Spectroscopy Study of n-Propyl Cyanide and Astronomical Detection of its Vibrationally Excited States

- BACKGROUND
- THEORY
- ANALYSIS
- PROGRESS
- FUTURE PLAN
- MINI-GAME: GUESS FILMS

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Advisor: Adam WALTERS
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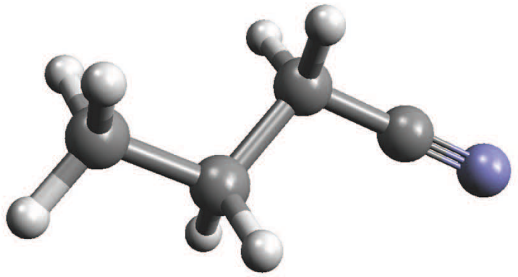
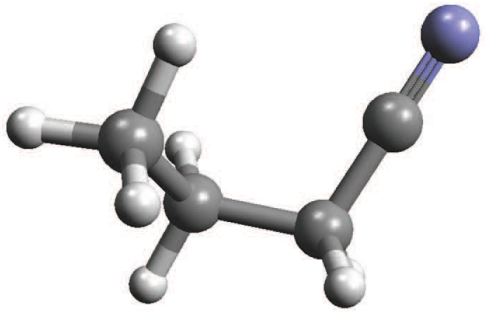
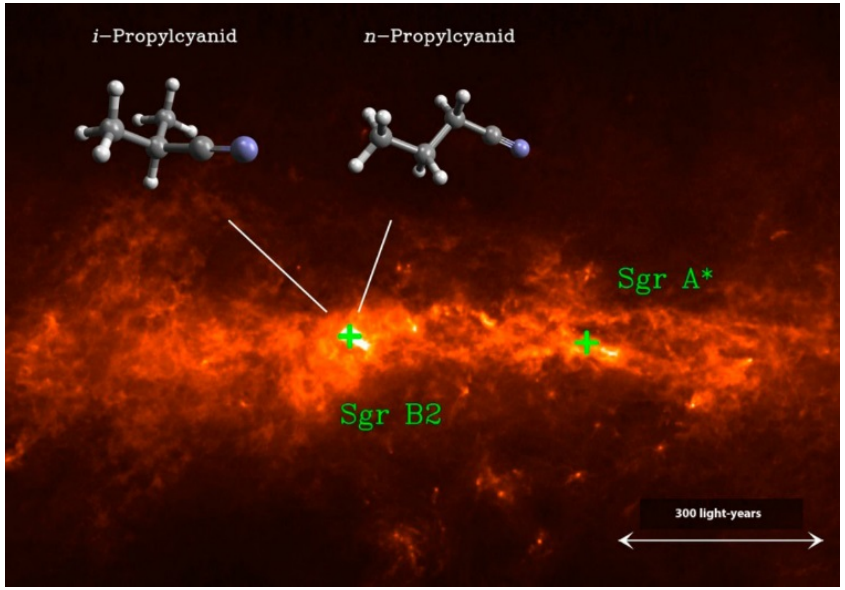
Background



Anti-normal-Propyl Cyanide



Gauche-normal-Propyl Cyanide



Chemical Formula: C_3H_7CN.

Largest molecule detected in Sagittarius B2.
Rotational transitions in vibrational states have been detected
by ALMA(Atacama Large Millimeter/Submillimeter Array), using our laboratory da

The good fit in lower energy range, within lower quantum number is always the beginning of a beautiful fitting.

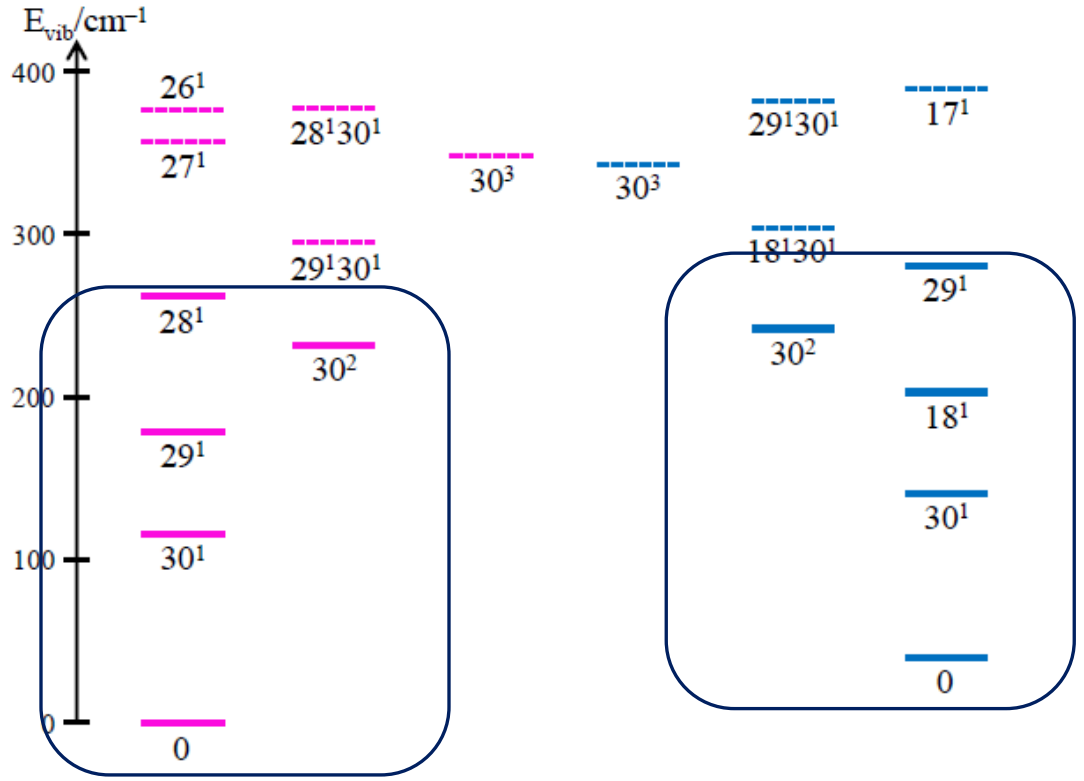
We fit the laboratory data to determine molecular parameters that can then be used to predict the spectrum in the ISM

