

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

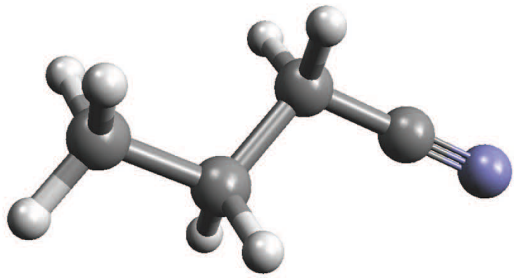
- BACKGROUND
- THEORY
- ANALYSIS
- PROGRESS
- FUTURE PLAN
- MINI-GAME: GUESS FILMS

LIU Delong

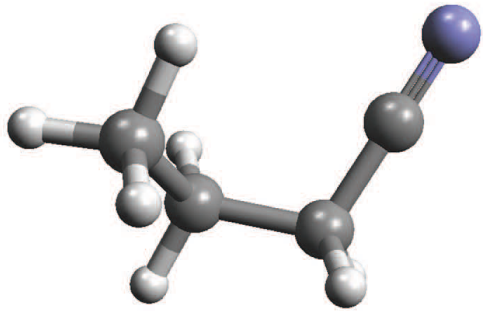
Advisor: Adam WALTERS

21/June/2017

Background



Anti-normal-Propyl Cyanide



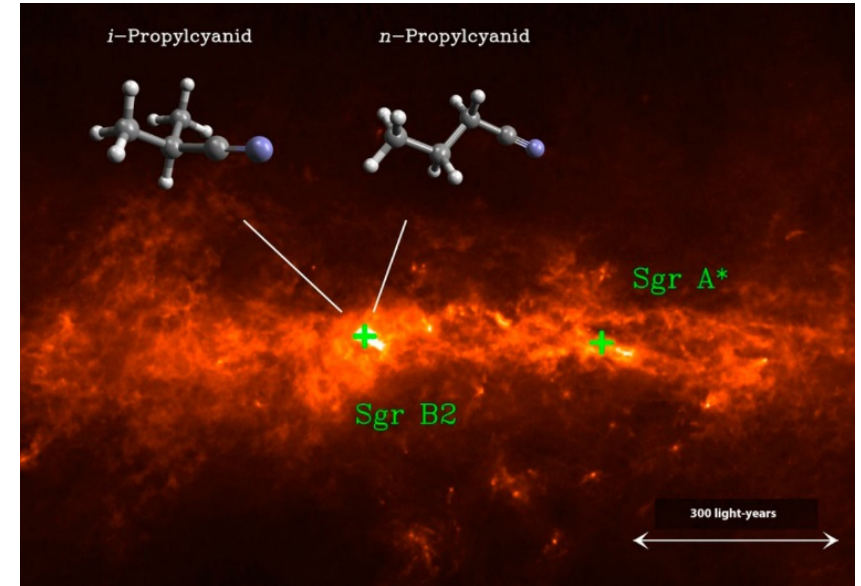
Gauche-normal-Propyl Cyanide

Chemical Formula: $\text{C}_3\text{H}_7\text{CN}$.

Largest molecule detected in Sagittarius B2.

Rotational transitions in vibrational states have been detected by ALMA (Atacama Large Millimeter/Submillimeter Array), using our laboratory data.

