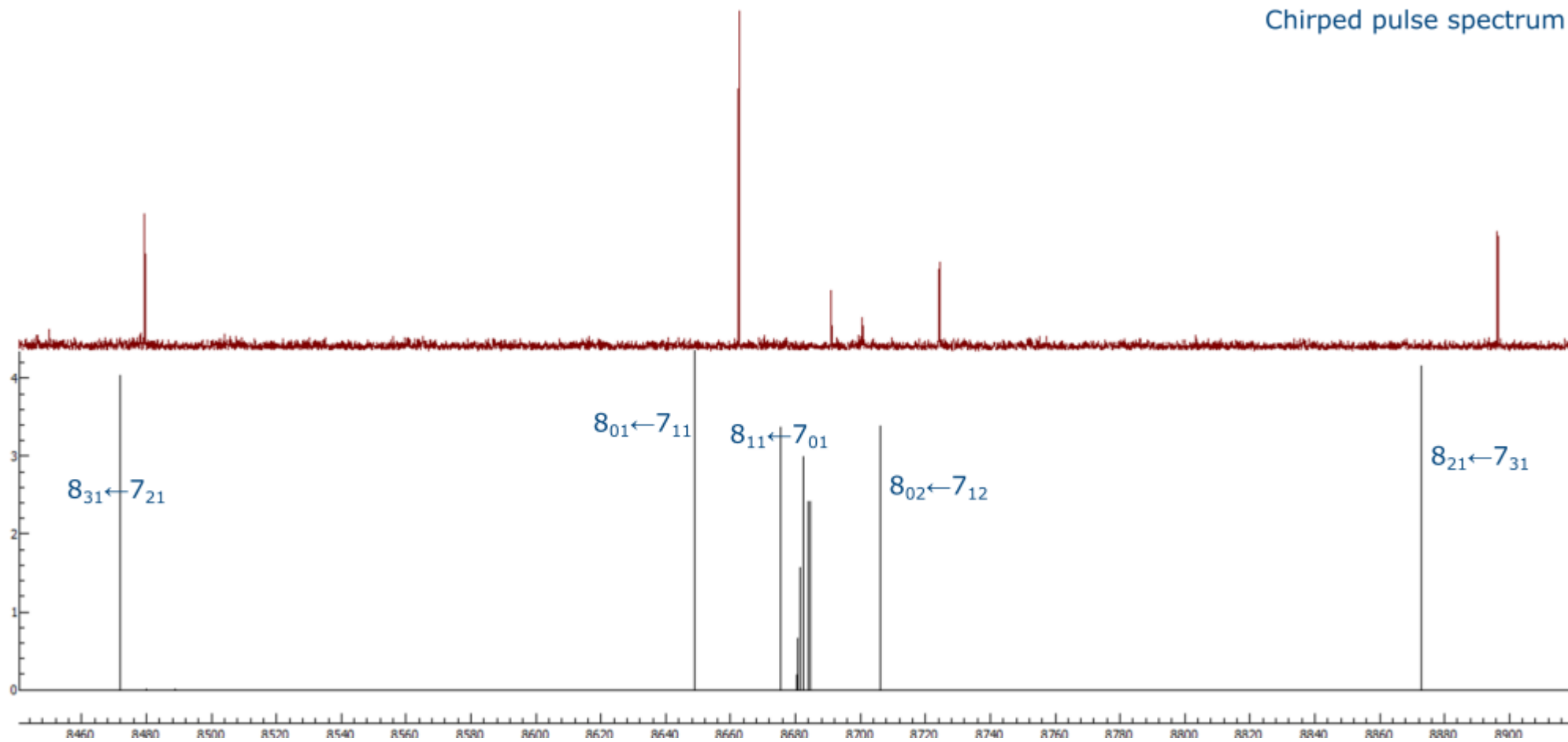


Experiment

Chirped pulse spectrum

Simulation

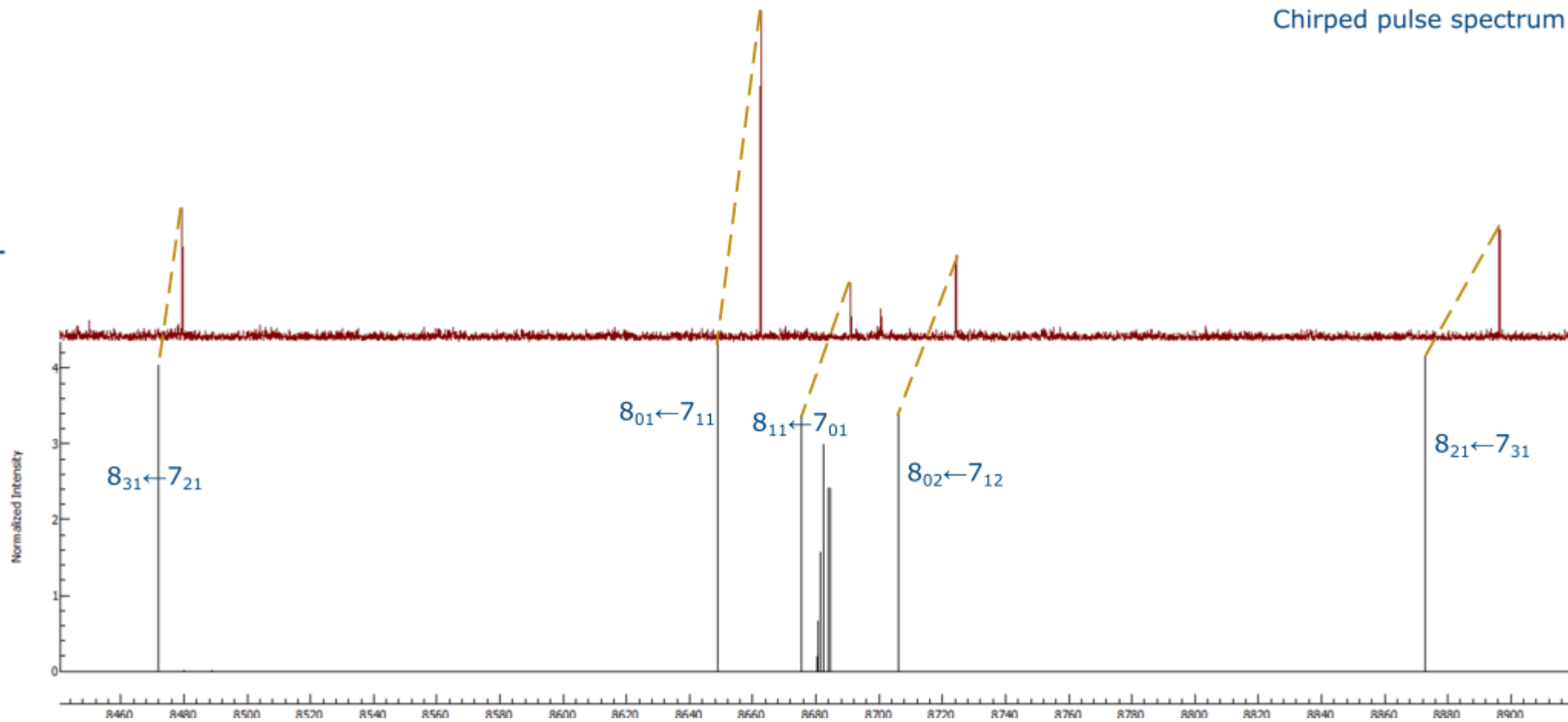