Asymmetric Rotor
Approximate expression ***for near Prolate Top***

$$F(J,K) \approx \bar{B}J(J+1) + (A-\bar{B})K^2 - D_J K^0 J^2(J+1)^2 - D_{JK}K^2 J(J+1) - D_k K^4 J^0 (J+1)^{\,0} - H_{KJ}K^4 J(J+1) - H_{JK}K^2 J^2(J+1)^2 - H_J K^0 J^3 (J+1)^3 \cdots$$

$$\bar{B} = \frac{1}{2}(B+C),\ B = \frac{h}{8\pi^2 I_b}$$

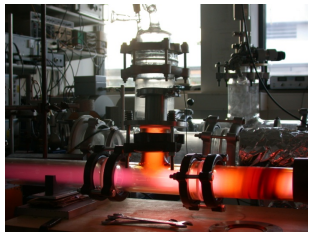
Content of the study



Vibrational states of normal-propyl cyanide up to vibrational energies of 400 cm^{-1} (575 K).

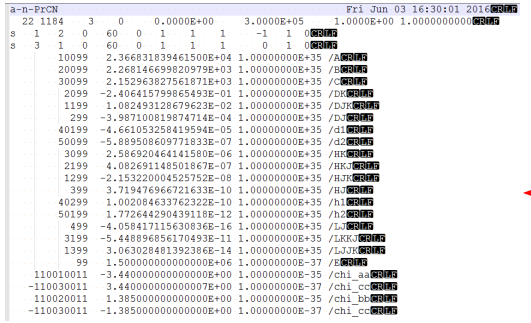
The *gauche* states are shown on the left-hand side, those of *anti* on the right.

