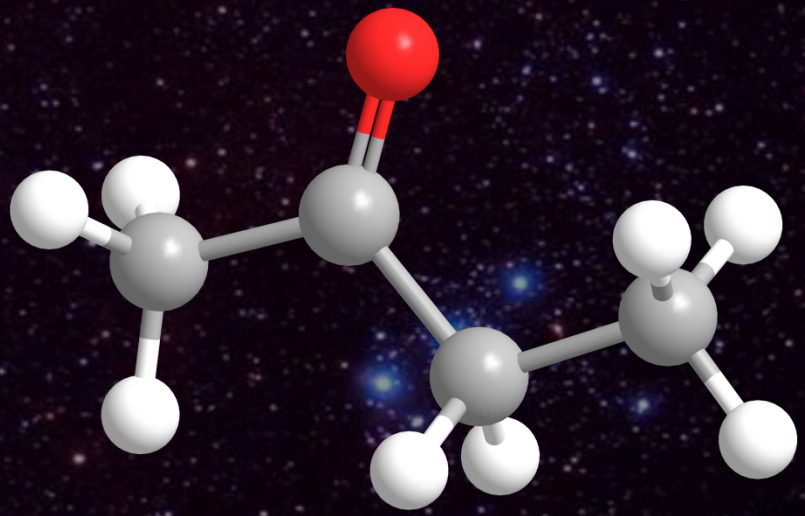
LABORATORY STUDY OF THE ROTATIONAL SPECTRUM OF 2-BUTANONE



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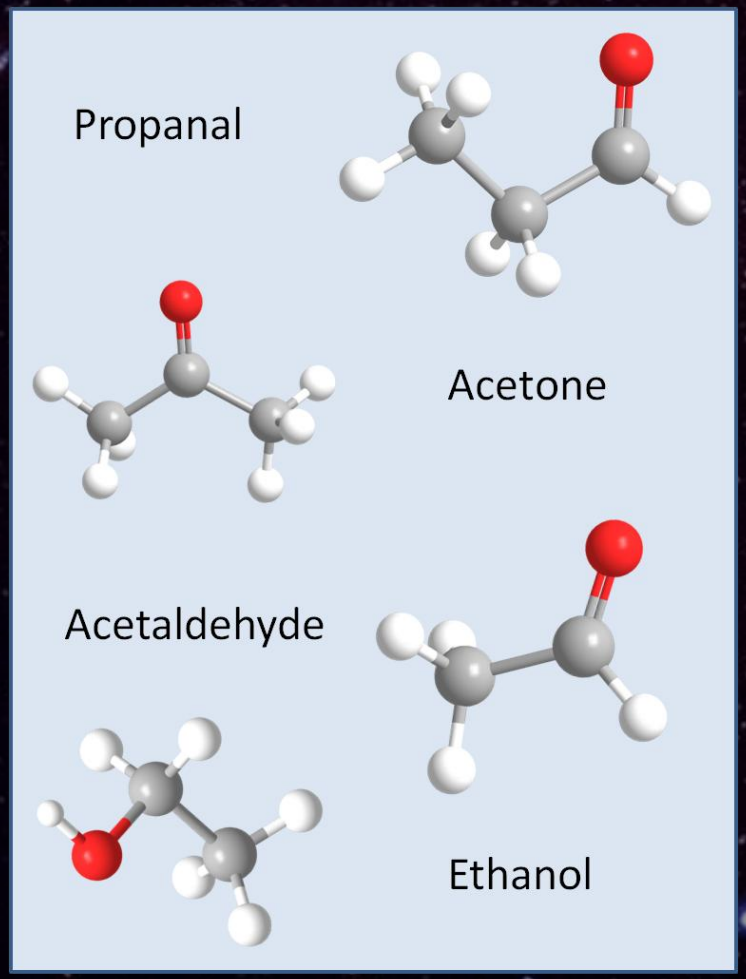
Division of Natural Sciences New College of Florida

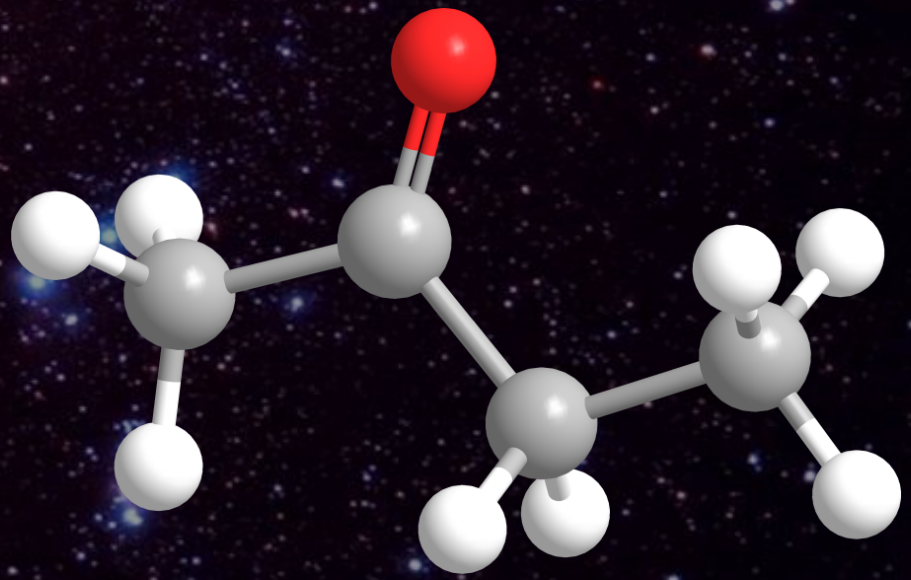
http://apod.nasa.gov/apod/ap030207.html

Why MEK?

Previously Detected Molecules



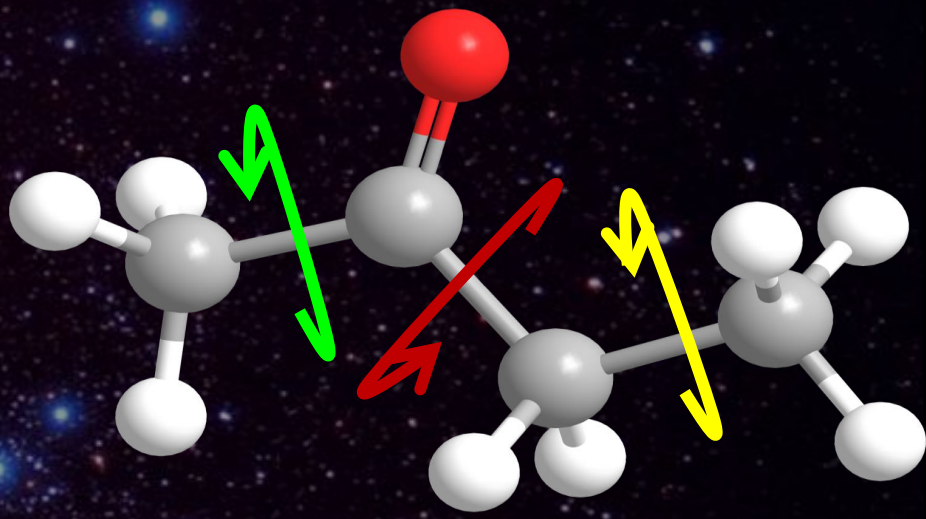
Methyl Ethyl Ketone



Hollis, J.M. P. R. Jewell, F. J. Lovas, A. Remijan, and H. Møllendal, Astrophys. J. 610, L21–L24 (2004).
Fourikis,N., M. W. Sinclair, B. J. Robinson, P. D. Godfrey, and R. D. Brown, Aust. J. Phys. 27, 425–430 (1974).
Zuckerman,B., B. E. Turner, D. R. Johnson, F. O. Clark, F. J. Lovas, N. Fourikis, P. Palmer, M. Ap. J Let. 196, L99. (1975)
Combes, F., M. Gerin, A. Wooten, G. Wlodarczak, F. Clausset, and P. J. Encrenaz, Astron. Astrophys. 180, L13–L16 (1987)

