First detection of the ammonium ion in space supported by an improved determination of the 1_0-0_0 rotational frequency of NH_3D^+ from the ν_4 infrared band

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OUTLINE

1. MOTIVATION
2. EXPERIMENTAL SET-UP
3. MEASUREMENTS
4. RESULTS
5. CONCLUSIONS

MOTIVATION

Why NH_4^+ ?

Hierarchy of protonated ions

Molecule	Proton affinity (kJ mol^{-1})	Protonated ion
NH_3	**853.6**	**NH_4^+**
H_2O	691	H_3O^+
N_2	493.8	N_2H^+
H_2	422.3	H_3^+
O_2	421	HO_2^+

Astronomical environments

NH_4^+ is the starting point to form NH_3 and amine prebiotic molecules in Space.

WARM:

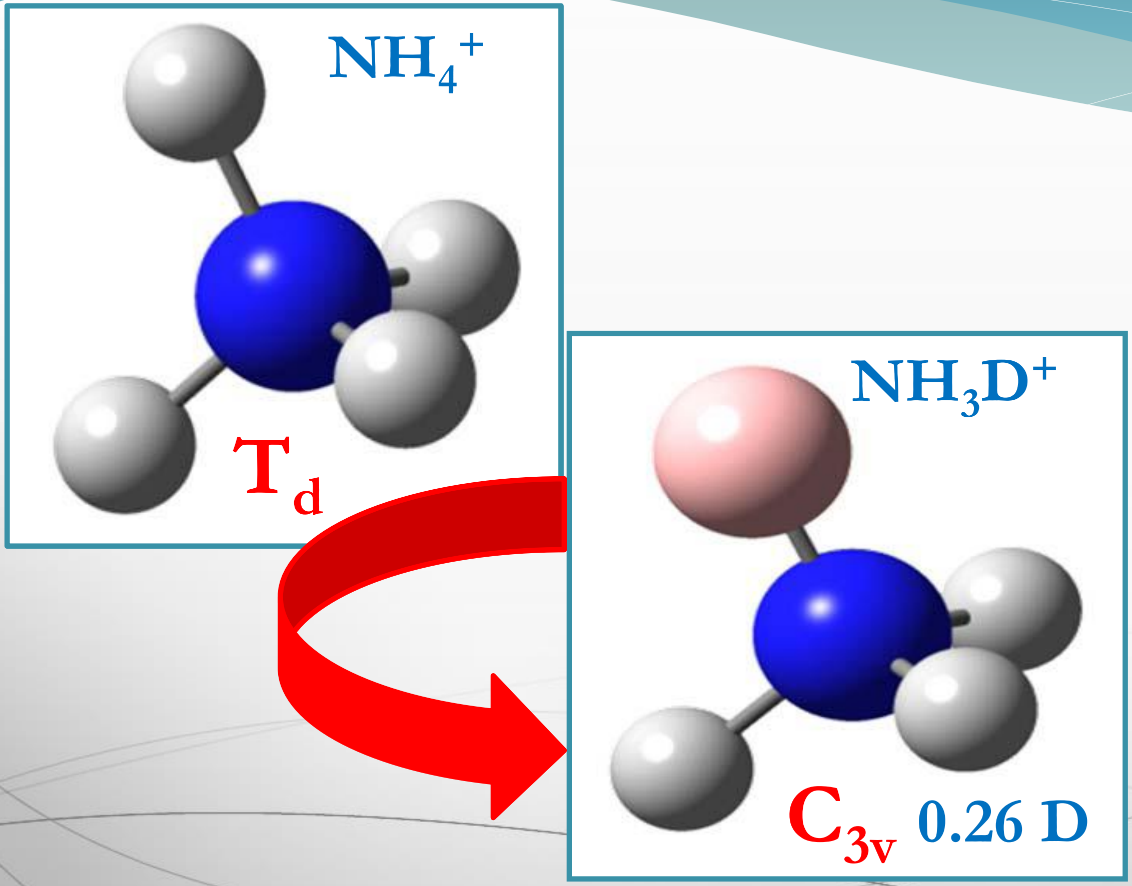
$$NH_3 + H^+ \rightarrow NH_4^+$$

COLD clouds:

$$N^+ + H_2 \rightarrow NH^+ + H$$
$$NH^+ + H_2 \rightarrow NH_2^+ + H$$
$$NH_2^+ + H_2 \rightarrow NH_3^+ + H$$
$$NH_3^+ + H_2 \rightarrow NH_4^+ + H$$
$$NH_4^+ + e^- \rightarrow NH_3 + H$$

MOTIVATION

… and NH_3D^+?

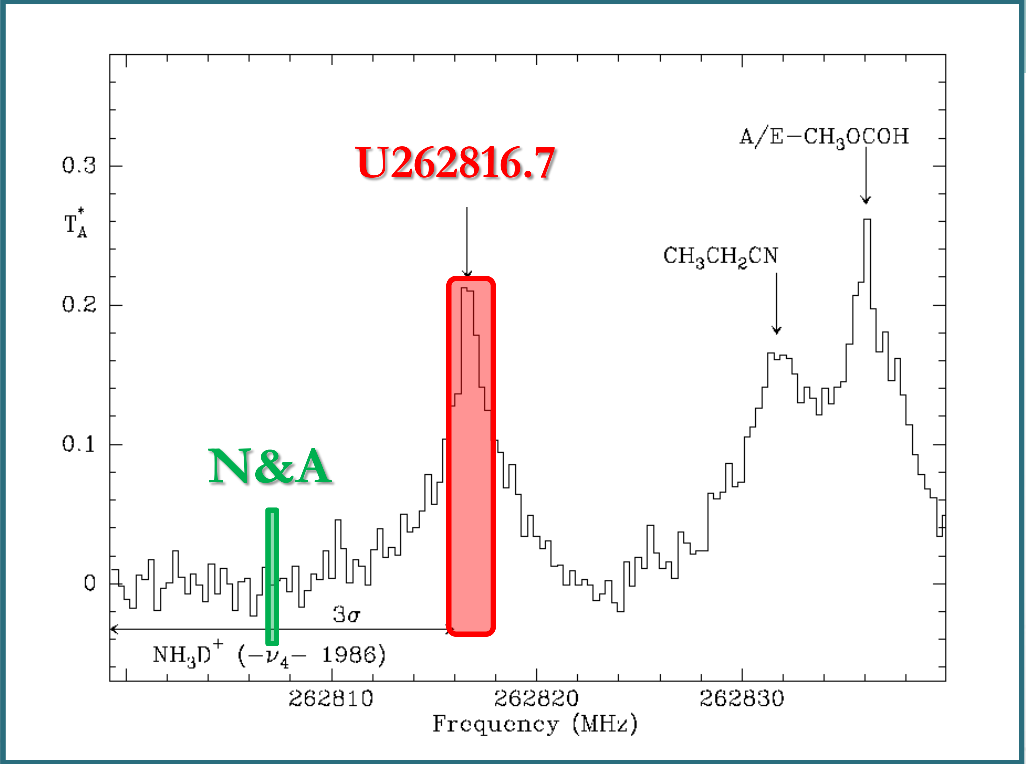


From the analysis of the ν_4 infrared band of NH_3D^+ **Nakanaga & Amano** predicted the **1_0-0_0** transition at **262807±9 MHz** (±3σ)

There is **no laboratory rotational spectrum** (mm-wave) of NH_3D (recently tried by J. Pearson & Amano in JET Propulsion Laboratory, NASA).