Content of the study



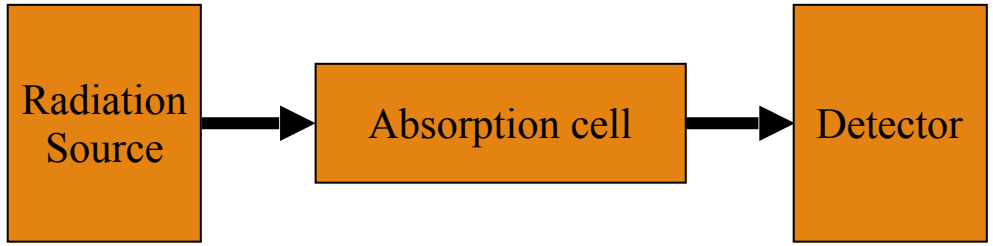
Laboratory Measurements

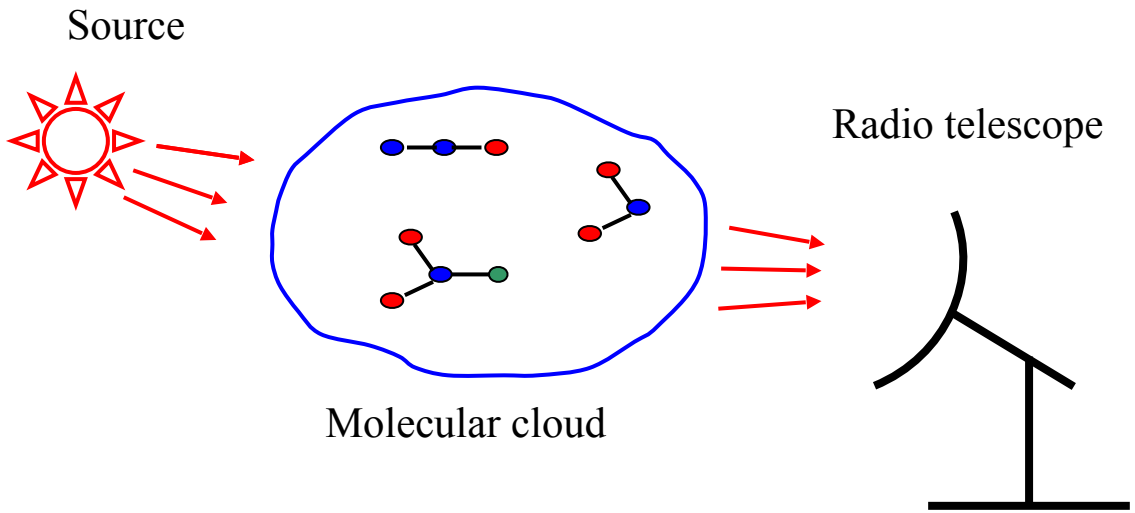
Analysis & Simulations