Previous Work

- 2 Previous Studies in the Microwave Region
  - 9-33 GHz
  - 36 Transitions Assigned
  - J_{max}=21
- No Previous Submillimeter Studies Conducted
  - Not enough information to accurately extrapolate to the submm region



183 cm^{-1}

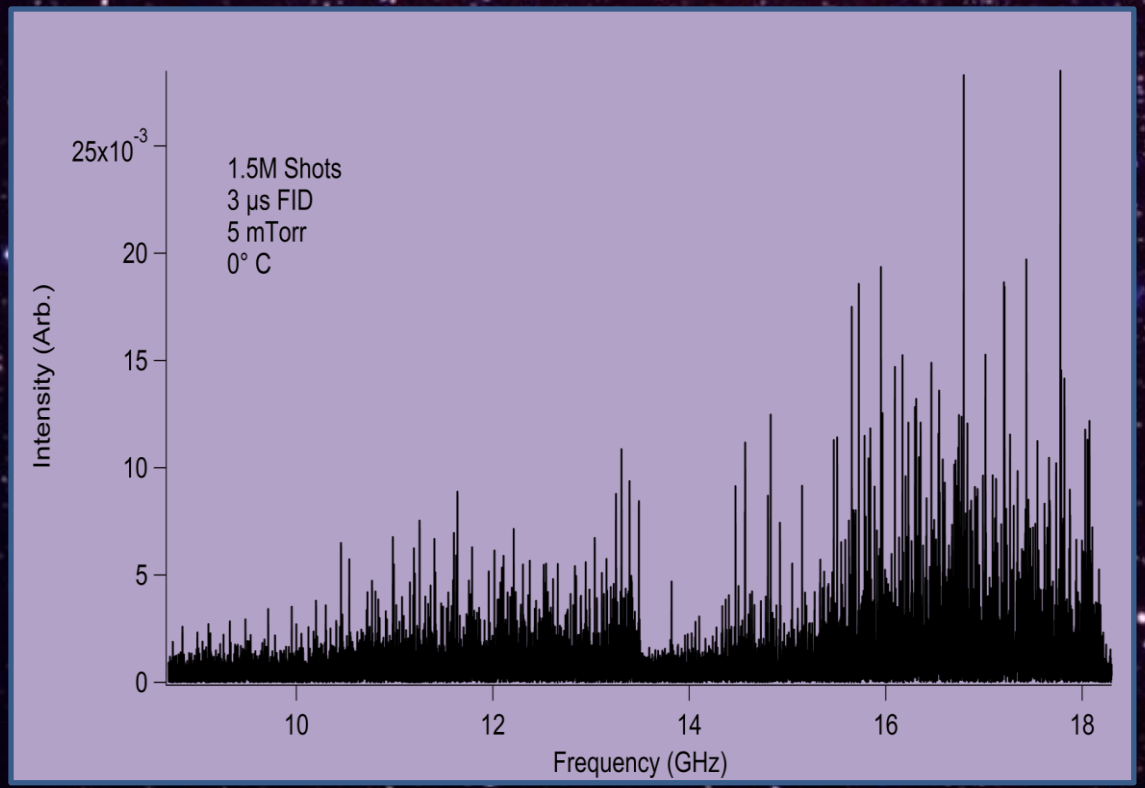
795 cm^{-1}

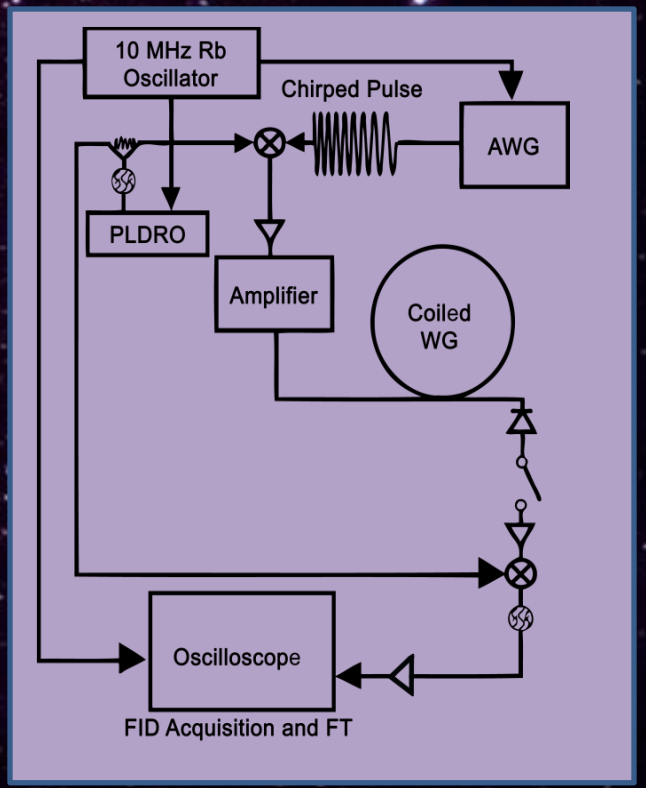
~ 5500 cm^{-1}

Pierce L.C., Chang, K., Hayashi, M., and Nelson R., JMS, 5, 449-457, (1969).
Pozdeev, N.M., Mamleev, A. Kh., Gunderova, L. N., and Galeev, R.V., J. Stuc.Chem, 52-58, (1988).