MOTIVATION

Observations towards proto-star region Orion-IRc2

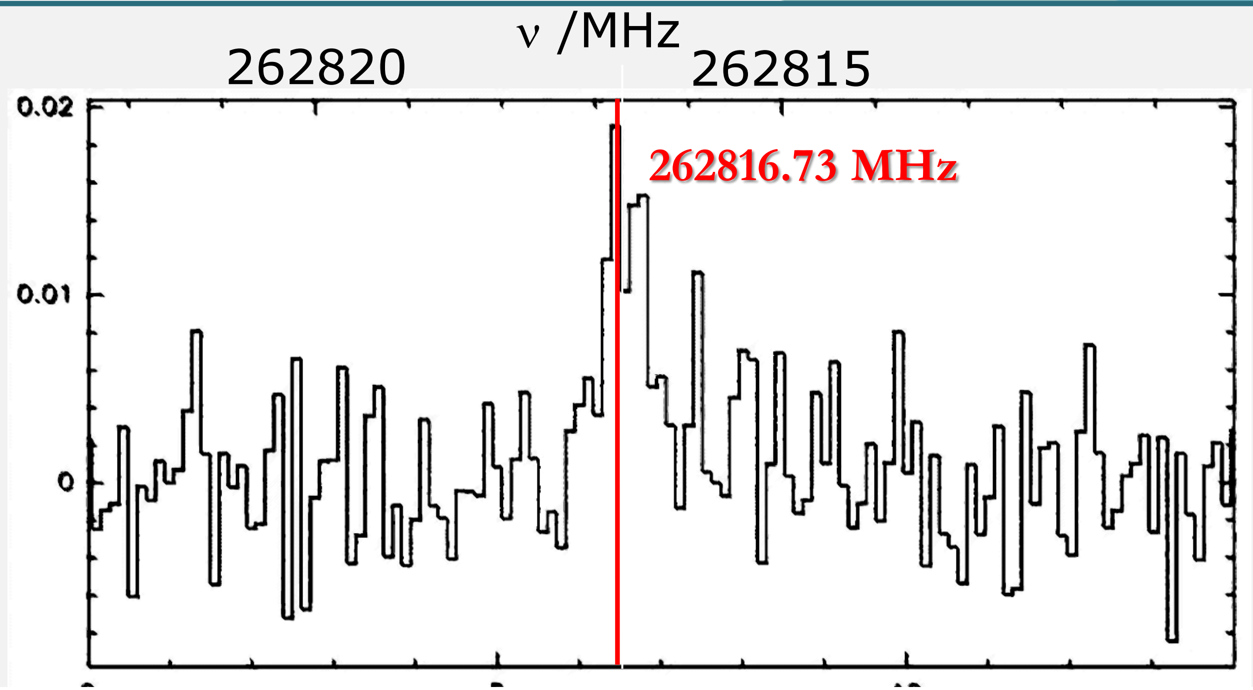


Tercero, B., Cernicharo, J., Pardo, J. R., & Goicoechea, J. R., 2010, A&A, 517, 96
Nakanaga, T., & Amano, T., 1986, Can. J. Phys., 64, 1356

- Surveys by IRAM 30m telescope (Sierra Nevada, Granada)
- > 8000 unidentified features. 4400 lines assigned already.
- A narrow unassigned peak at 262816.73 MHz, close to the predicted frequency for the 1_0-0_0 NH_3D^+ transition at 262807±9 MHz (±3σ).
- Is U262816.7 MHz NH_3D^+???
- Having 3600 unidentified features in Orion…extremely risky!!