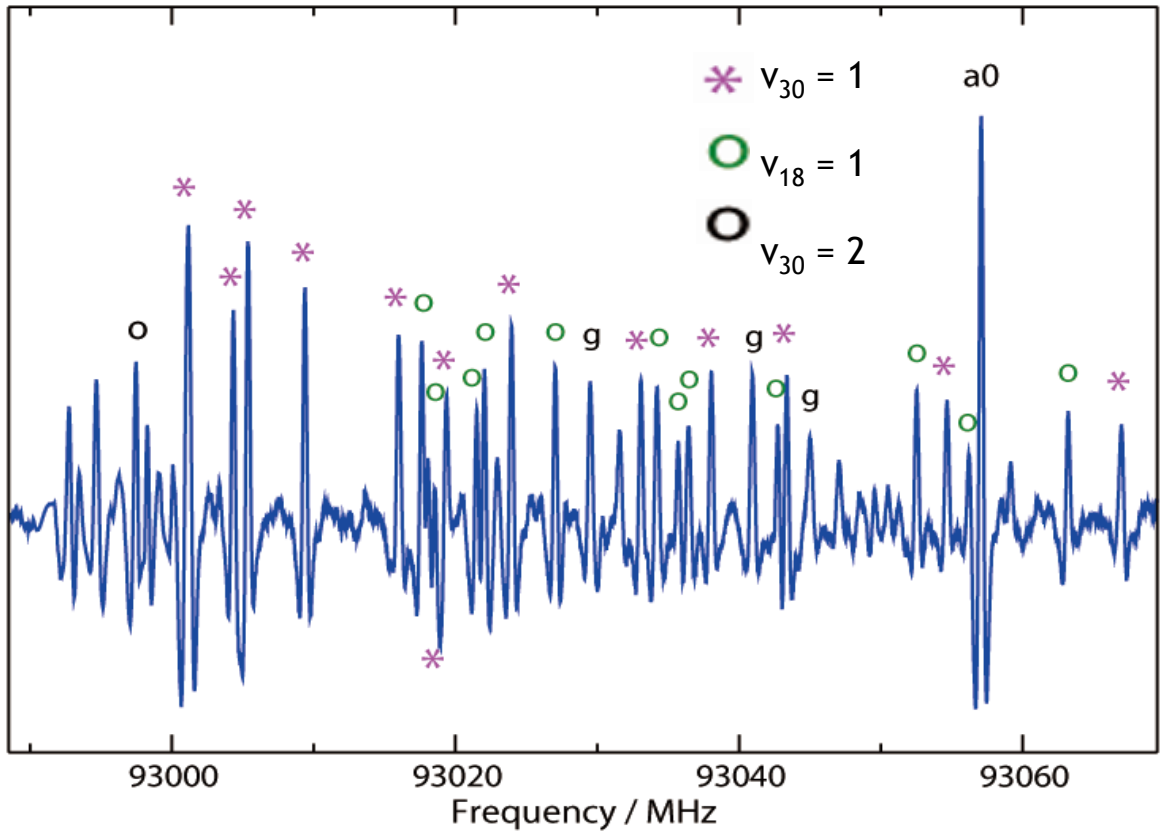
Next molecules interested

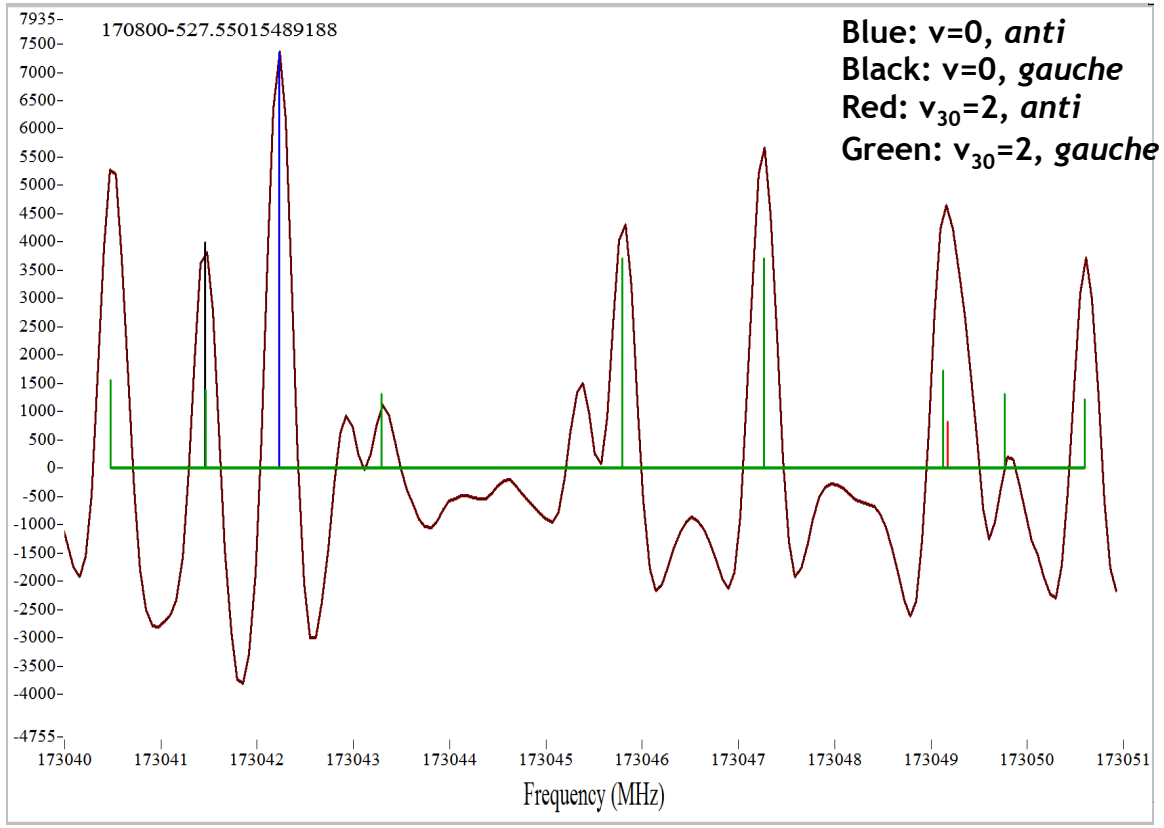
Astronomy Observation