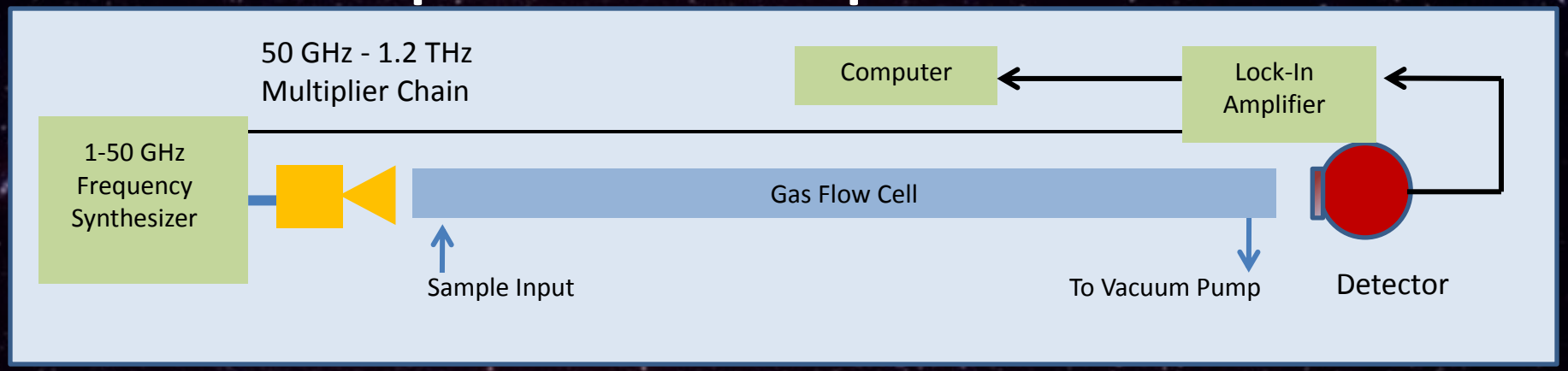
Spectral Acquisition

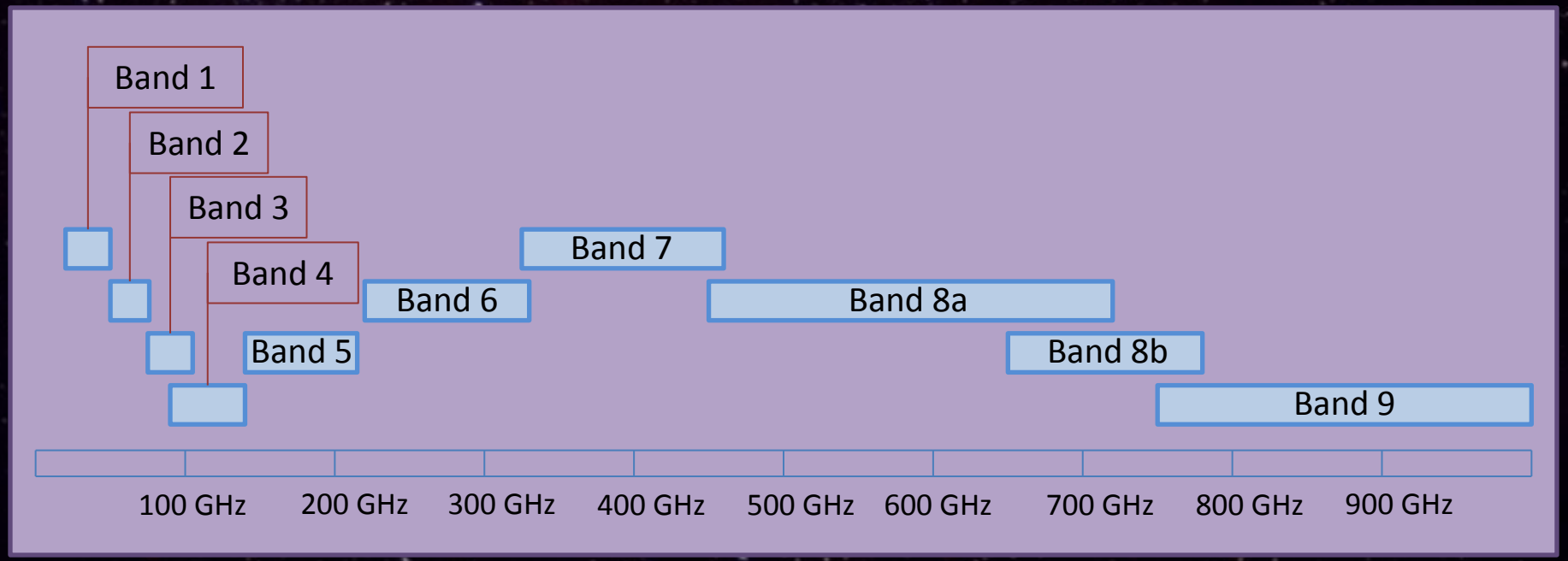
- 8.7 to 18.3 GHz
- Chirped-Pulse Waveguide Fourier Transform Microwave (FTMW) spectrometer
- New College of Florida