MOTIVATION

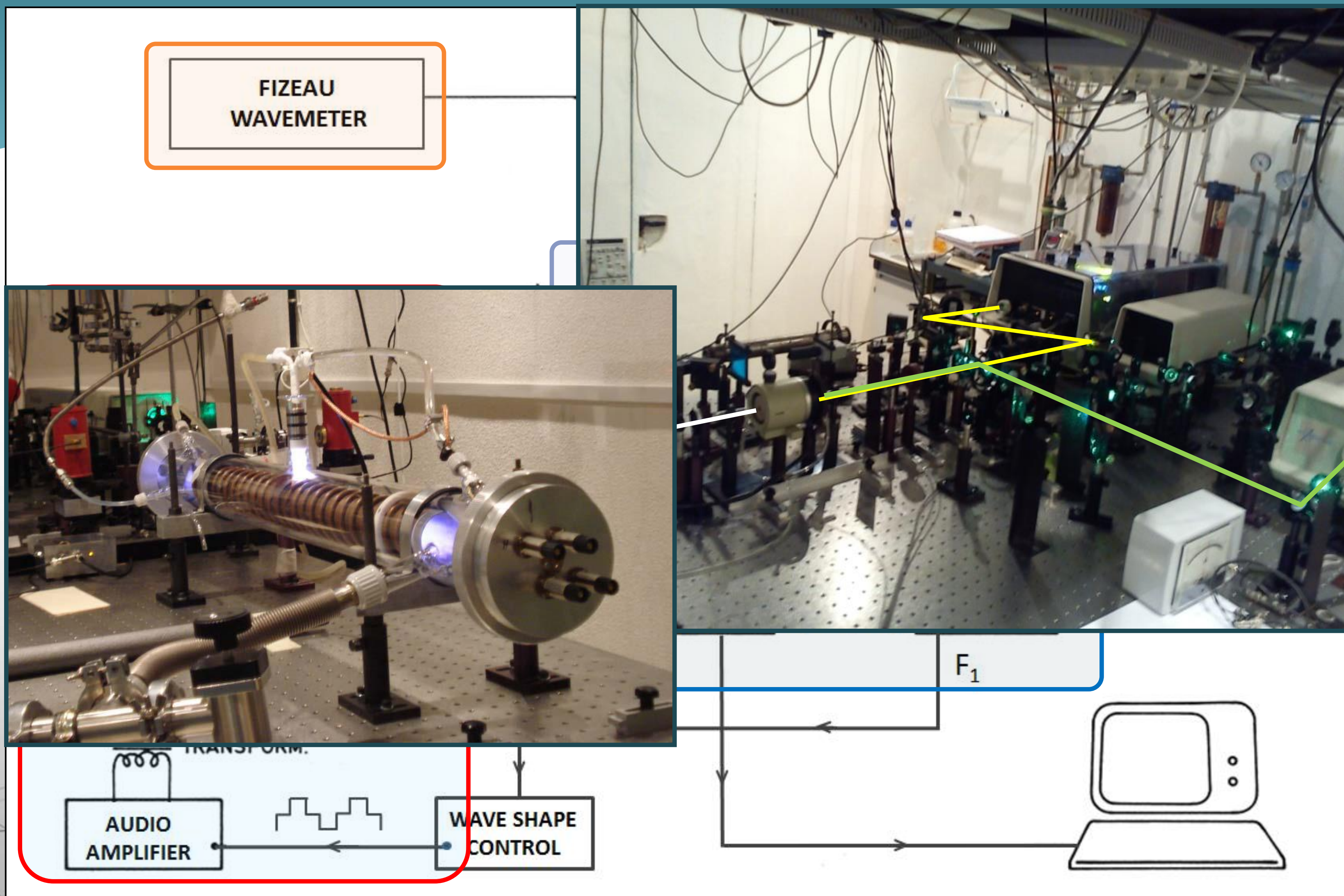
Observations towards cold Prestellar core B1-bS