Normalized Intensity



Experiment

Simulation

Chirped pulse spectrum

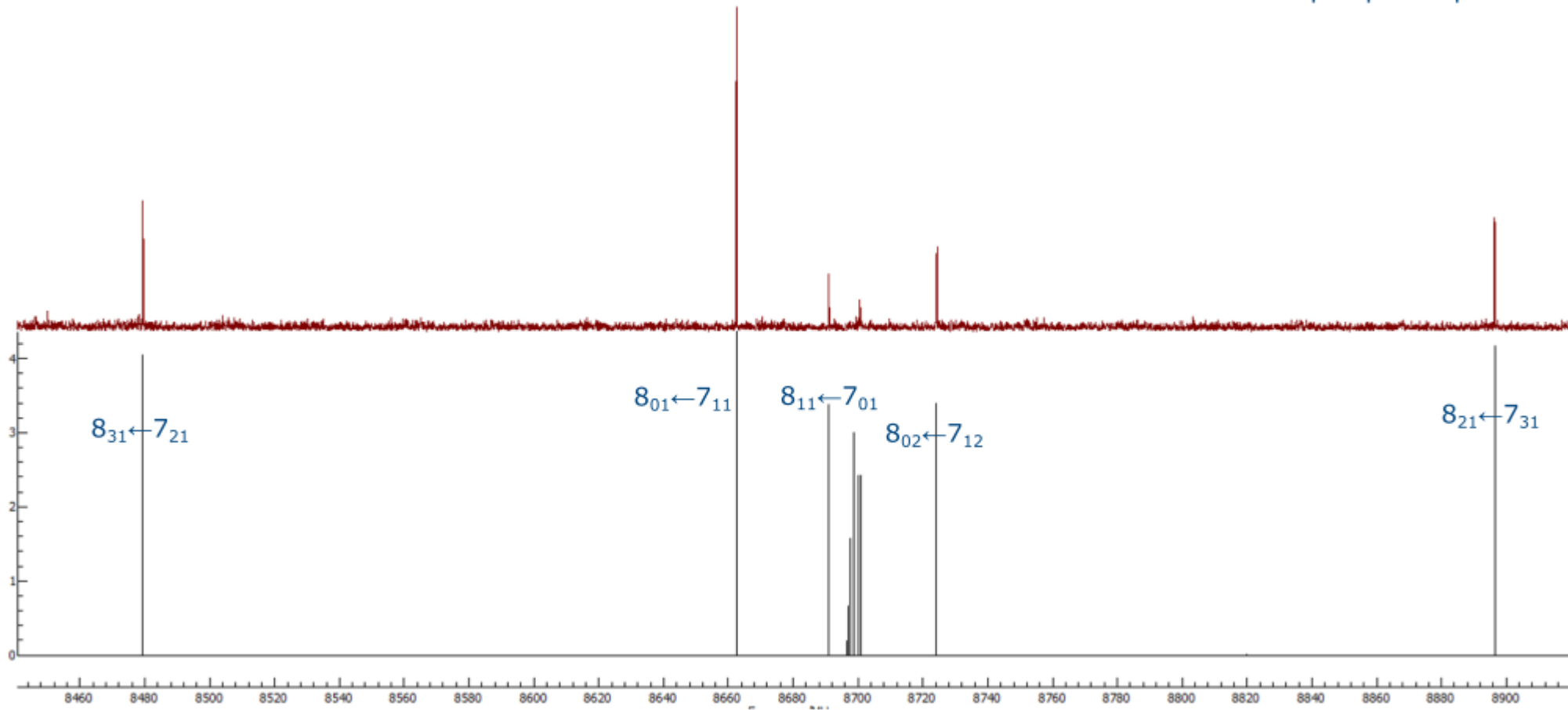