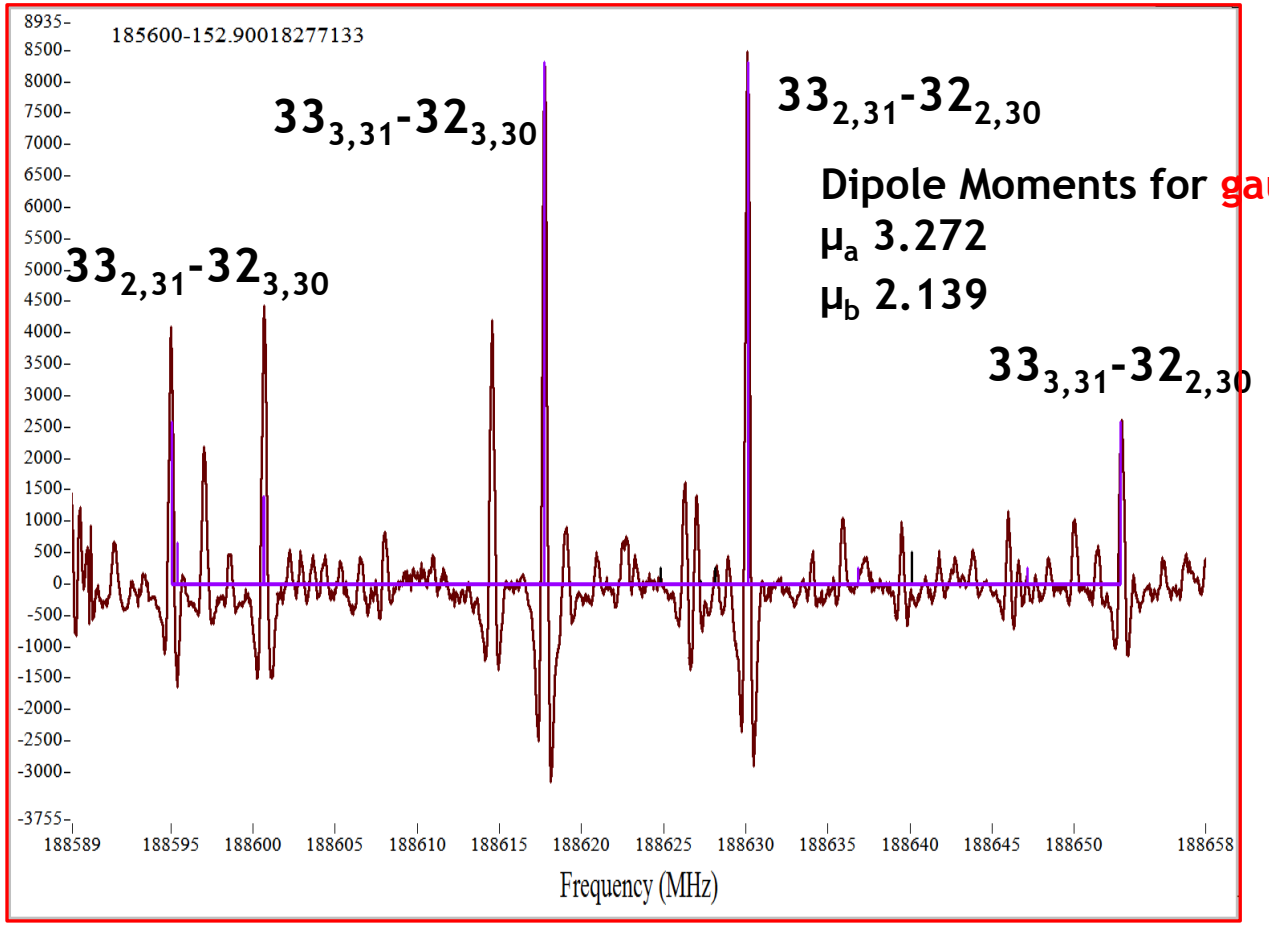
Analysis



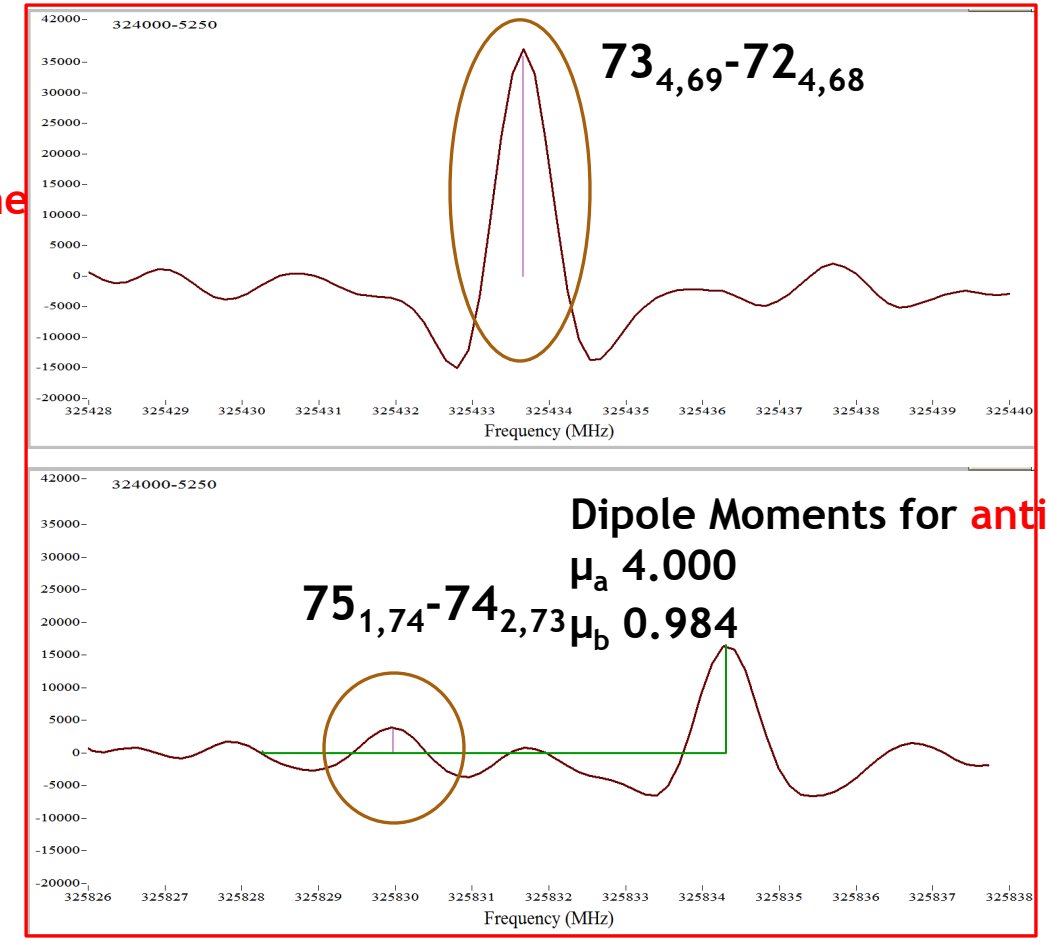


Extract of Laboratory Spectrum

μ_a and μ_b transitions