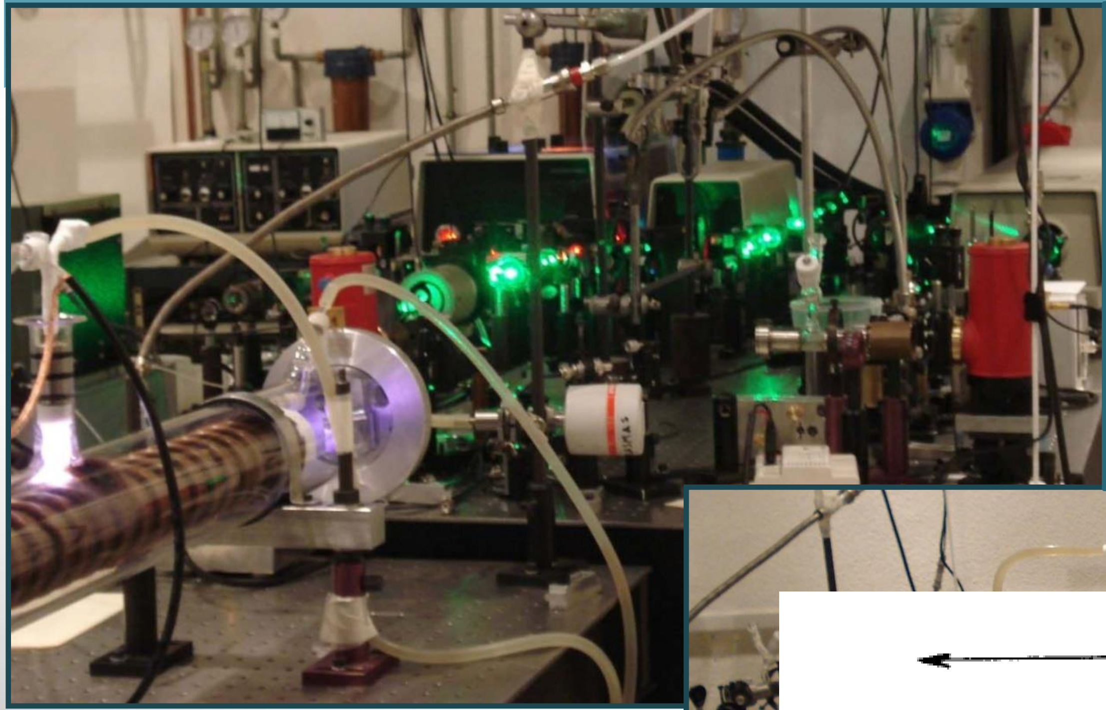
- Narrow and isolated feature (no more lines in 3.8 GHz)
- Kinetic temperature 12 K, the carrier has to be a light species.
- NH_3, $^{15}NH_3$, NH_2D, $^{15}NH_2D$, ND_2H, ND_3 … detected, …$^+$, NND^+, …, $N^{15}NH^+$.