Chirped pulse spectrum

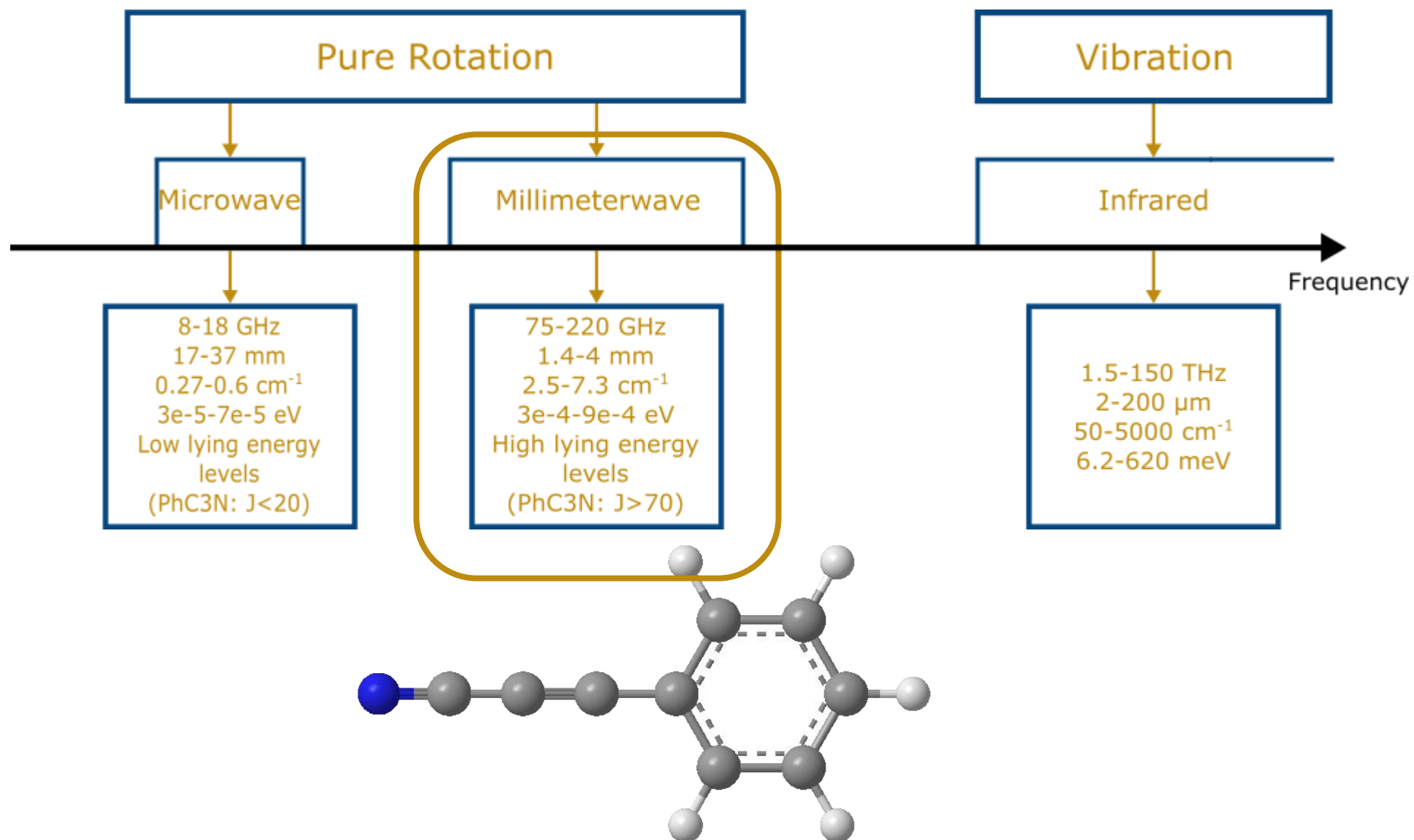
Experiment

Simulation

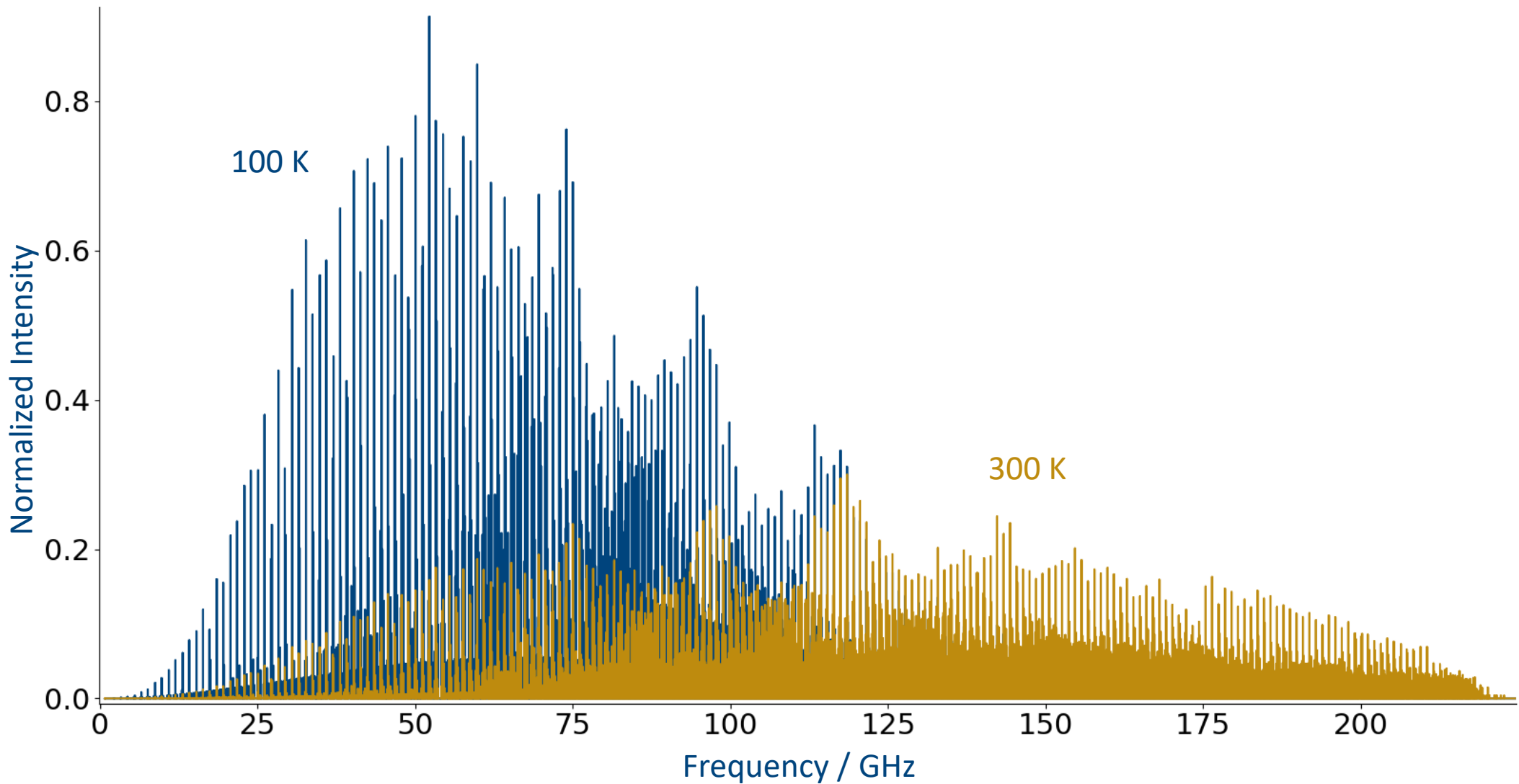