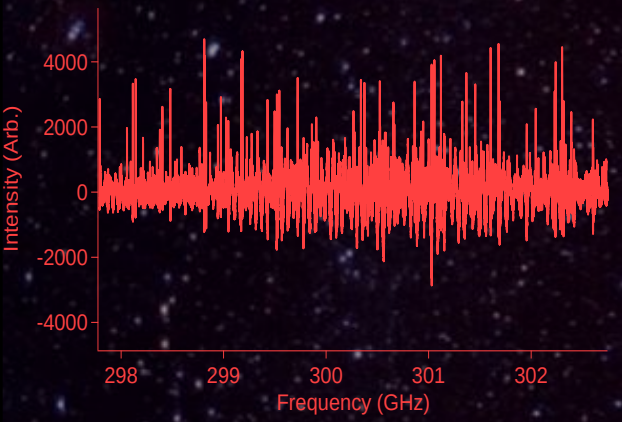
Spectral Acquisition

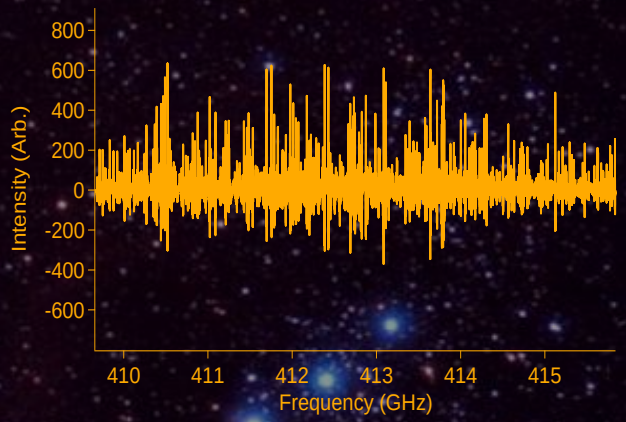


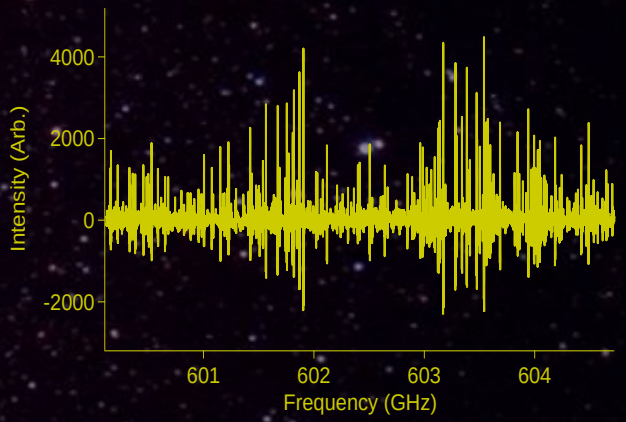


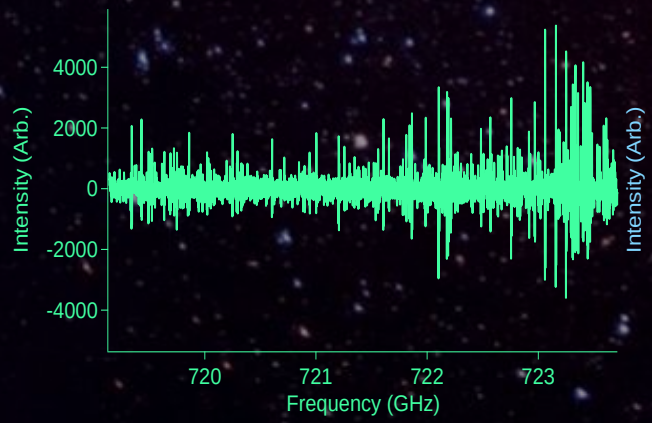
33 GHz - 1 THz

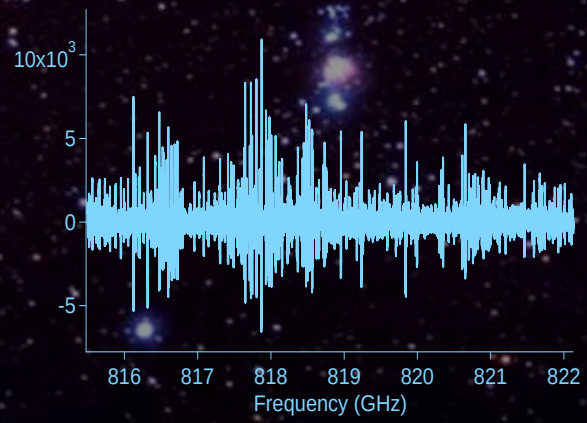
Sample Spectra Across the Submm Range

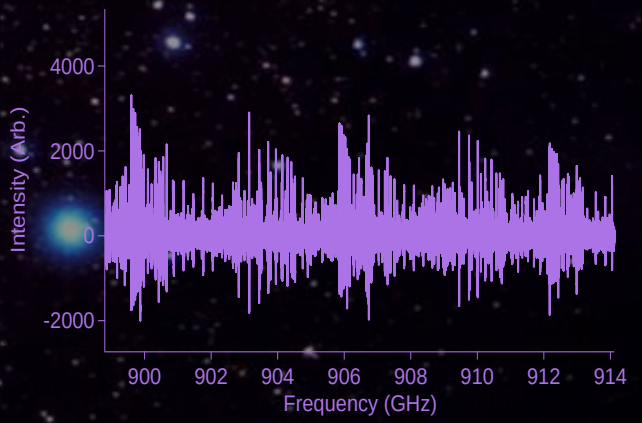




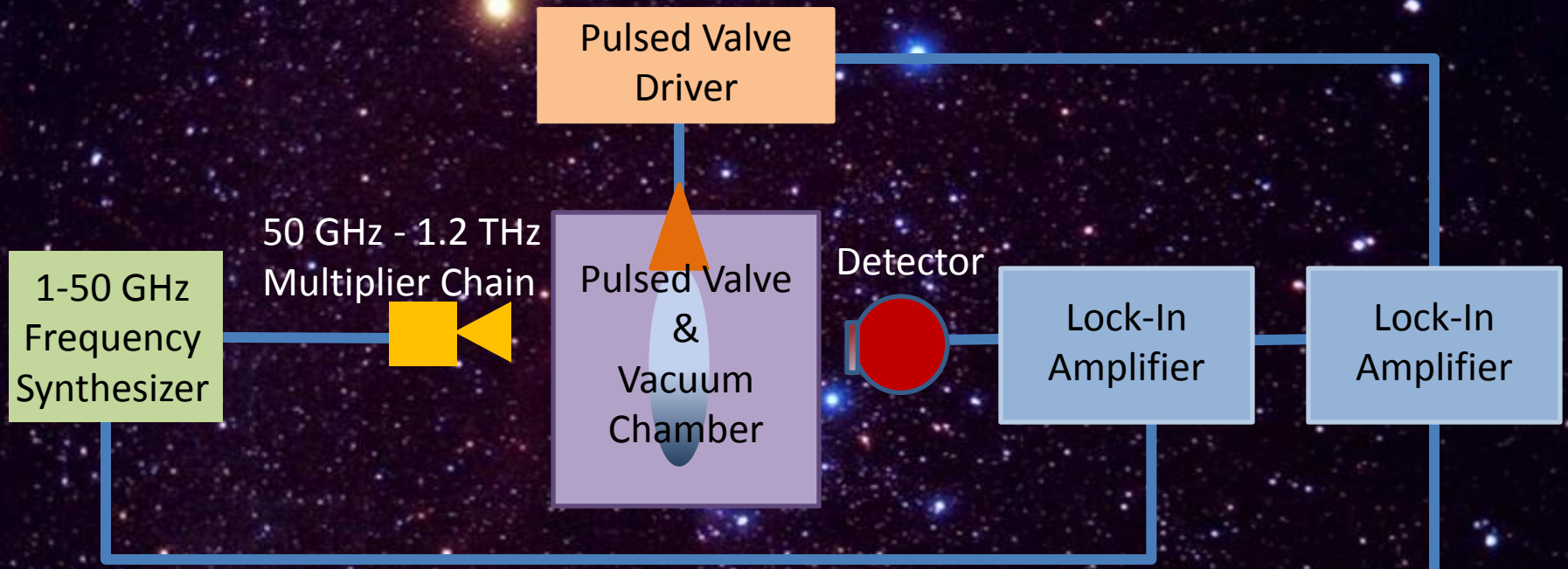


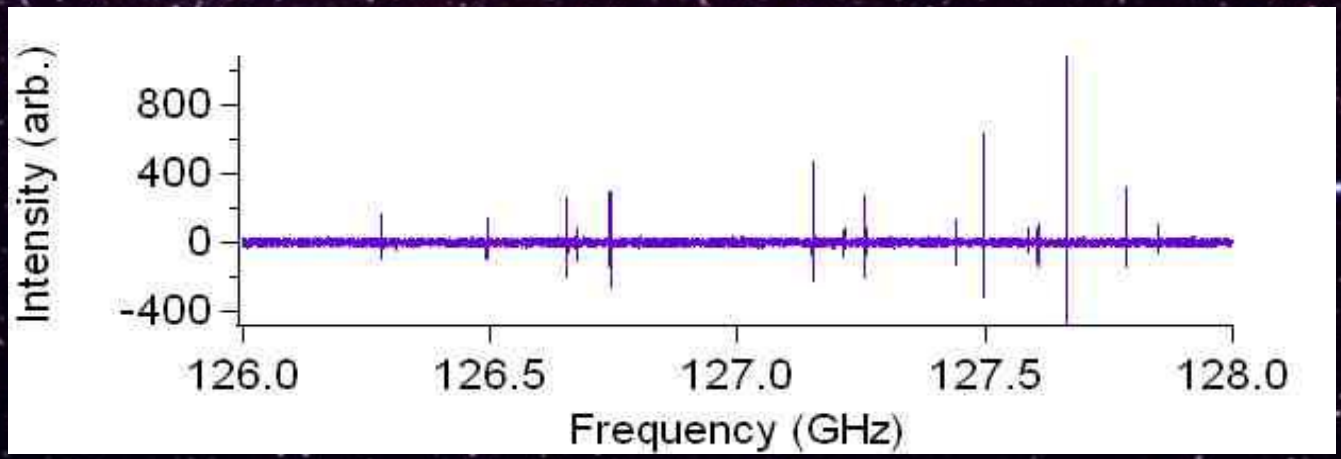




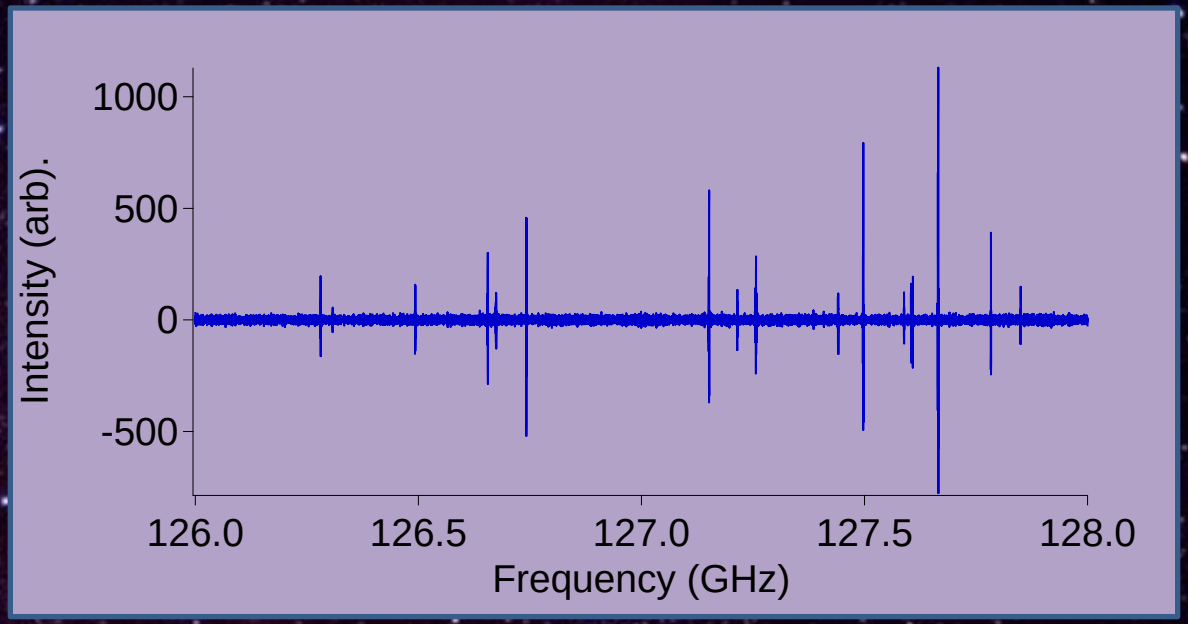


Acquisition of Cold Spectra

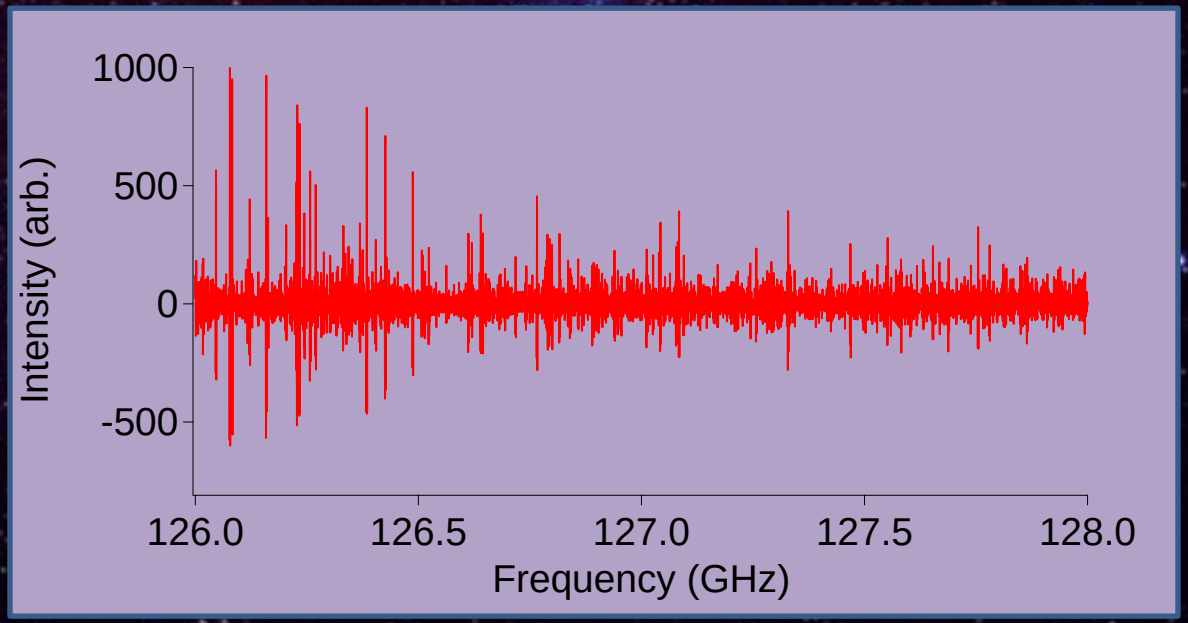




Cold

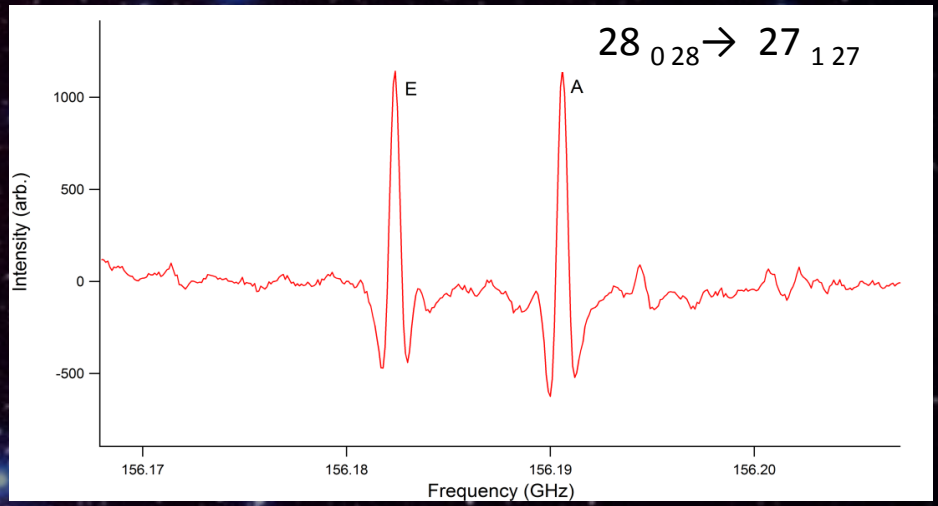