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

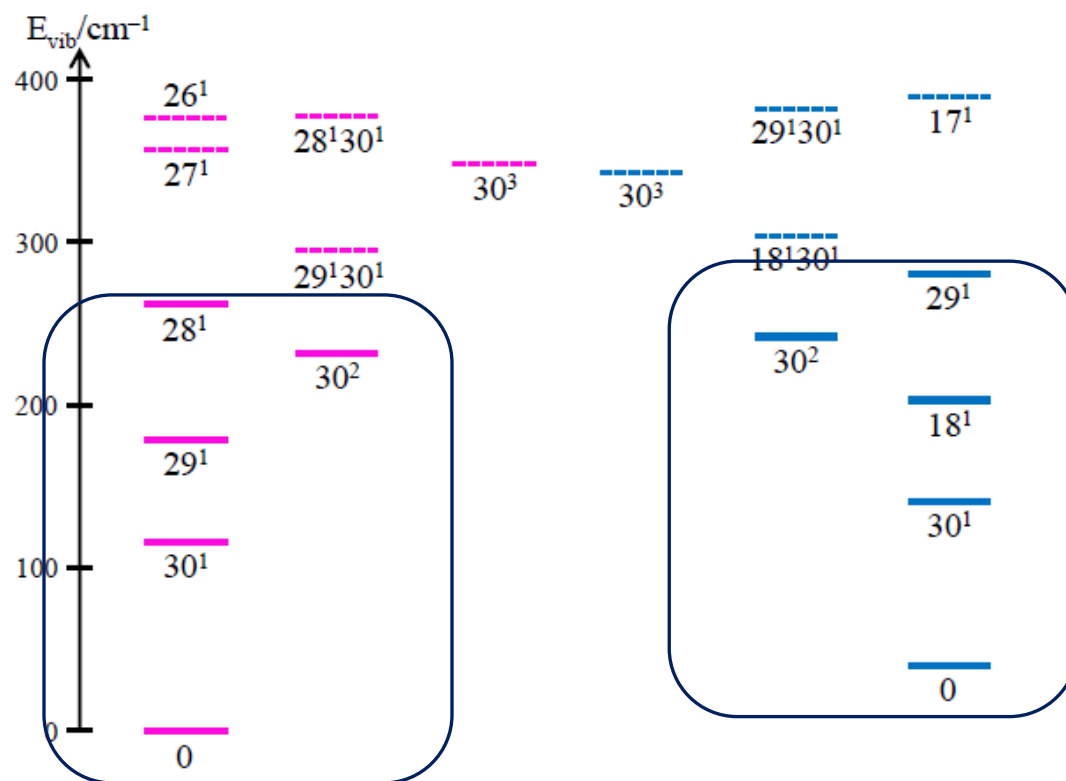
Asymmetric Rotor

Approximate expression *for near Prolate Top*

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

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

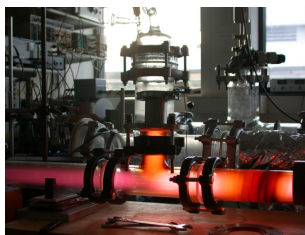
Content of the study



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

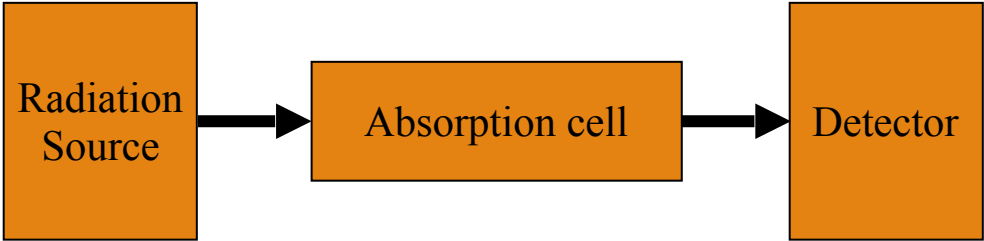
The *gauche* states are shown on the left-hand side, those of *anti* on the right.