Normalized Intensity



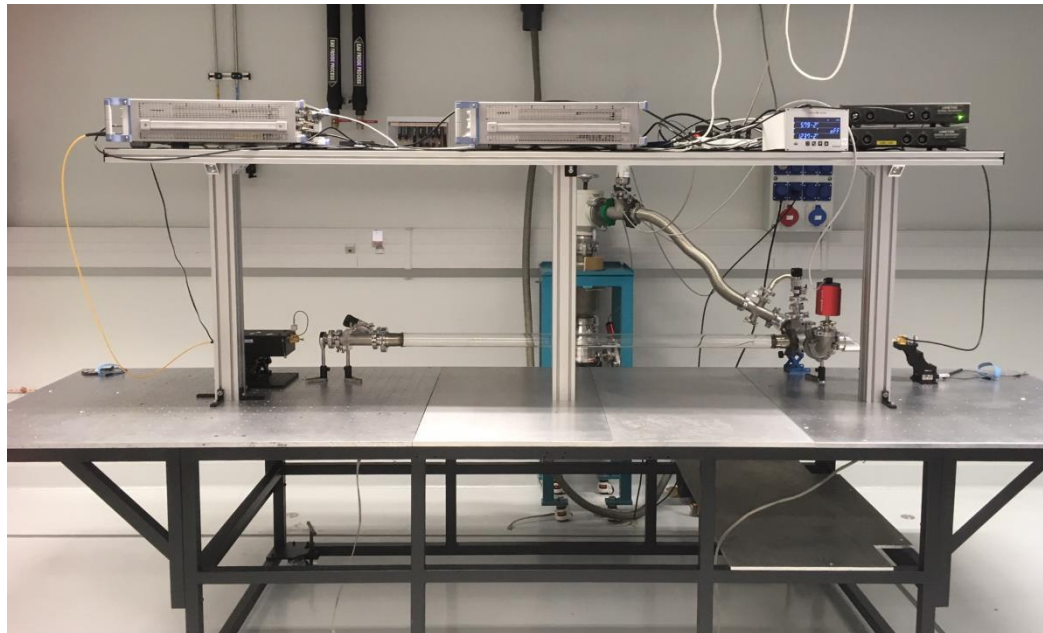
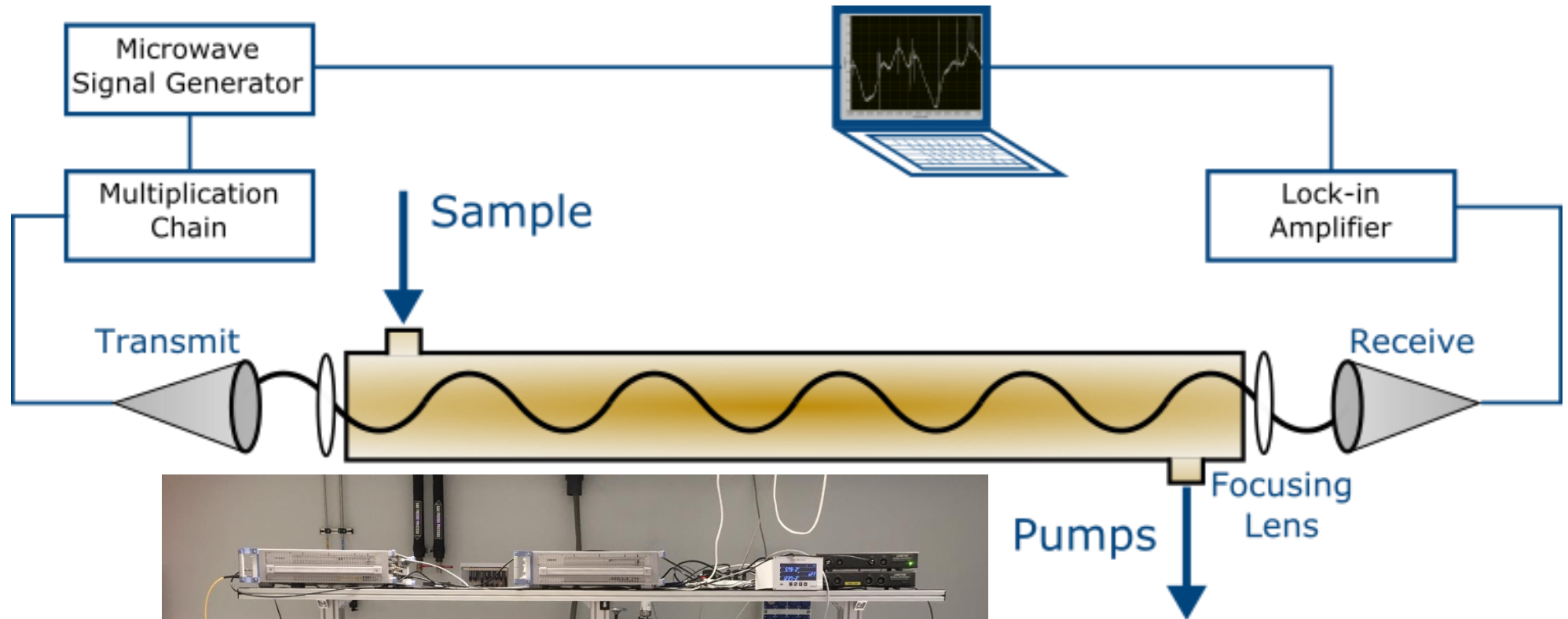
Outline