1000
500
0
-500
Intensity (arb).
126.0
126.5
127.0
127.5
128.0
Frequency (GHz)

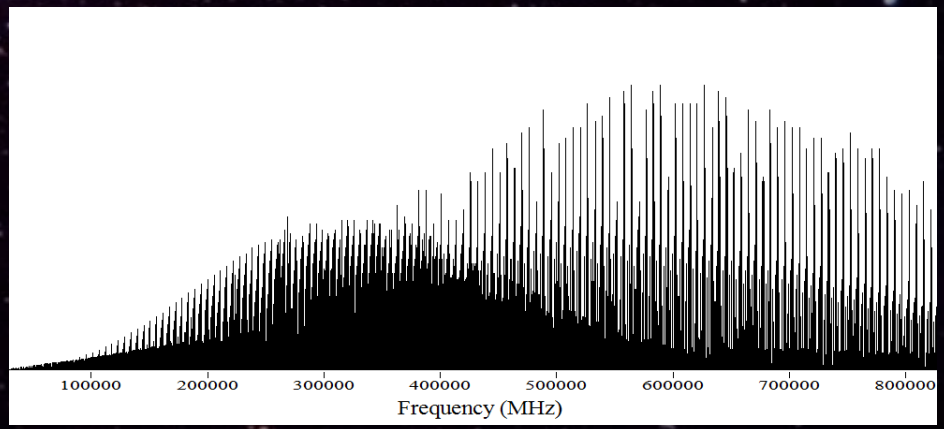
Hot


1000
500
0
-500
Intensity (arb.)
126.0
126.5
127.0
127.5
128.0
Frequency (GHz)

Analysis

- Initial A state fit performed using the CALPGM Suite of Programs (SPFIT/SPCAT)*
  - Information from previous studies used as the initial parameters of the fit.†
- XIAM‡ used to perform initial fit of the combined A and E states and to assign easily observed E state transitions
  - Straightforward conversion between constants in XIAM and constants in SPFIT