We need more laboratory evidence

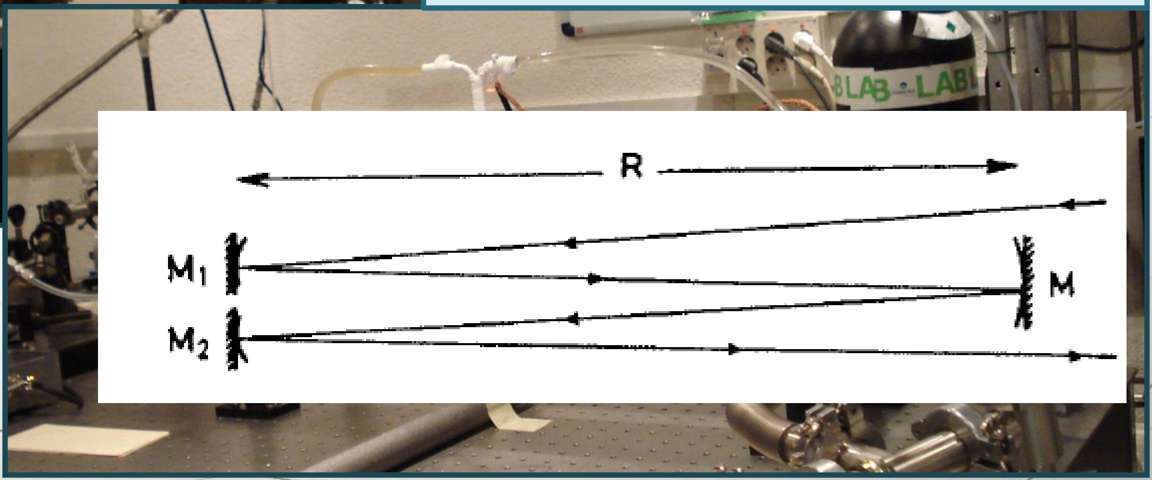
EXPERIMENTAL SET-UP



EXPERIMENTAL SET-UP



- Precursors: $NH_3 : D_2 = 2 : 3$
- Total pressure: 0.34 mbar
- 380 V, 200 mA
- White cell ~9 m inside the cathode
- $F_1 = 5.5$ kHz, $F_2 = 14.2$ kHz
- Lock-in detection at 19.7 kHz

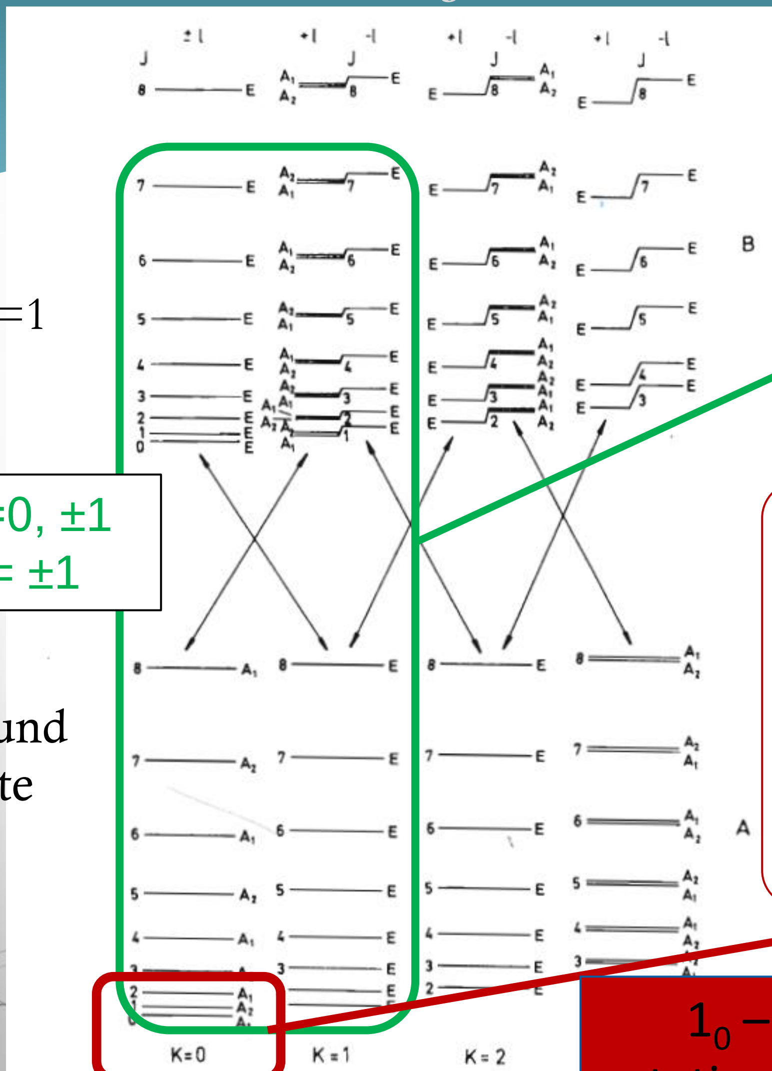


Main differences	This work	N & A
IR frequency scale	A high accuracy wavemeter (10 MHz) for the dye laser and a I_2-stabilized Ar^+ laser	Calibration with N_2O IR absorption lines with 30 MHz accuracy
$NH_3 : D_2$	~ 2 : 3	~ 1 : 10
Absorption path length (m)	9	20
IR power available (µW)	~ 1	~ 10
Detection	$F_1 + F_2$	F_1
Discharge frequency (kHz)	5.5	17