Temperature dependence of rotational spectra



75-220 GHz experimental setup

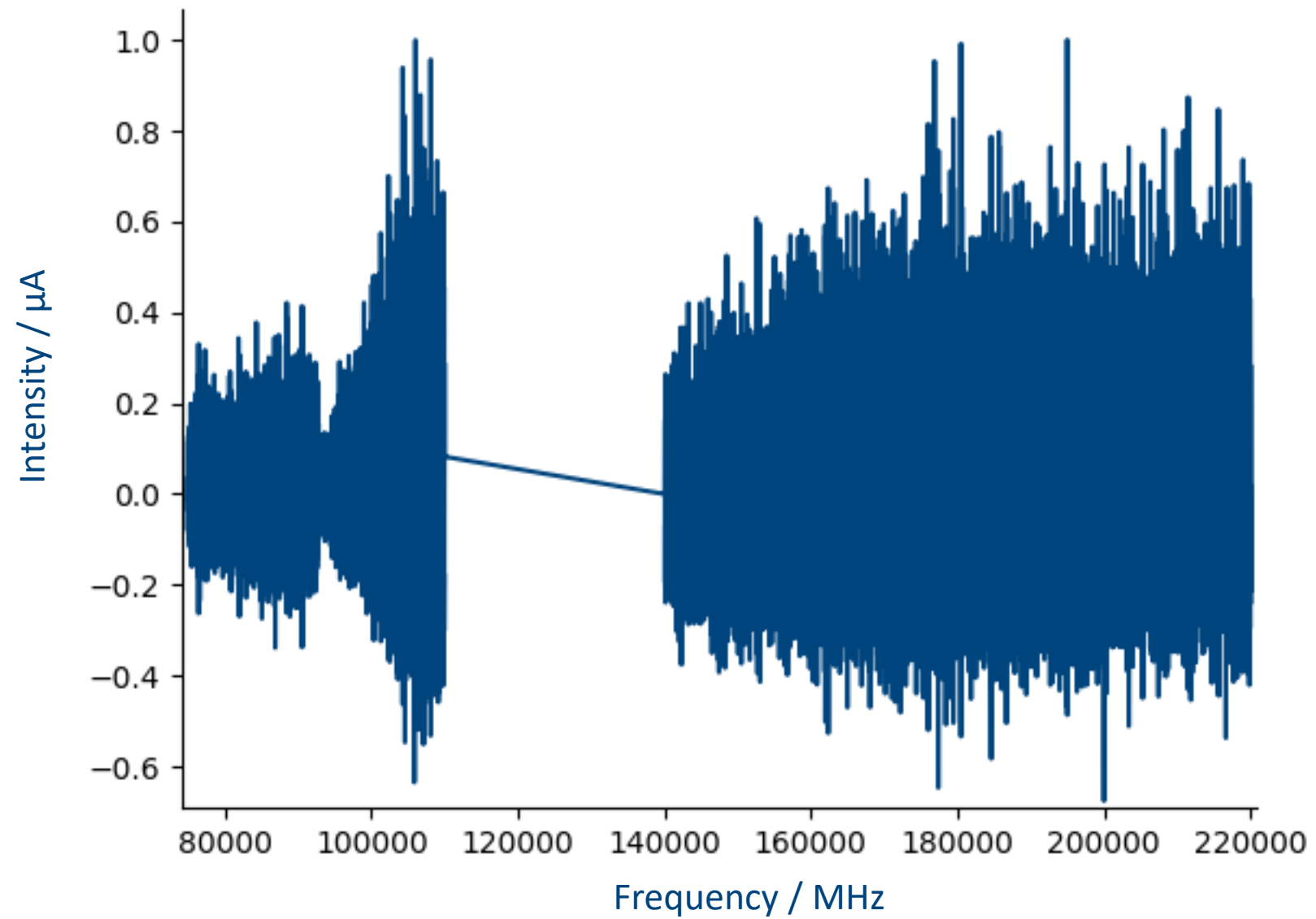


Pumps

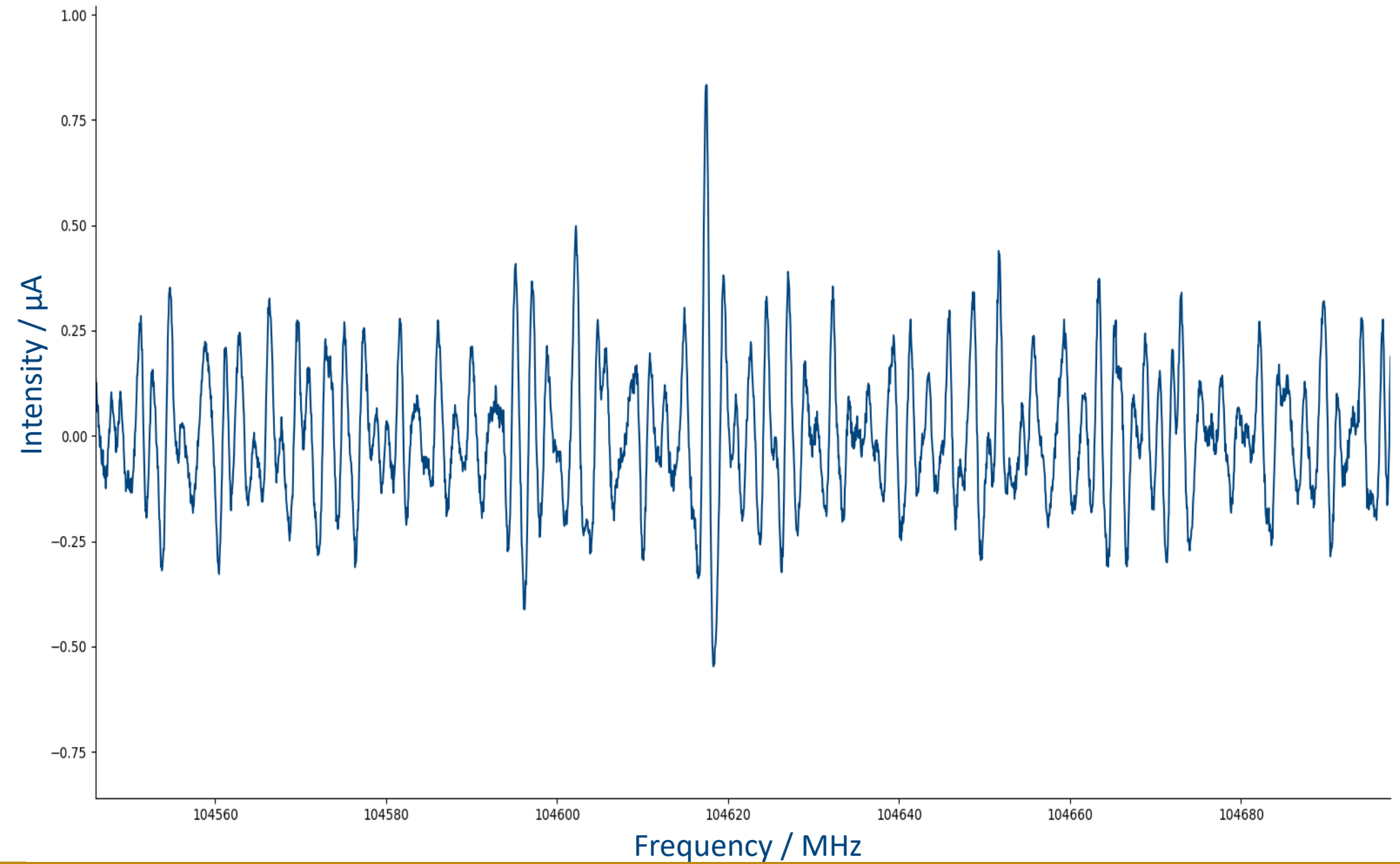
Focusing
Lens

- Room temperature
- 2 m path length
- 5 μ bar pressure