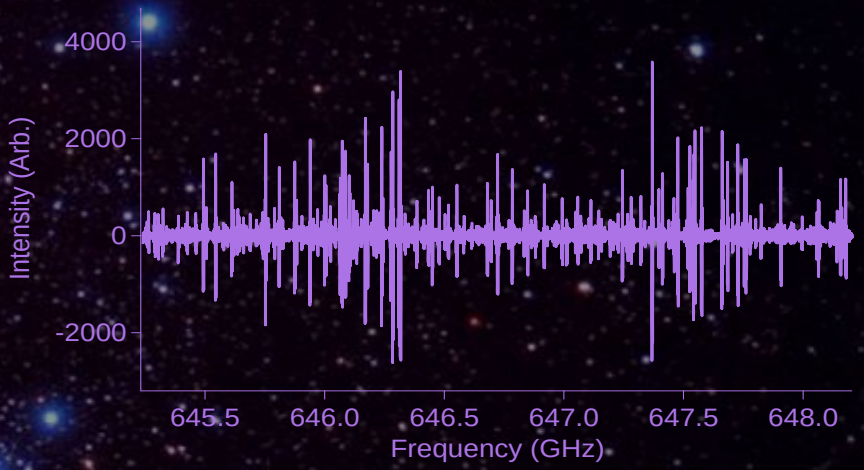


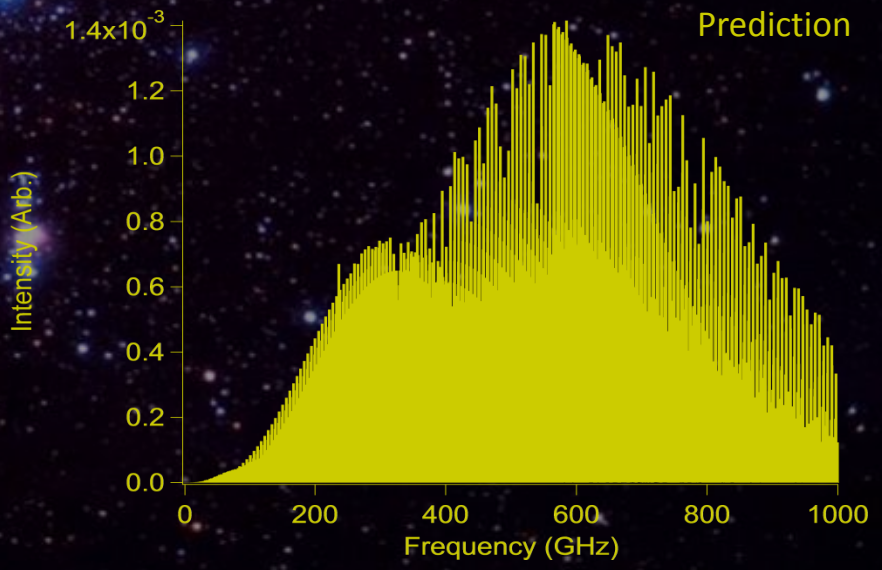


*Pickett, H. M., J. Molec. Spectroscopy 148 (1991) 371-377.
†Pierce et al., J. Mol . Spec., 5 (1969), 449-457.
‡ Hartwig, H. and H. Dreizler, Z. Naturforsch, 51a (1996) 923.

Analysis

- ERHAM*
  - Known to be powerful tool for spectral fitting of molecules with internal rotors
- 4440 Transitions Assigned
- J_{max}=100
- $K_{a\ max}$=11
- Max Frequency=568.611 GHz
- RMS = 192.4 kHz





*Groner,P., J. Chem. Phys. 107(1997) 4483-4498.

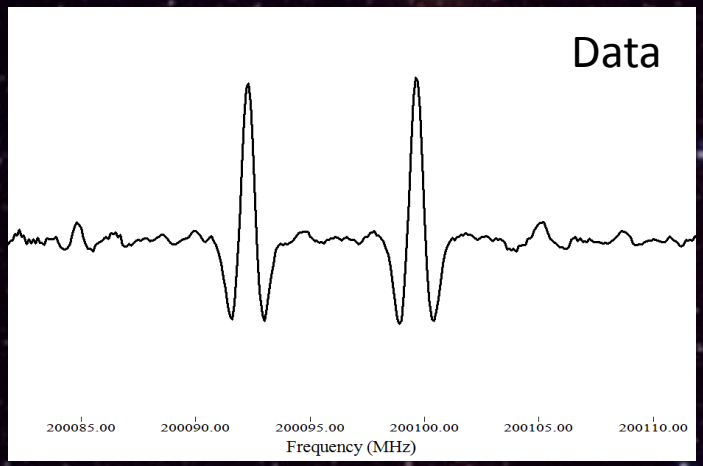
Resulting Fit Values from ERHAM

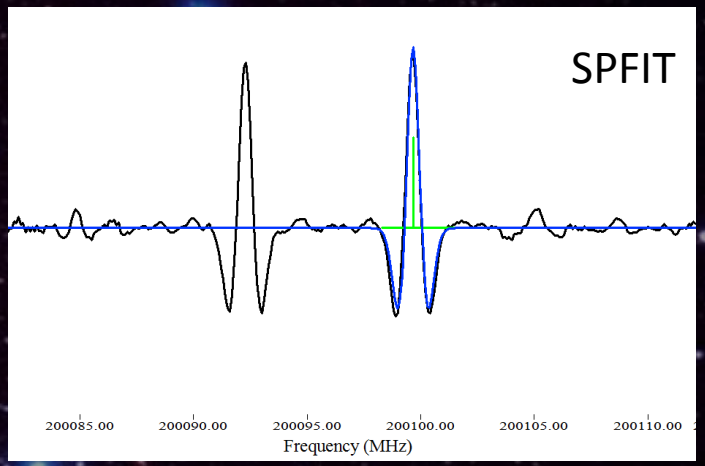
Parameter	Fit Value	Error
A (MHz)	9.545E+03	1.717E-02
B (MHz)	3.597E+03	2.380E-03
C (MHz)	2.747E+03	3.920E-04
Δ_J (kHz)	6.722E-01	3.950E-04
Δ_{JK} (kHz)	3.214E+00	1.163E-02
δ_J (kHz)	1.620E-01	2.075E-04
δ_K (kHz)	9.509E-01	8.091E-03
Φ_J (Hz)	-5.156E-04	1.804E-05
Φ_{KJ} (Hz)	4.766E-01	3.877E-02
φ_J (Hz)	-2.553E-04	1.029E-05
φ_K (Hz)	2.973E-01	2.312E-02

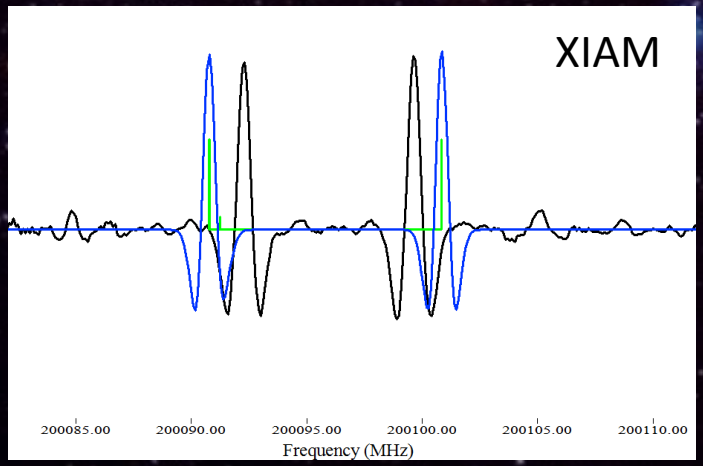
Resulting Fit Values from ERHAM

Splitting Tunneling Parameters		
Parameter	Value	Standard Error
ε_{10}	-2.791E+03	1.320E+01
$[A-(B+C)/2]_{10}$	1.022E+00	3.416E-02
$\Delta_{K\ 10}$	-1.151E-03	7.387E-05
$\Delta_{JK\ 10}$	3.179E-04	1.155E-05
$\Delta_{J\ 10}$	1.001E-05	6.200E-08
$[B-C]/4_{10}$	9.659E-03	8.278E-05
$\delta_{K\ 10}$	1.524E-04	5.967E-06
$\delta_{J\ 10}$	5.010E-06	3.485E-08