Content of the study



Laboratory Measurements

Analysis & Simulations



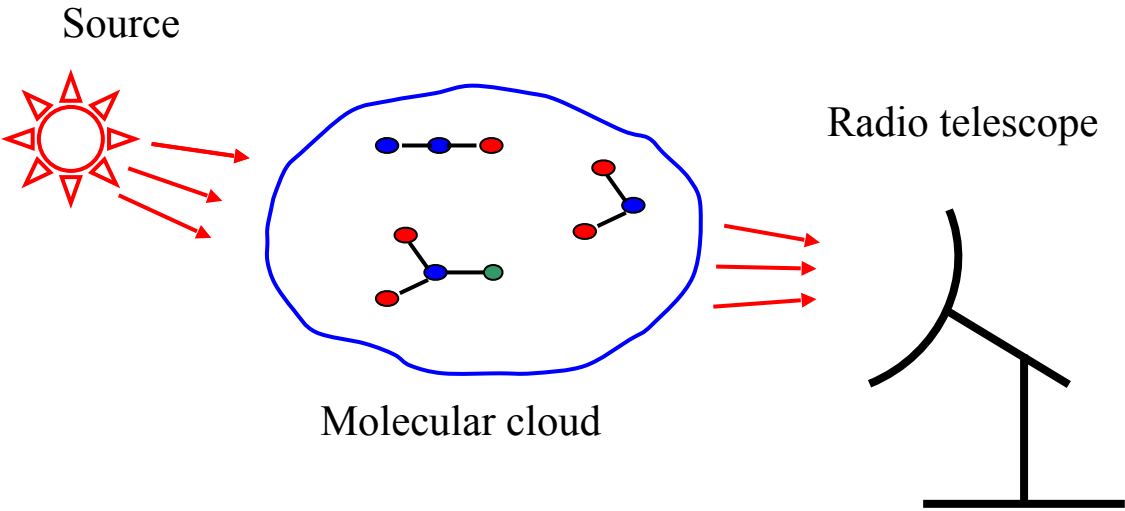
Next molecules interested



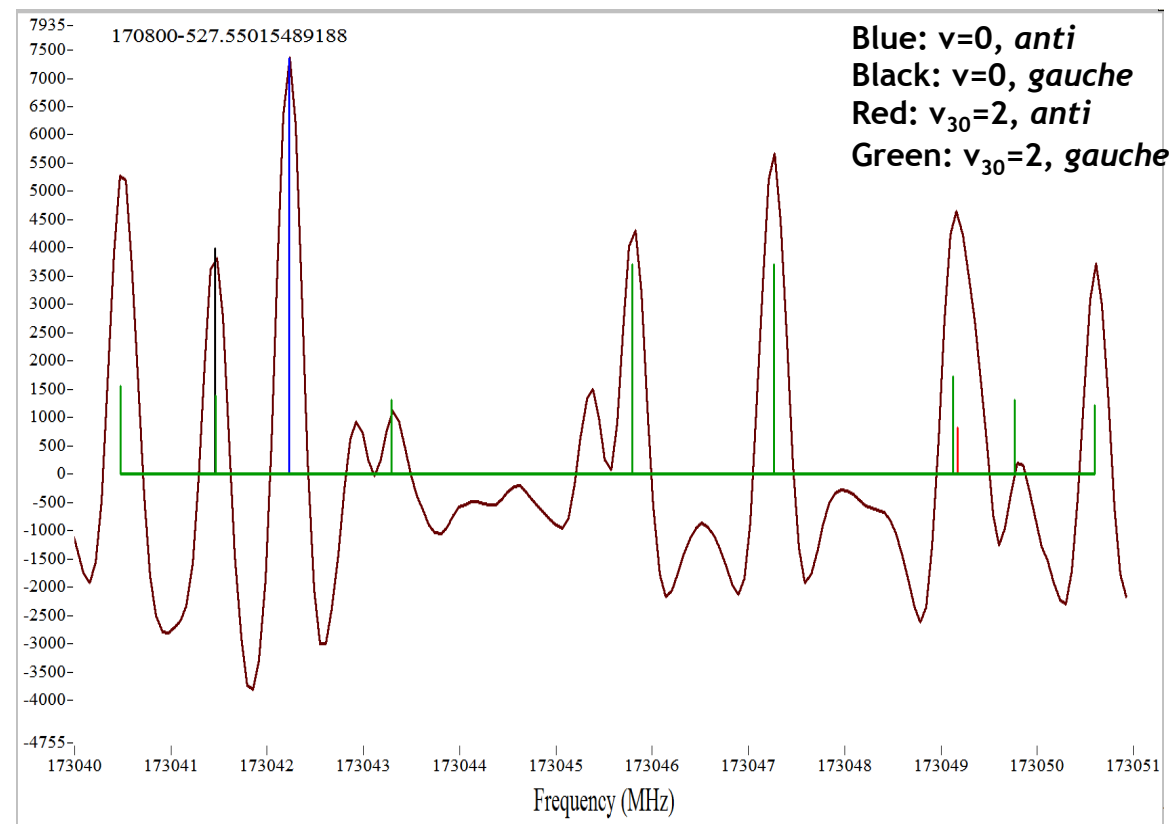
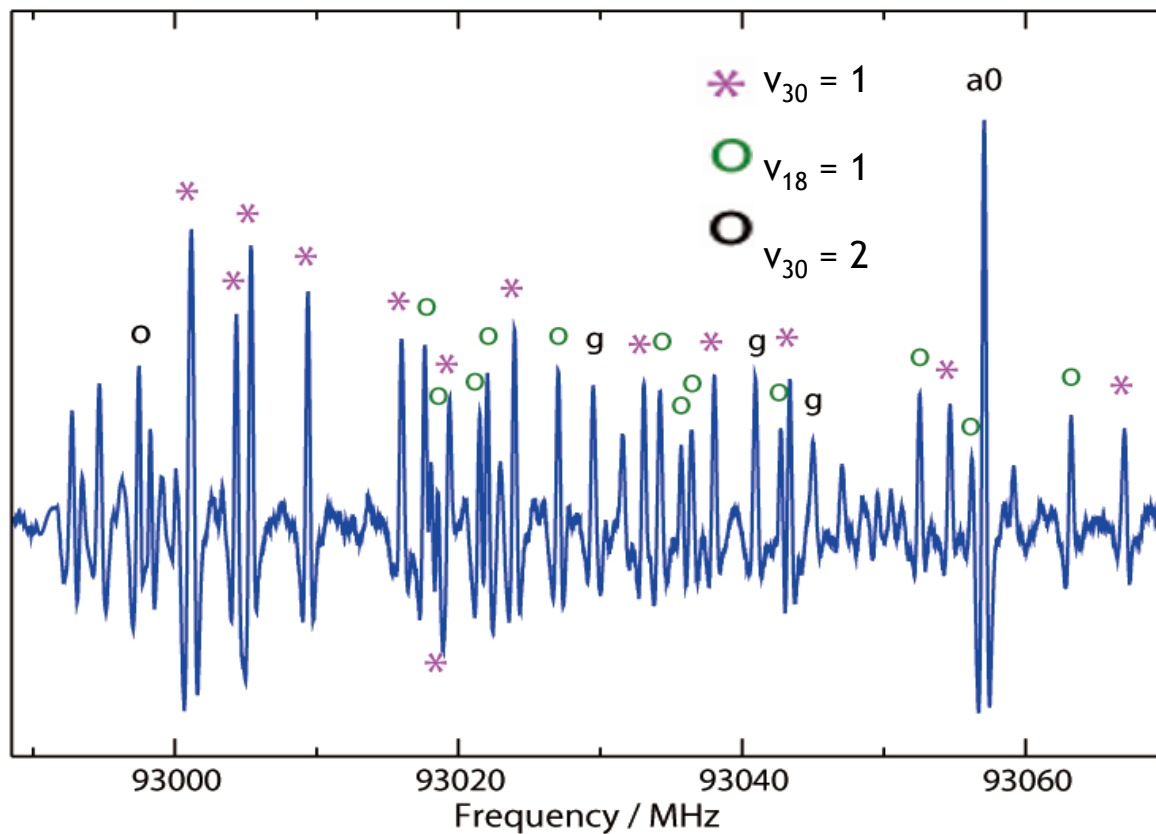
Astronomy Observation