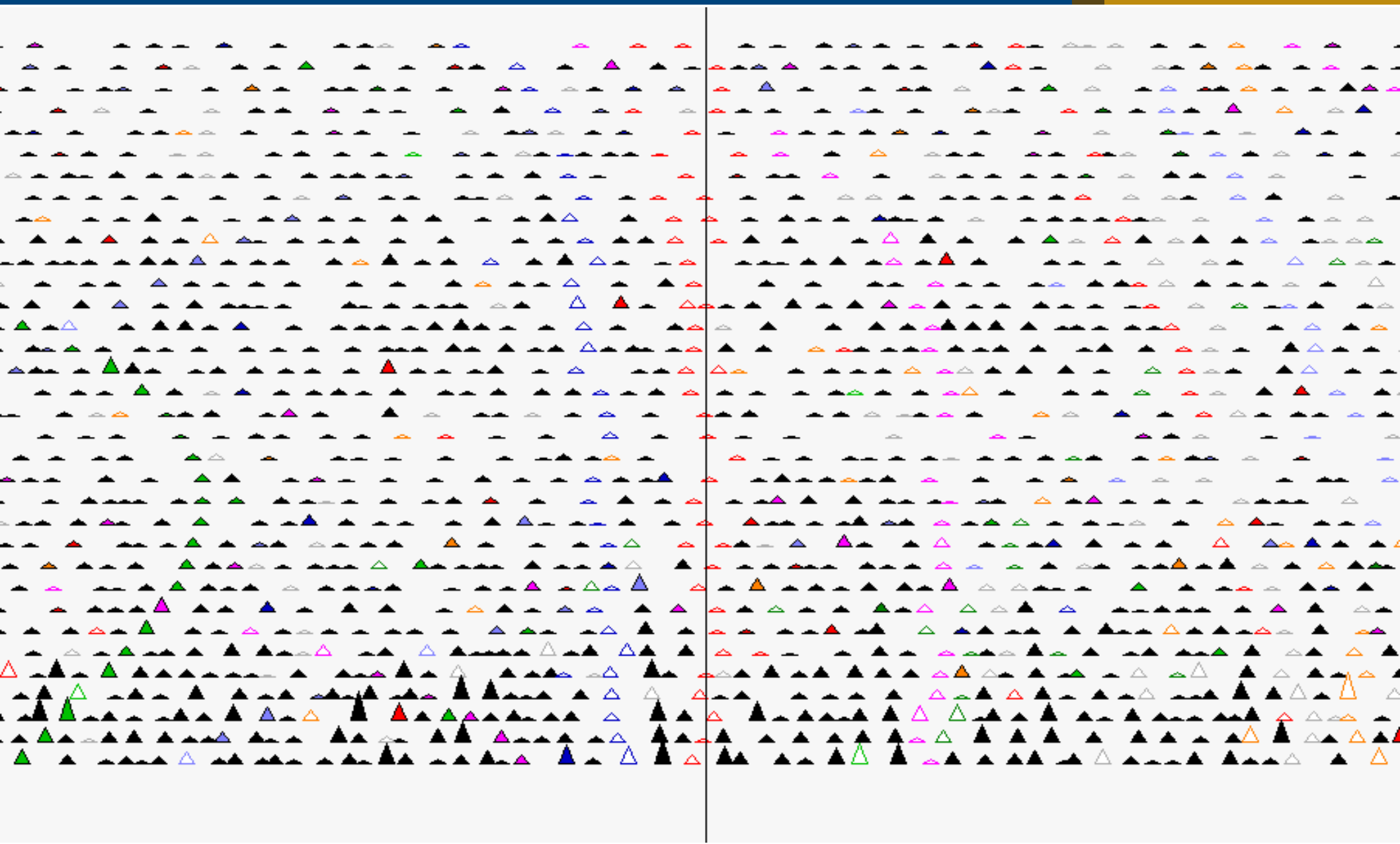
Millimeterwave spectrum



Millimeterwave spectrum

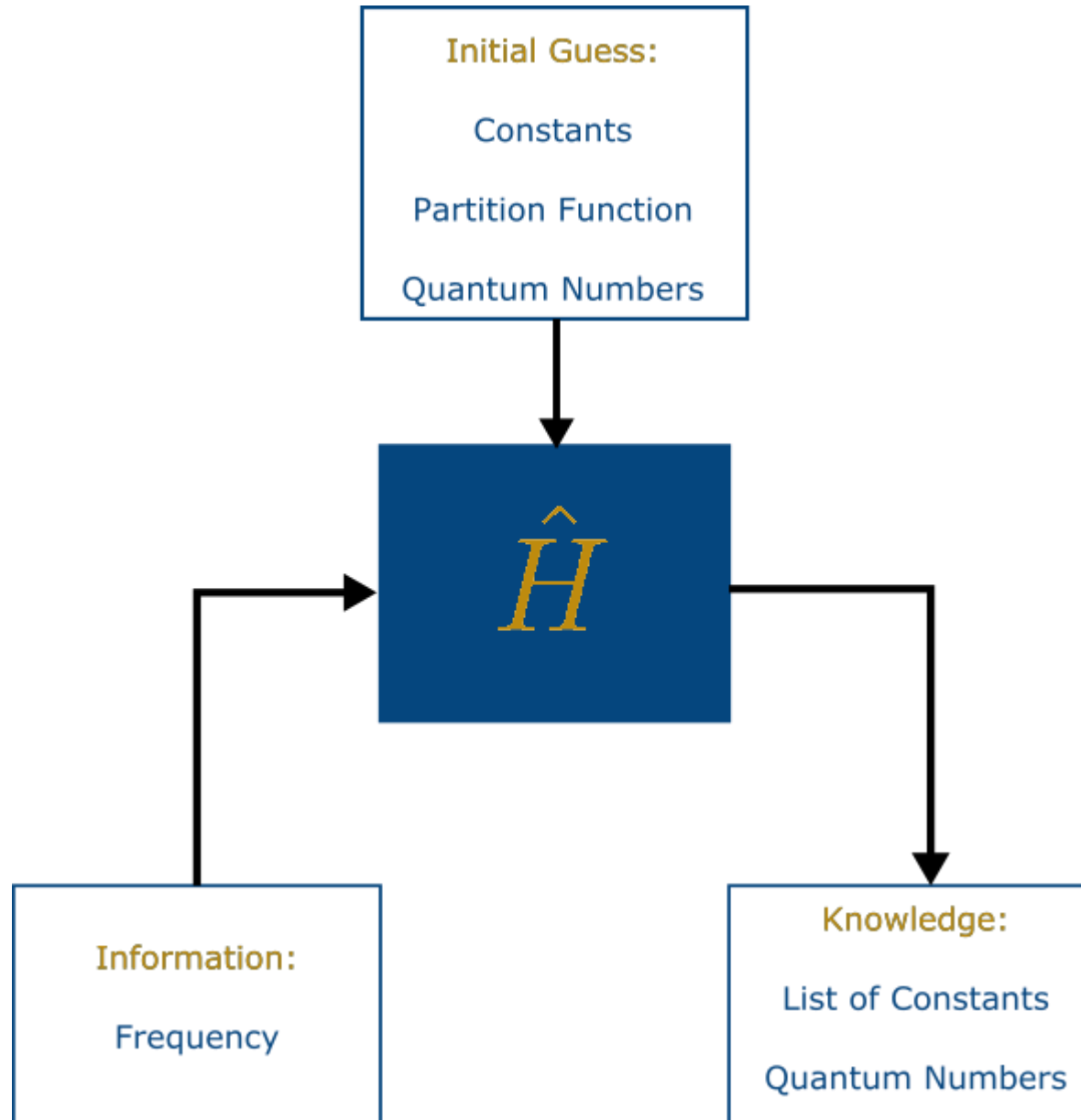


Loomis-wood plot



Loomis-wood plot





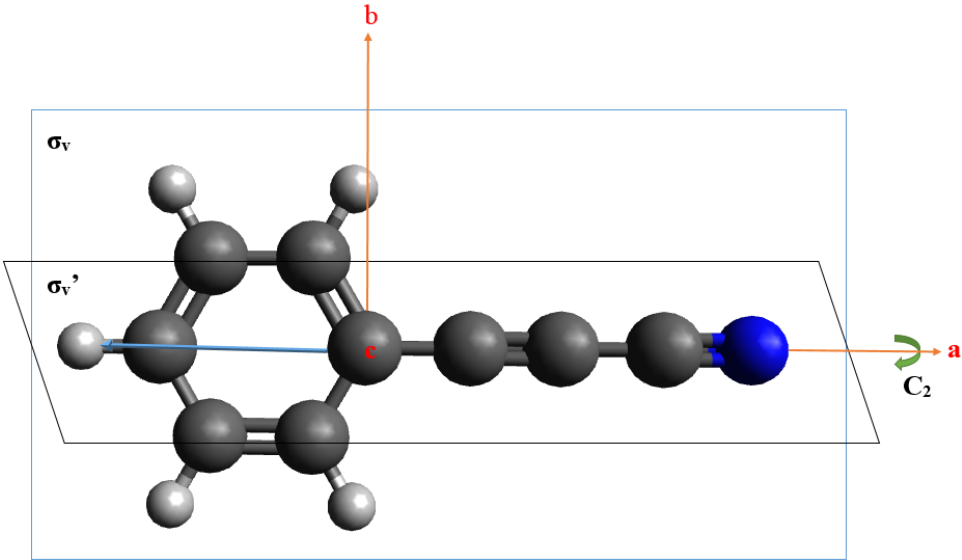
Rotational Hamiltonian

Parameter	Calc. (MHz)	Exp. (MHz)	% Diff.
A	5705	5660	-0.79
B	573	570	-0.66
C	521	517	-0.69
ΔJ	5E-06	5E-06	6.39
ΔJK	8E-04	8E-04	7.16
ΔK	5E-04	2E-03	326.44
δJ	5E-07	6E-07	13.72
δK	4E-04	4E-04	3.02
ϕ_{KJ}		-4E-08	
ϕ_{JK}		9E-10	
ϕ_J		-2E-12	