Levels involved in the ν_4 band of NH_3D^+

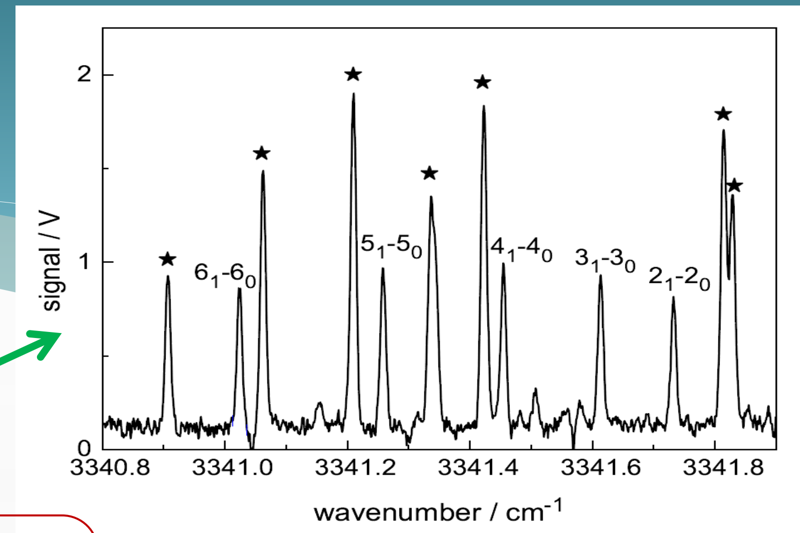
MEASUREMENTS

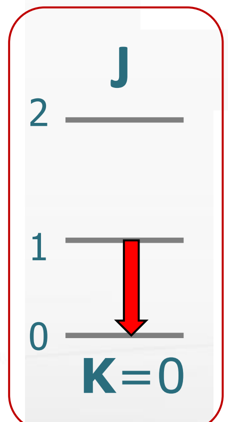
v_4=1



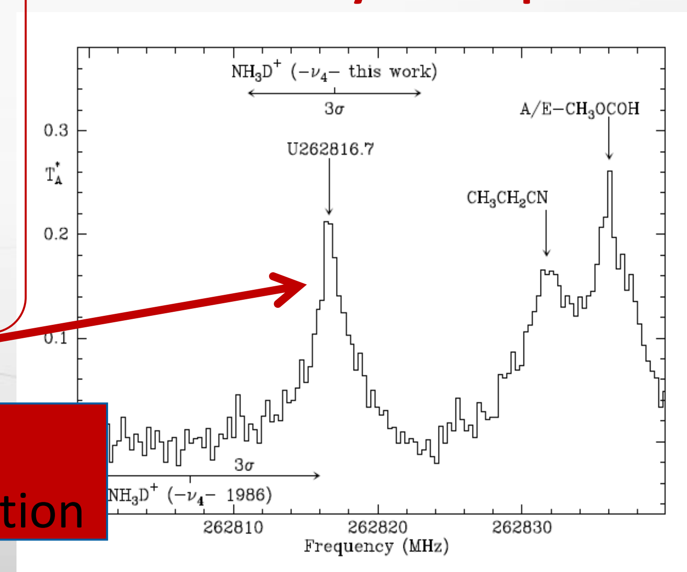
Ground state