Comparing the Fits

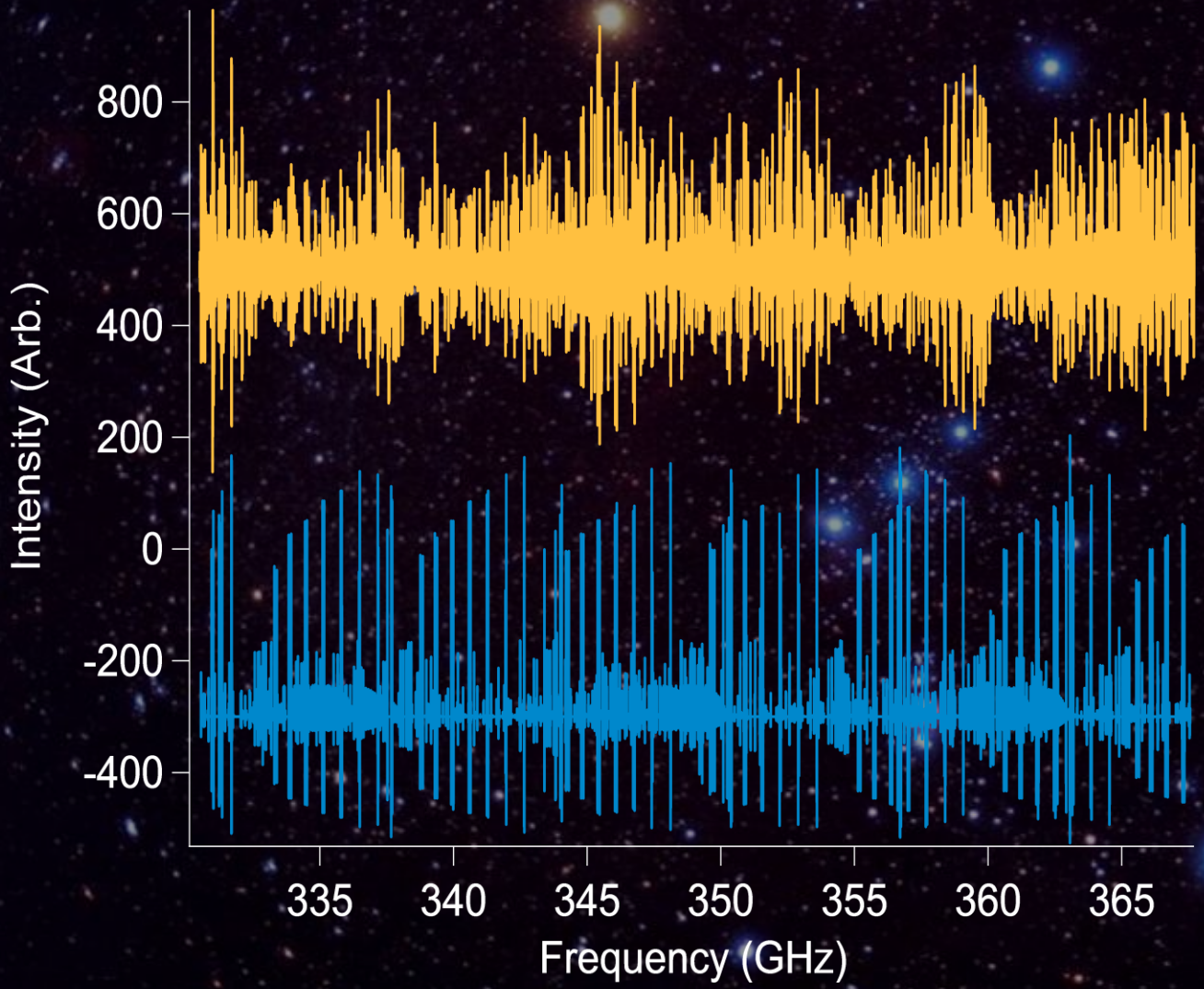






$$J_{Ka\,Kc} = 36_{1\,36} \leftarrow 35_{0\,35}$$

More Lines To Assign



Lab Spectrum
4175 Lines
Observed

Predicted
Spectrum
211 Lines
Assigned

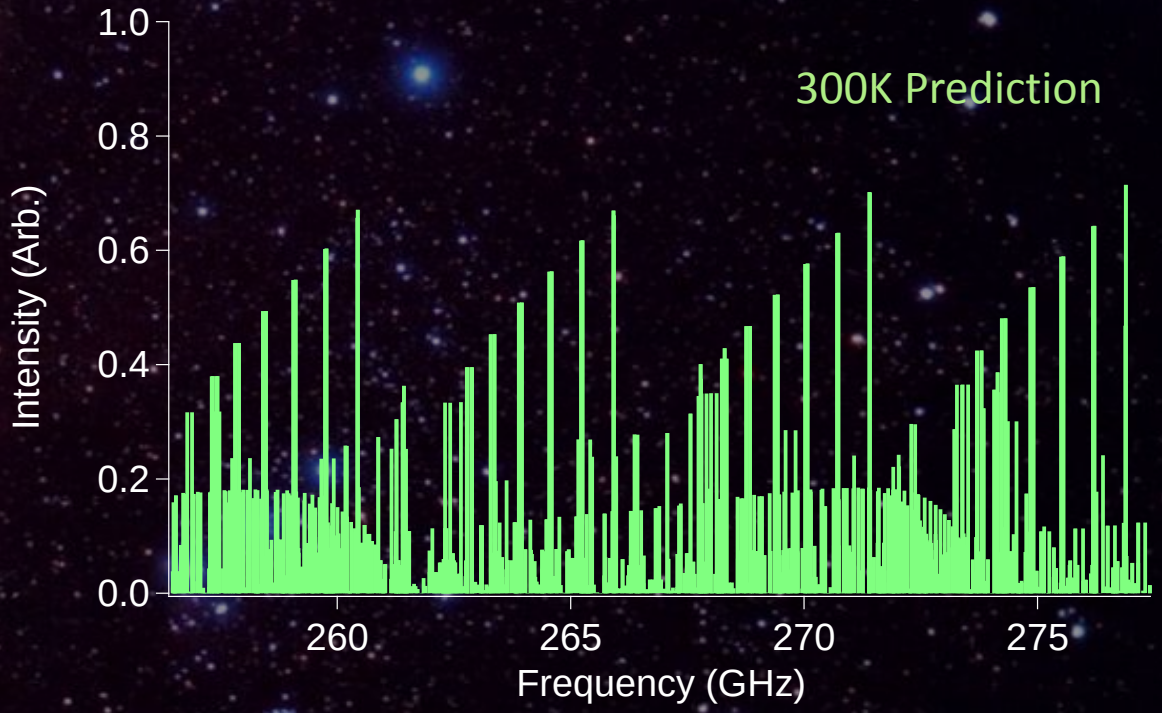
Future Work

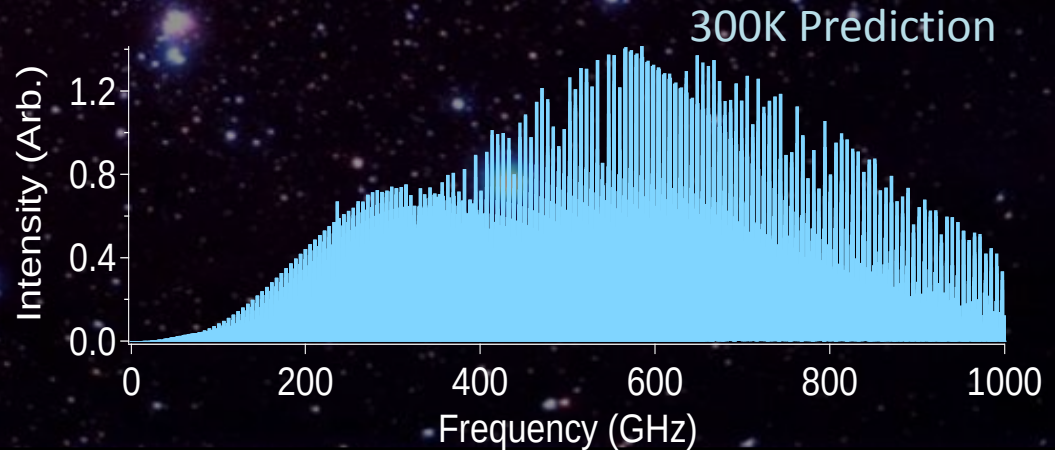
Strong R type lines assigned

Lower intensity Q branches not assigned

Rotationally cold spectra are helping with line ID

Prediction at higher K_a does not match laboratory spectra



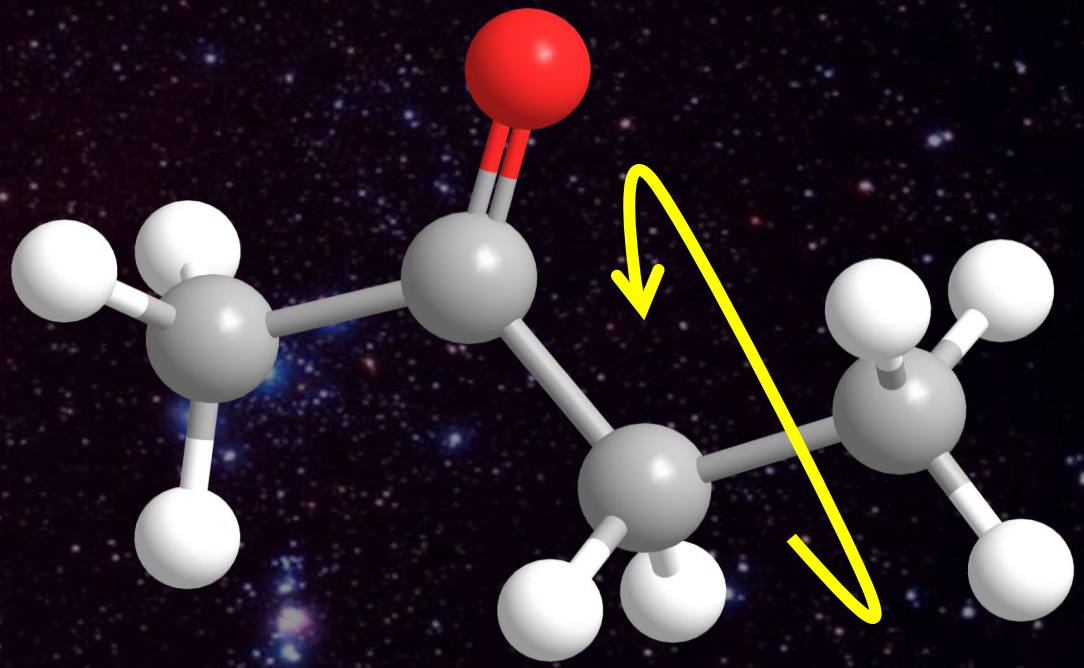


Future Work

Internal rotation of the second methyl group
$V_3 = 795\ cm^{-1}$

ERHAM is capable of fitting this