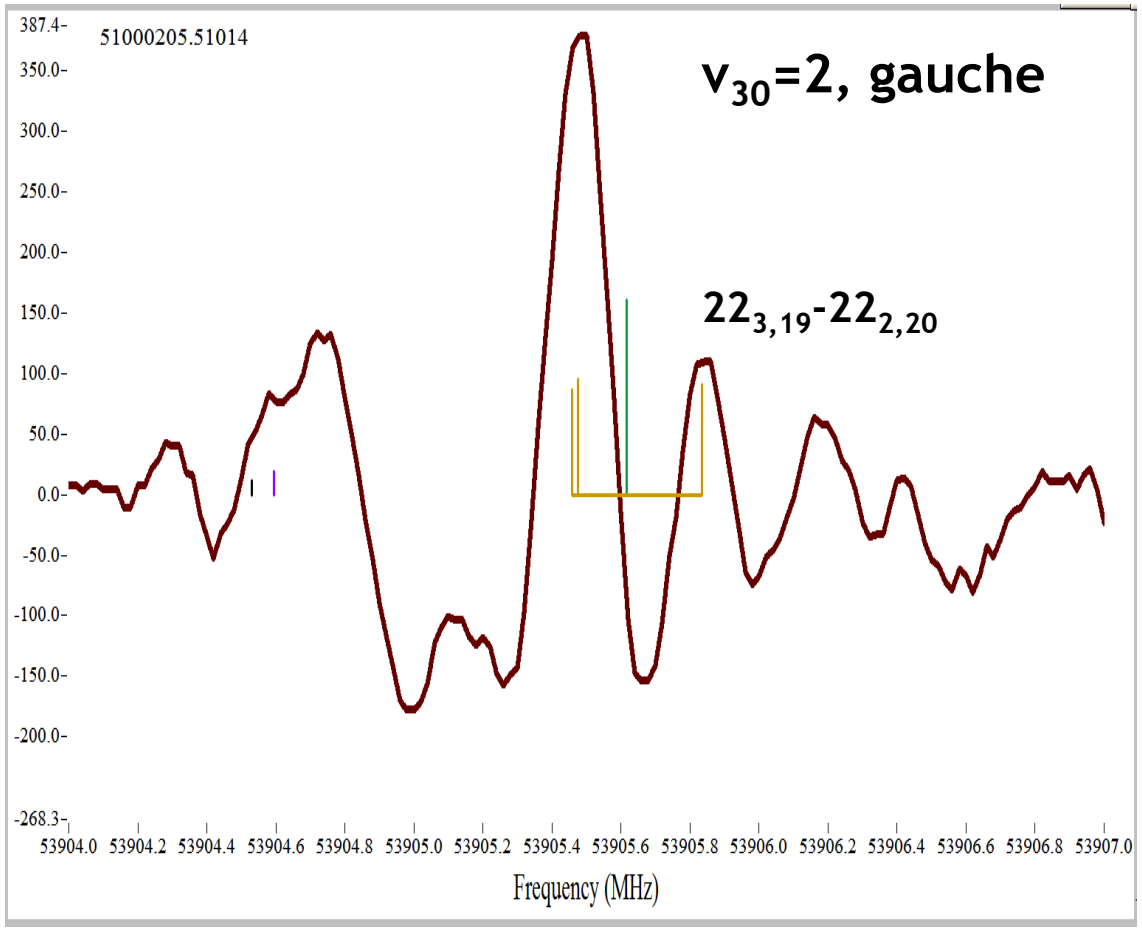


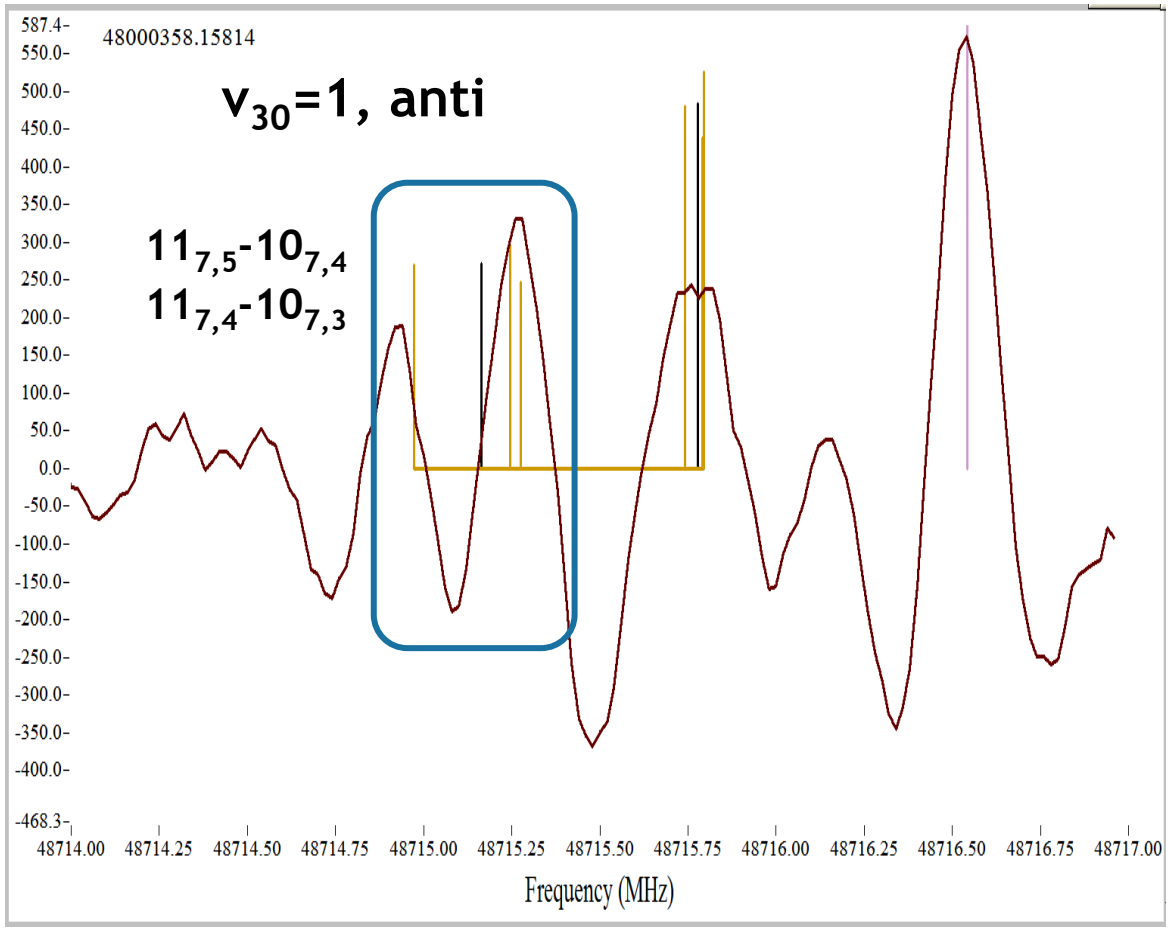
Dipole Moments for gauche
μ_a 3.272
μ_b 2.139