a-n-PICN Fri Jun 03 16:30:01 2016

| | | | | | | | | |
|------------|------------------------|----------------|---------|------------|------------|------------|------------------|------------|
| 22 | 1184 | 3 | 0 | 0.0000E+00 | 3.0000E+05 | 1.0000E+00 | 1.0000000000E+00 | 0.0000E+00 |
| 8 | 1 | 2 | 0 | 60 | 0 | 1 | 1 | 1 |
| 8 | 3 | 1 | 0 | 60 | 0 | 1 | 1 | 1 |
| 10099 | 2.366831839461500E+04 | 1.00000000E+35 | /A | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 20099 | 2.268146699620979E+03 | 1.00000000E+35 | /B | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 30099 | 2.152963827561871E+03 | 1.00000000E+35 | /C | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2099 | -2.406415799865493E-01 | 1.00000000E+35 | /D | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1199 | 1.082493128679623E-02 | 1.00000000E+35 | /E | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 299 | -3.967100819674714E-04 | 1.00000000E+35 | /F | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 40199 | -4.661053258419594E-05 | 1.00000000E+35 | /G | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 50099 | -5.889508609771833E-07 | 1.00000000E+35 | /H | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3099 | 2.586920464141580E-06 | 1.00000000E+35 | /I | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2199 | 4.082691148501867E-07 | 1.00000000E+35 | /J | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1299 | -2.153220004525752E-08 | 1.00000000E+35 | /K | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 399 | 3.719476966721633E-10 | 1.00000000E+35 | /L | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 40299 | 1.002084633762322E-10 | 1.00000000E+35 | /M | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 90199 | 1.772644290439110E-12 | 1.00000000E+35 | /N | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 499 | -4.058417115630836E-16 | 1.00000000E+35 | /O | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3199 | -5.448896856170493E-11 | 1.00000000E+35 | /P | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1399 | 3.063028481392386E-14 | 1.00000000E+35 | /Q | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 99 | 1.500000000000000E+06 | 1.00000000E+37 | /R | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 110010011 | -3.440000000000000E+00 | 1.00000000E+35 | /chi_a | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| -110030011 | 3.440000000000000E+00 | 1.00000000E+37 | /chi_c | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 110020011 | 1.385000000000000E+00 | 1.00000000E+35 | /chi_b | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| -110030011 | -1.385000000000000E+00 | 1.00000000E+37 | /chi_cc | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |

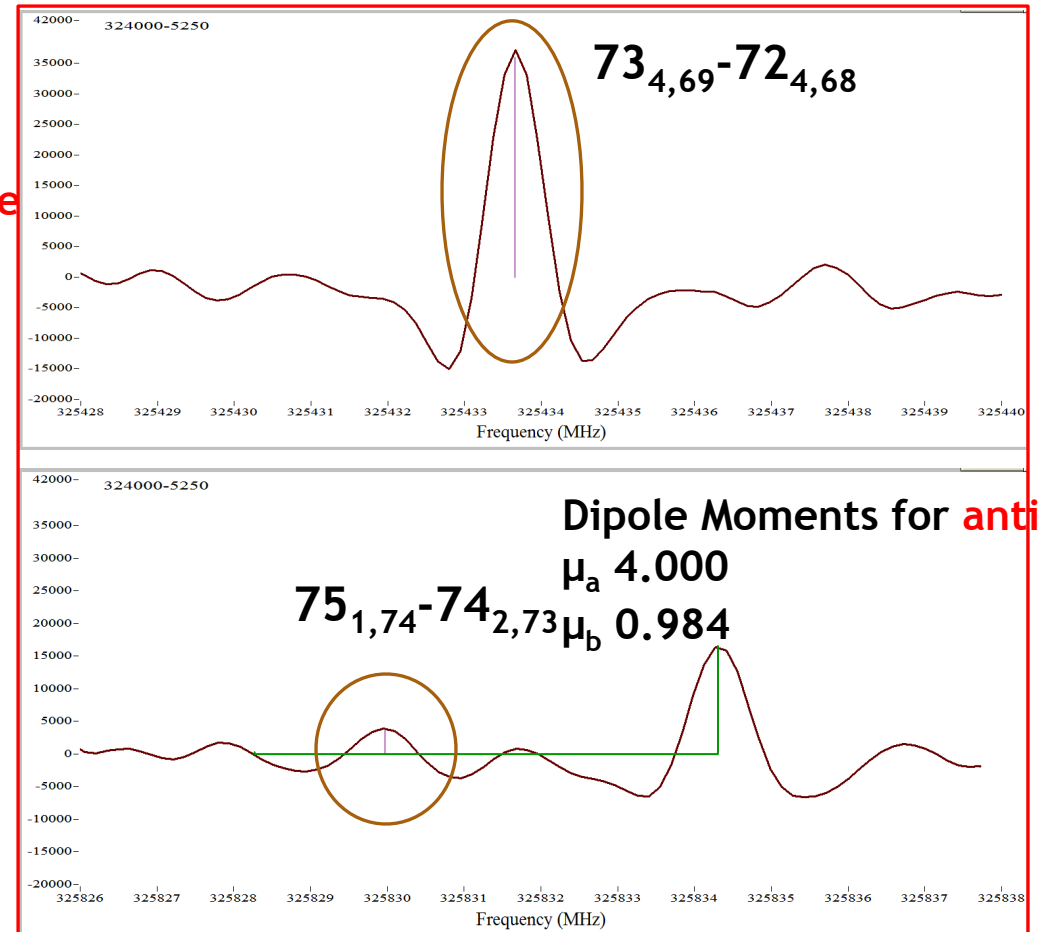
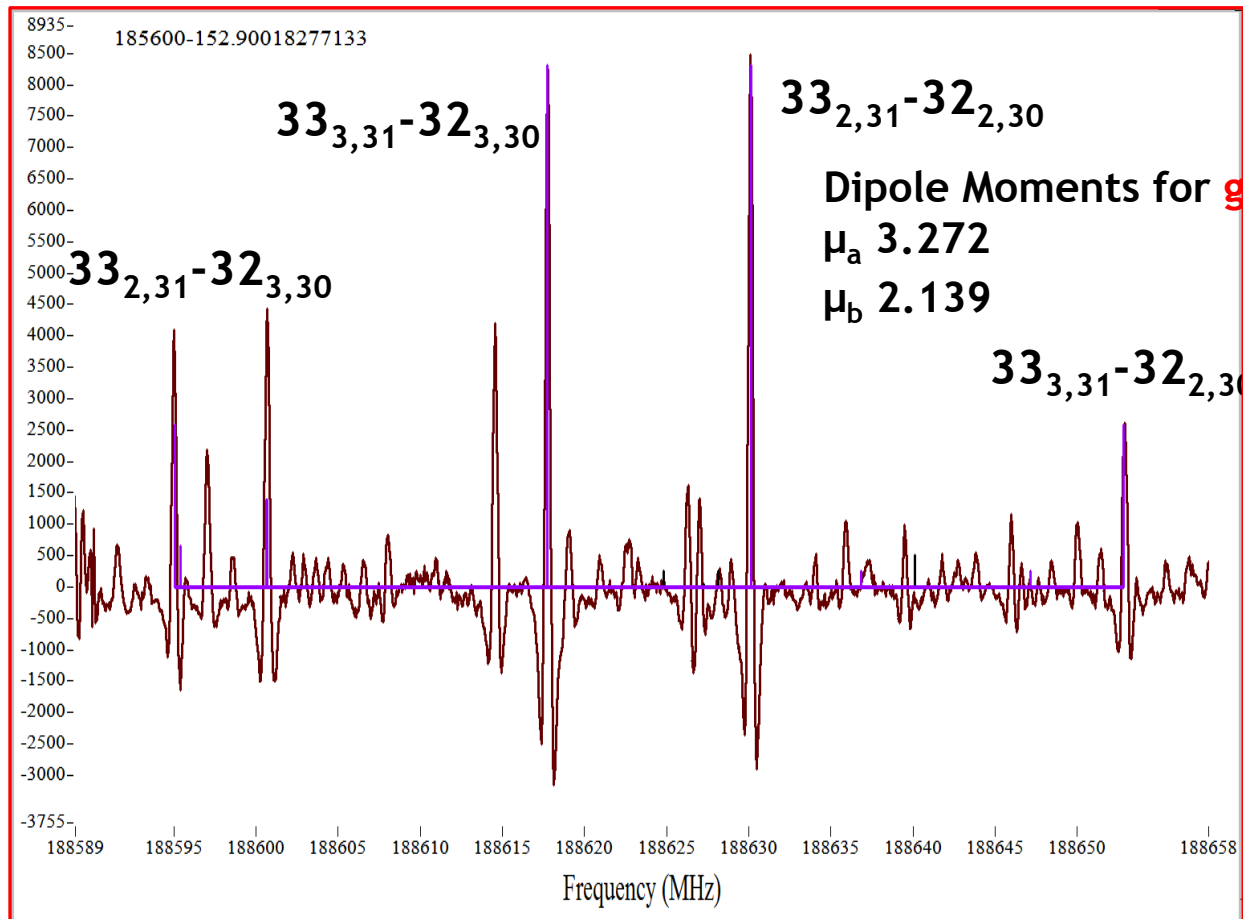