6329 Lines Assigned

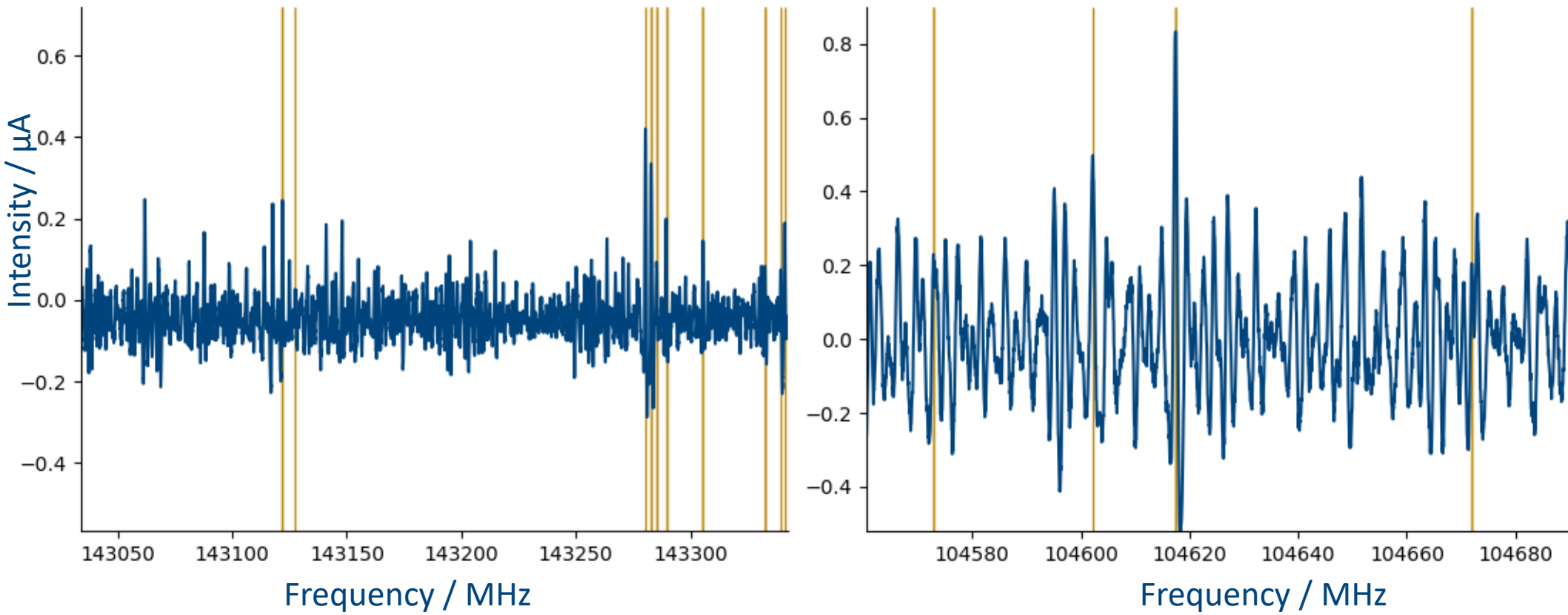
Max J = 200

Max Ka = 42

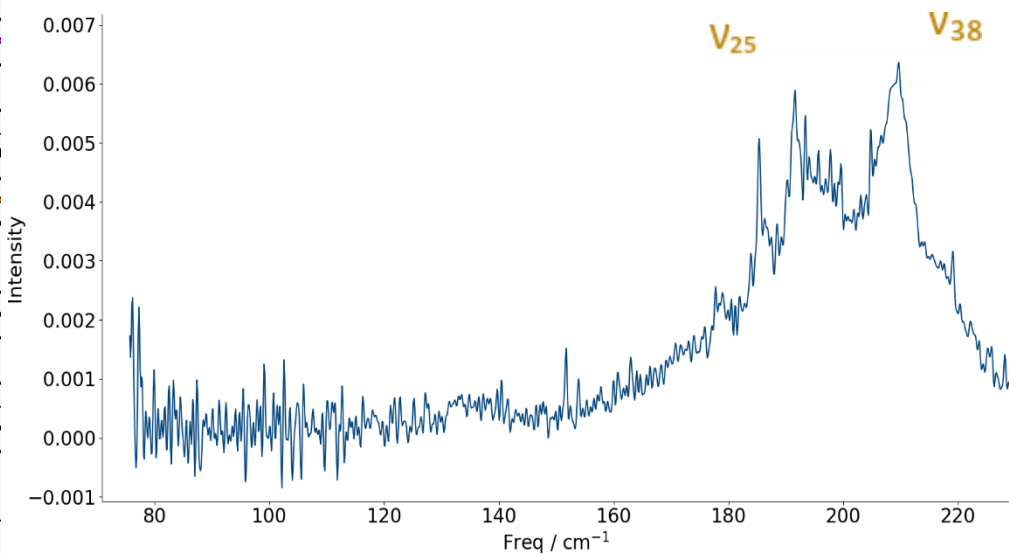


$$\begin{aligned}
 \hat{H} = & A\hat{J}_a^2 + B\hat{J}_b^2 + C\hat{J}_c^2 \\
 & -\Delta_J\hat{J}^4 - \Delta_{JK}\hat{H}\hat{J}_z^2 - \Delta_k\hat{J}_z^4 \\
 & + \frac{1}{2} \left[\delta_J\hat{J}^2 + \delta_K\hat{J}_z^2\hat{J}_+^2 + \hat{J}_-^2 \right] \\
 & + \Phi_J\hat{J}^6 + \Phi_{JK}\hat{J}^4\hat{J}_z^2 + \Phi_{KJ}\hat{J}^2\hat{J}_z^4
 \end{aligned}$$

Millimeterwave spectrum assigned



Future Work



Team members:

- ▶ Olivia Chitarra
- ▶ Olivier Pirali
- ▶ Marie-Aline Martin-Drumel

Harvard-Smithsonian Center for Astrophysics:

- ▶ Kelvin Lee
- ▶ Mike McCarthy

➤ Funding:

- ▶ Chateaubriand Fellowship of the Office for Science & Technology of the Embassy of France in the United States
- ▶ PCMI
- ▶ DIM-ACAV+