Currently no spectral evidence observed for splitting due to second rotor

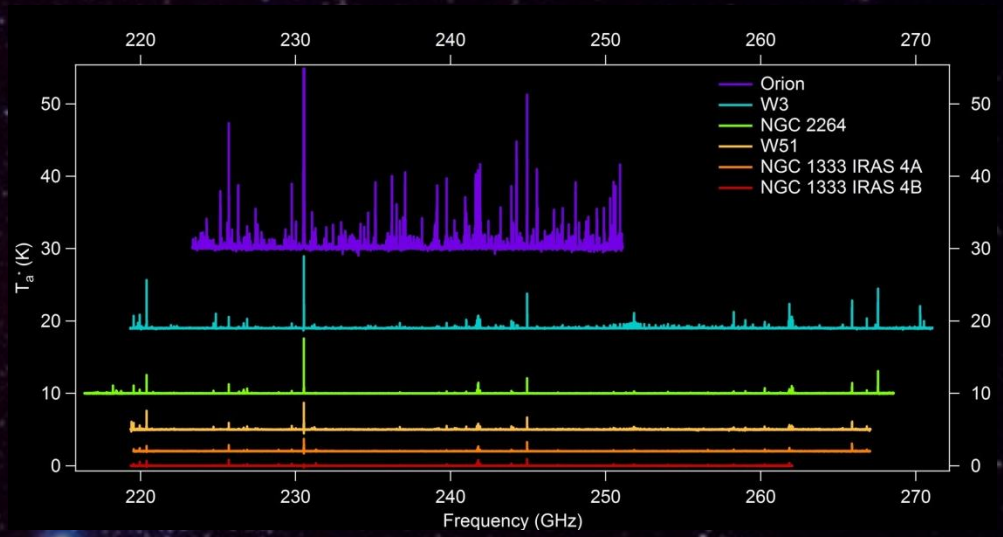


Pozdeev, N.M., Mamleev, A. Kh., Gunderova, L. N., and Galeev, R.V., J. Stuc.Chem, 52-58, (1988).

Future Work

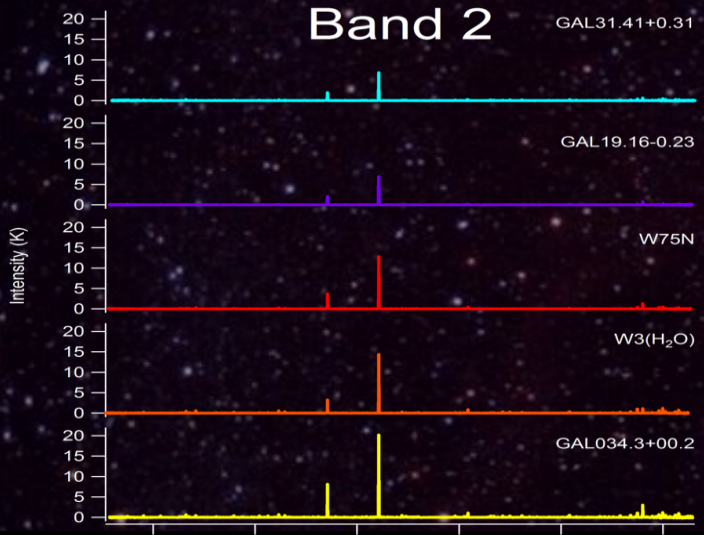
An initial search for MEK Orion, W3, and W52 has been performed using CSO data

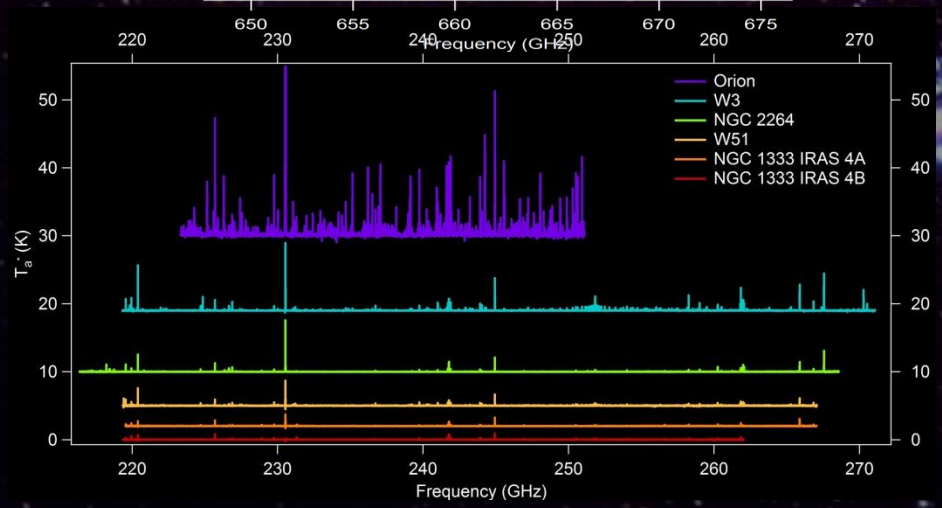
Due to line confusion problems in the dense spectra, we were unable to detect MEK or determine a upper limit for column density



Future Work

Interstellar Search





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NASA

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