Analysis

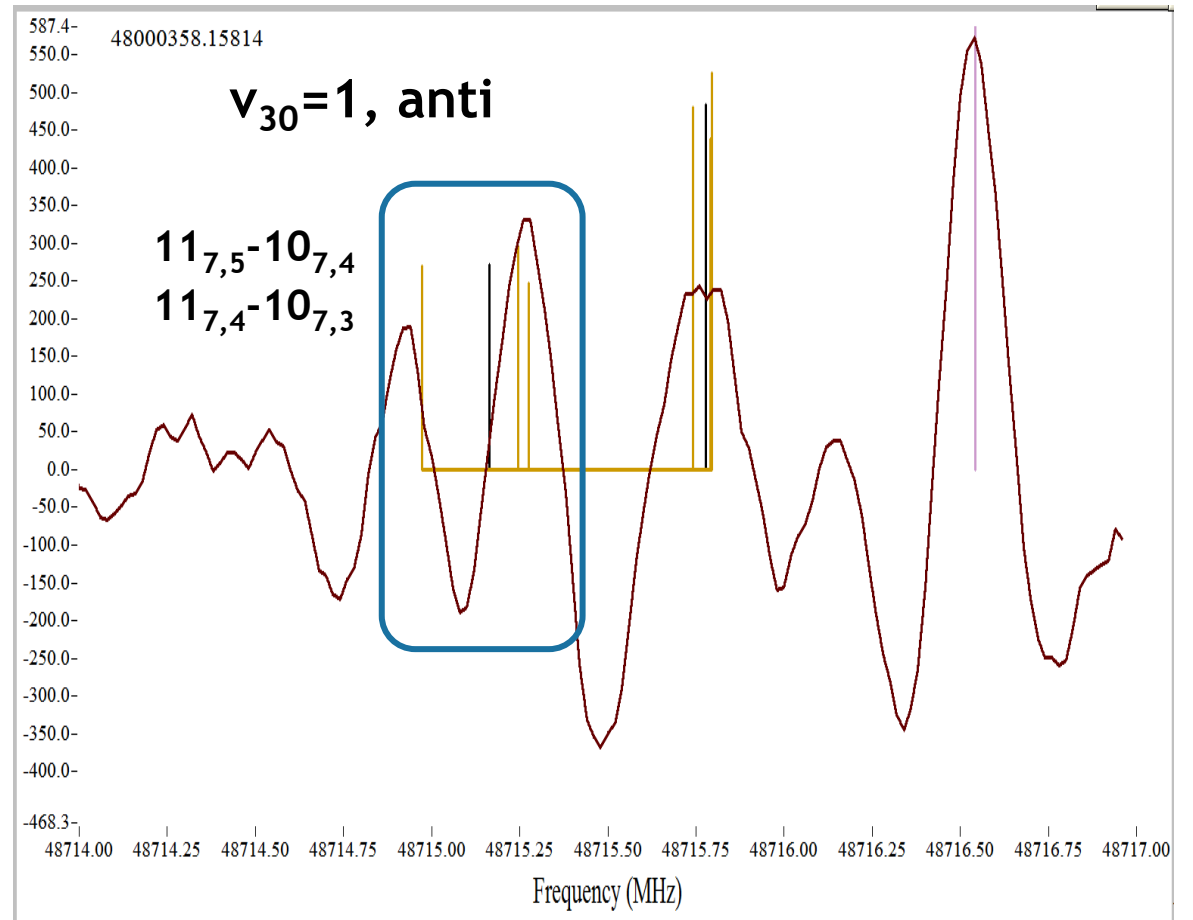
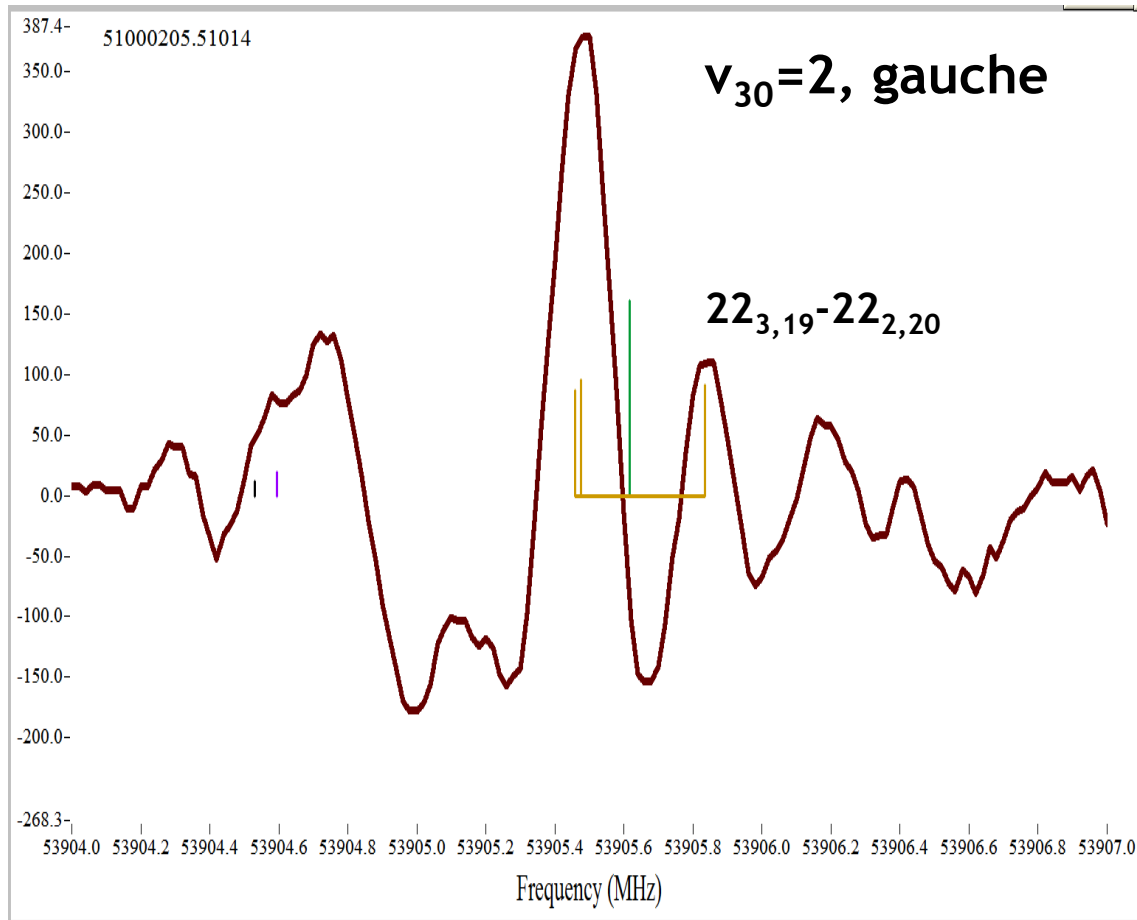