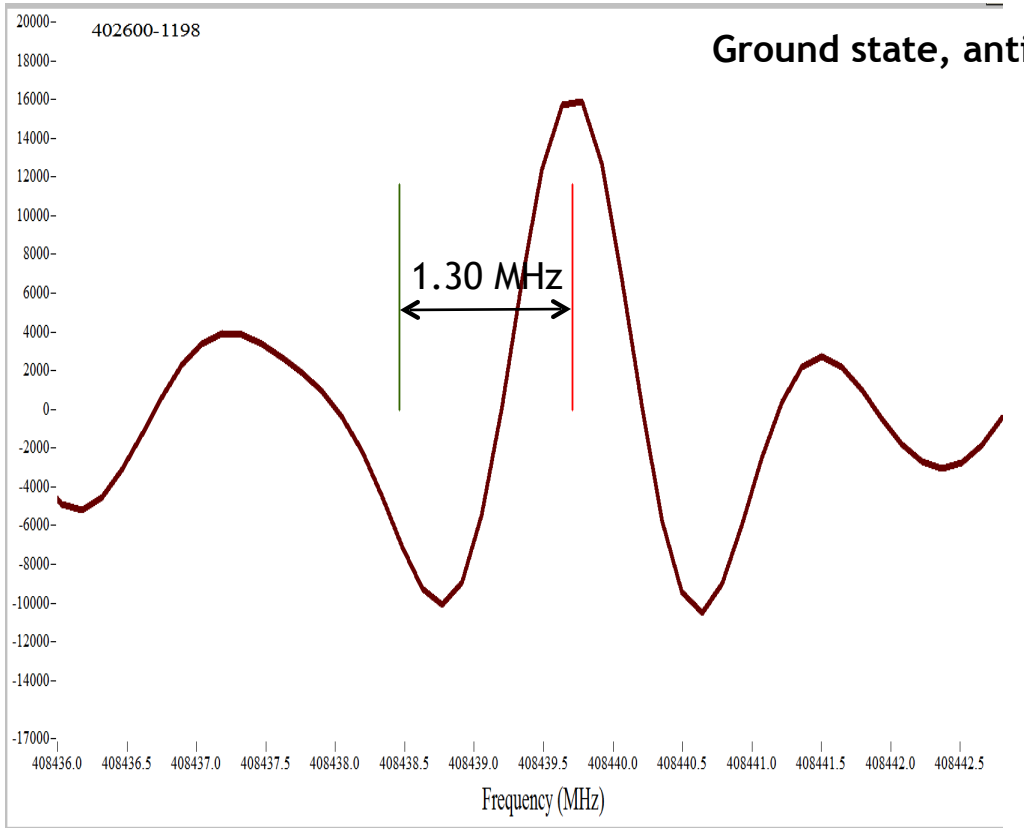
Dipole Moments for anti
μ_a 4.000
μ_b 0.984