Extract of Laboratory Spectrum

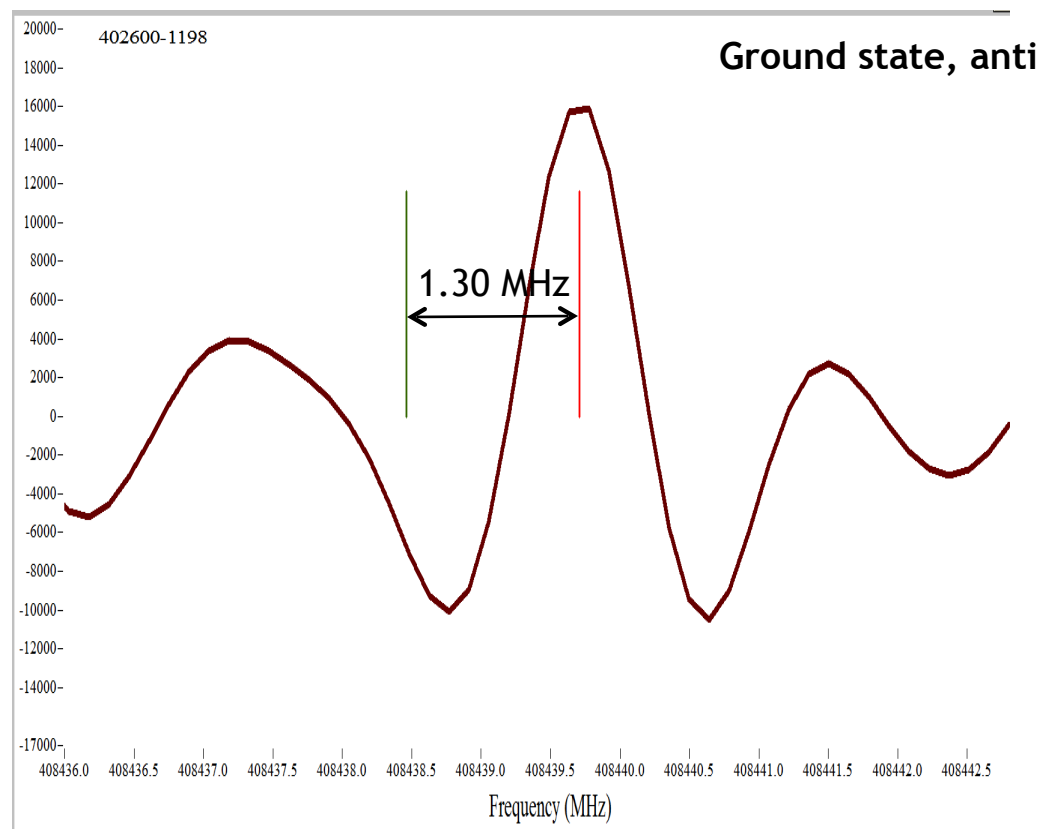
μ_a and μ_b transitions



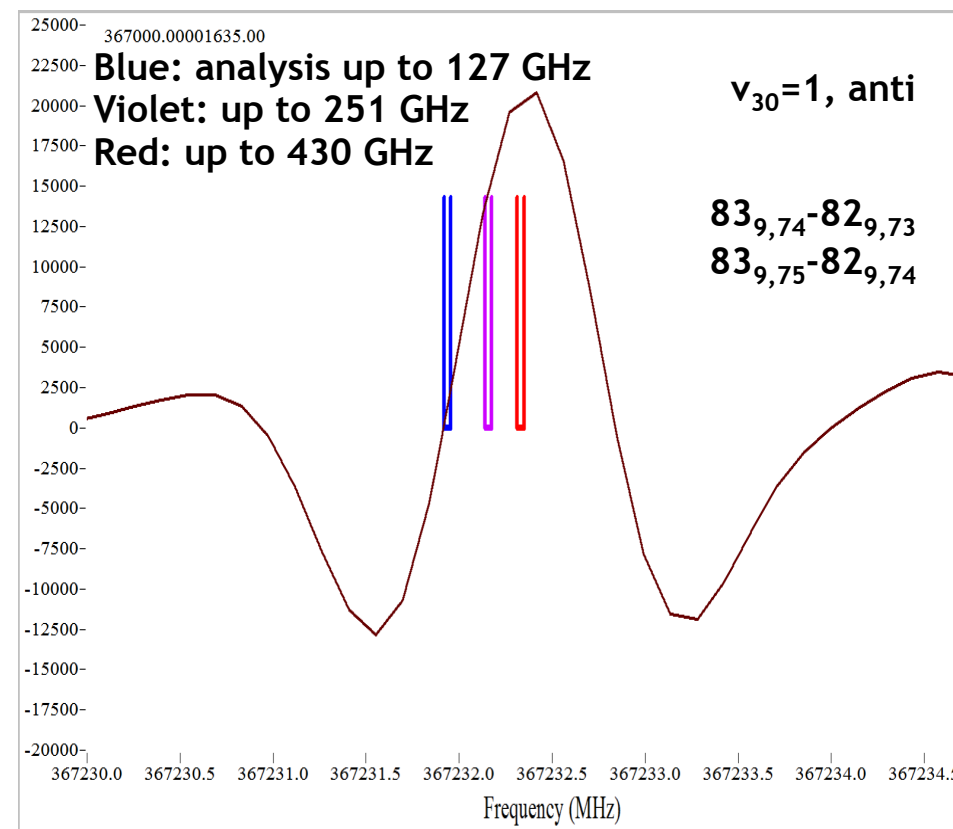
Hyperfine structure



progress

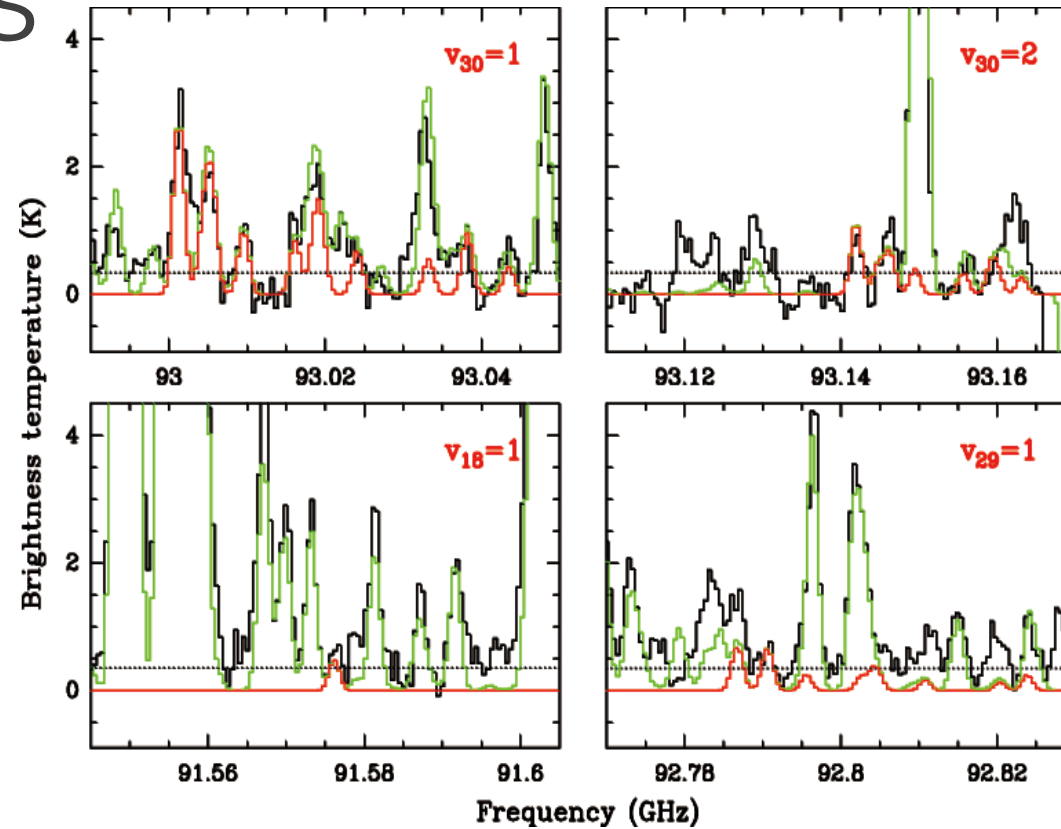


Old prediction (green) and our new prediction (red)



Prediction shifts at higher frequency

progress



Black-spectrum of Sagittarius B2 by ALMA, (Belloche et al.)

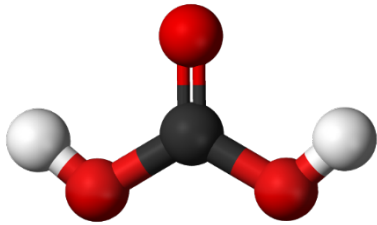
Red-simulated spectrum of Propyl Cyanide in vibrational states (from our work)

Green-simulated spectrum of all known molecules.

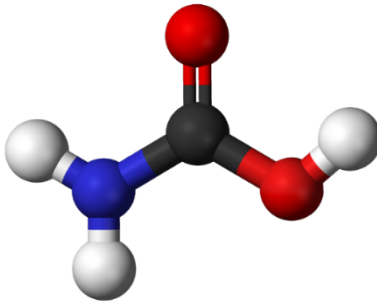
Future plan

Study another astronomical molecule,
eg, carbonic acid, carbamic acid, methylcarbamic acid...

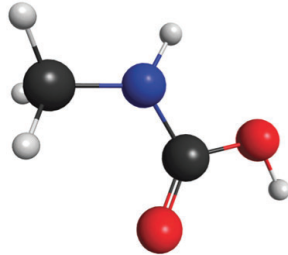
Though, you never know what you'er gone get, thank god, we can choose our targets



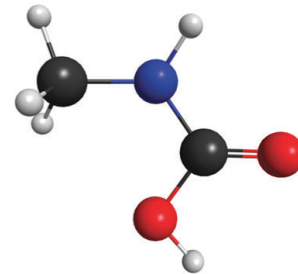
carbonic acid



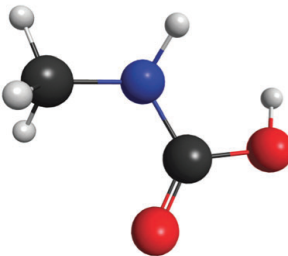
carbamic acid



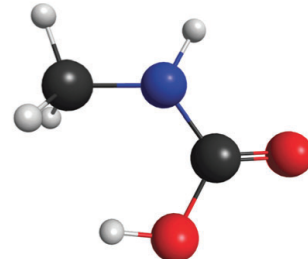
MCA-1



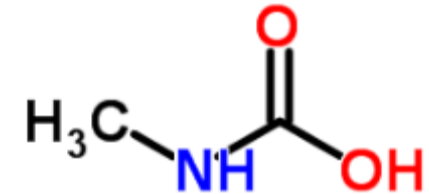
MCA-2



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