Hyperfine structure

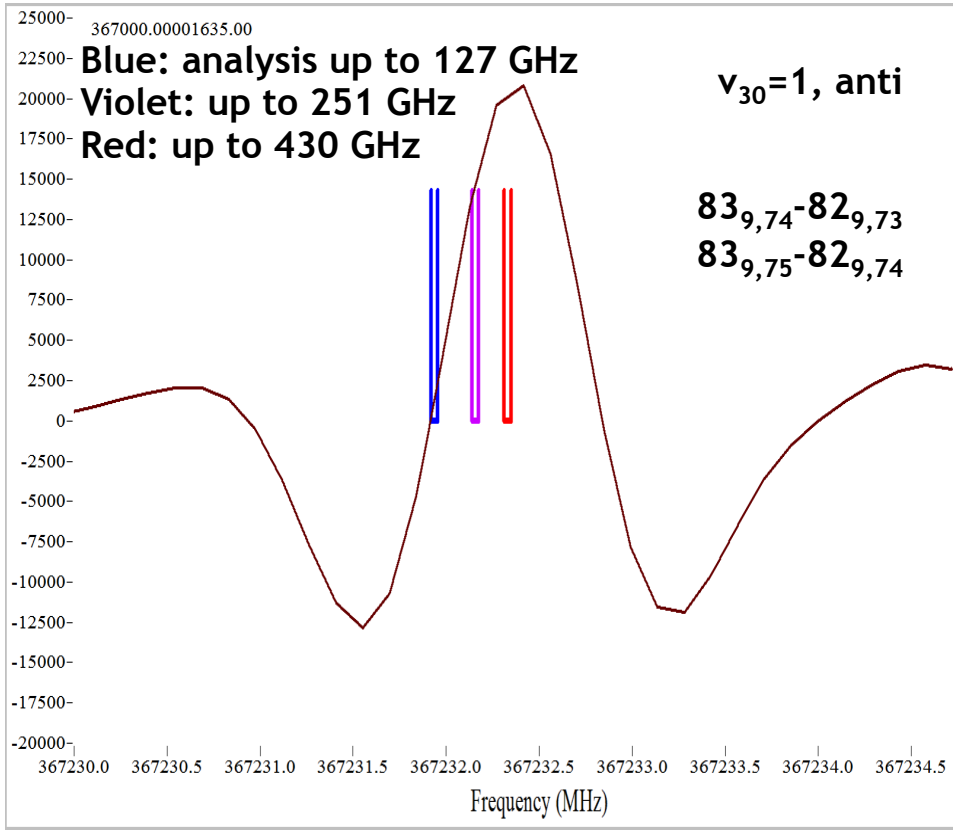




progress

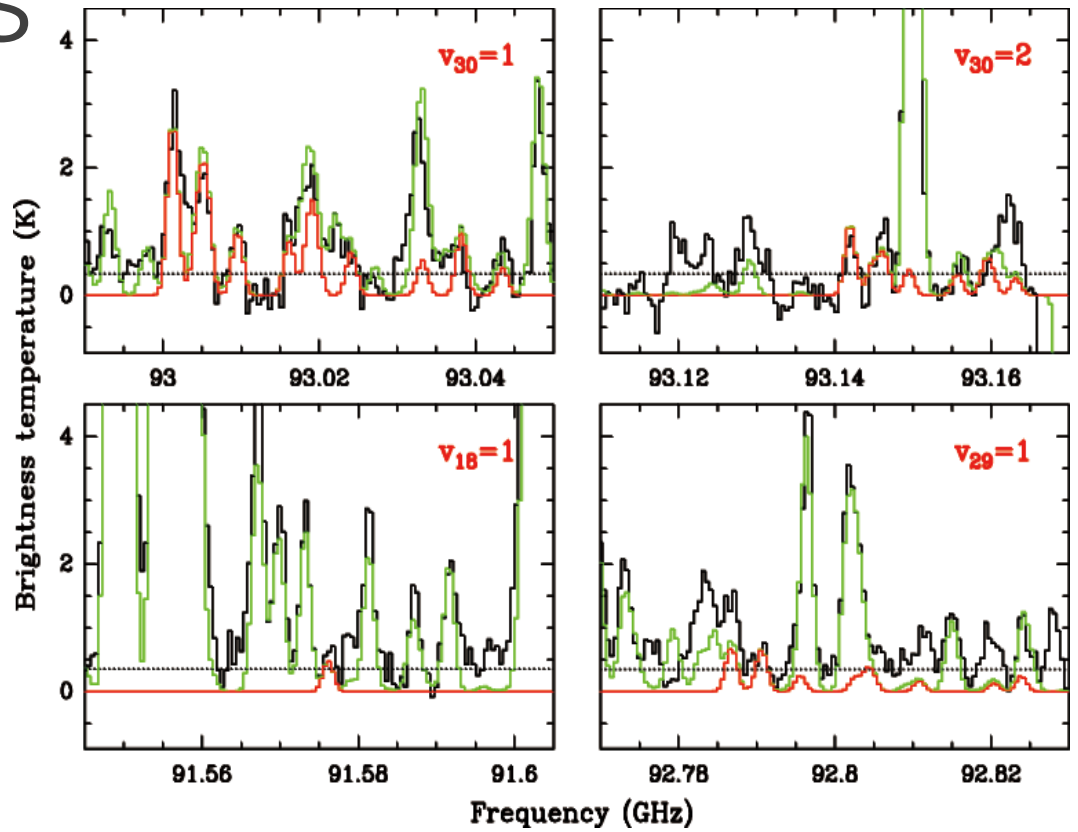


Old prediction (green) and our new prediction (red)



Prediction shifts at higher frequency

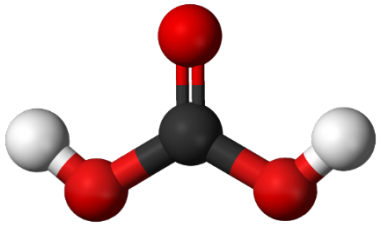
progress



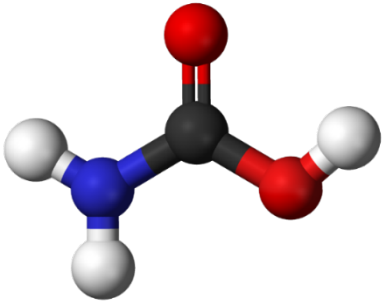
Black-spectrum of Sagitarius B2 by ALMA, (Belloche et al.)
Red-simulated spectrum of Propyl Cyanide in vibrational states (from our work)
Green-simulated spectrum of all known molecules.

Future plan

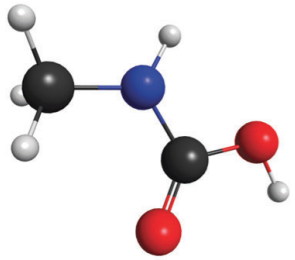
Study another astronomical molecule,
eg, carbonic acid, carbamic acid, methylcarbamic acid...
Though, you never know what you'er gonne get, thank god, we can choose our ta



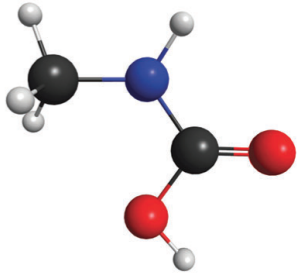
carbonic acid



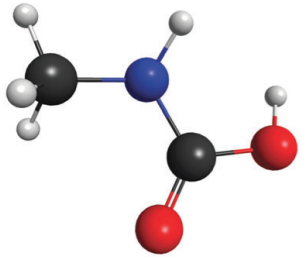
carbamic acid



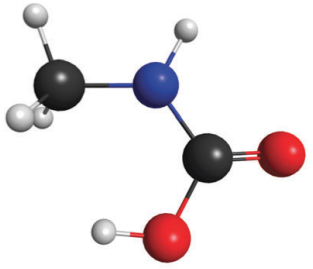
MCA-1



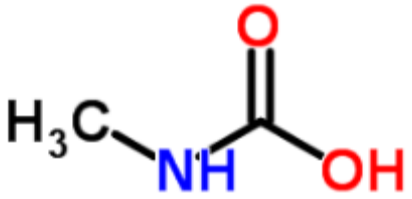
MCA-2



MCA-3



MCA-4



methylcarbamic acid

Guess films!

What's the first one?

So, what's the other one?

Merci, tout le monde

刘德龙