ΔJ=0, ±1
ΔK= ±1



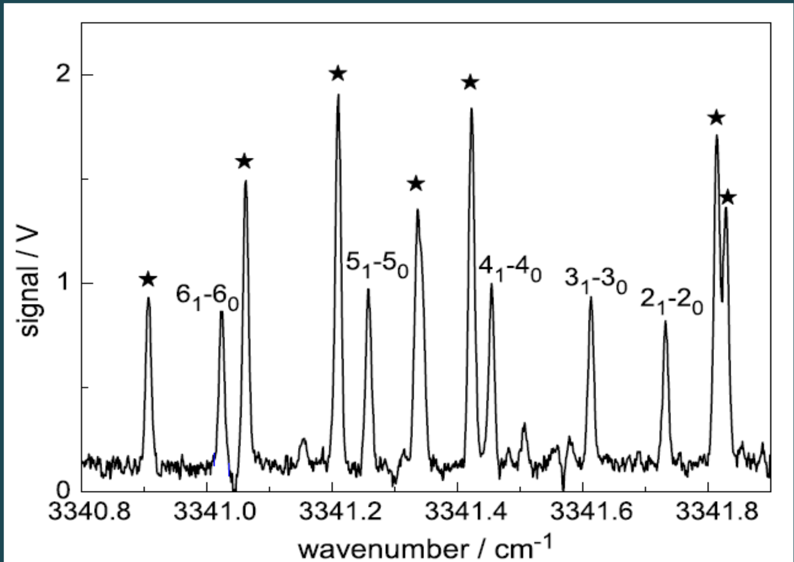


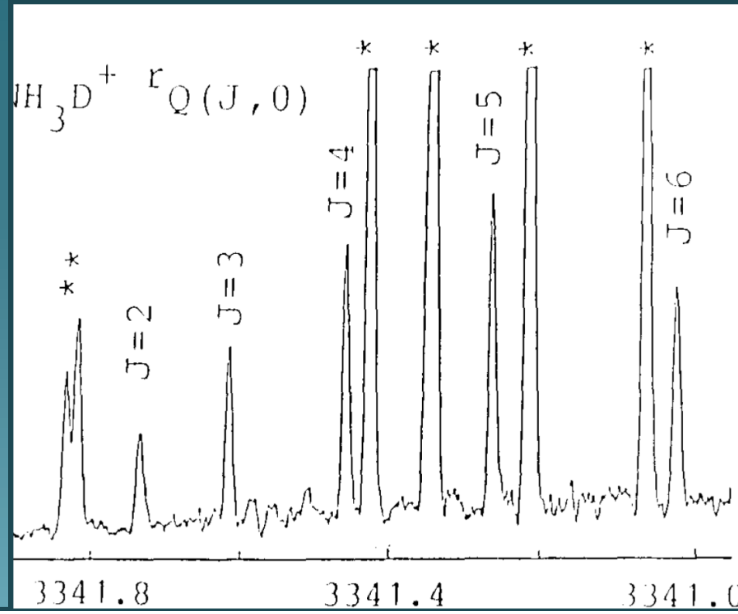
Orion survey: mm spectrum



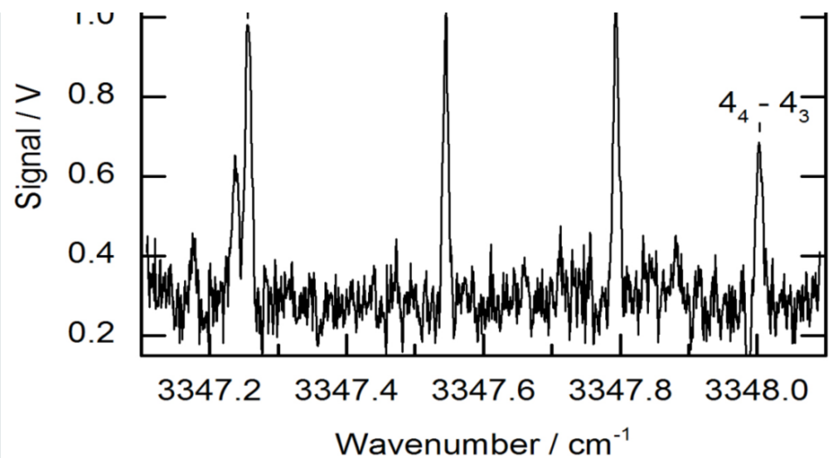
$1_0 - 0_0$ pure rotational transition

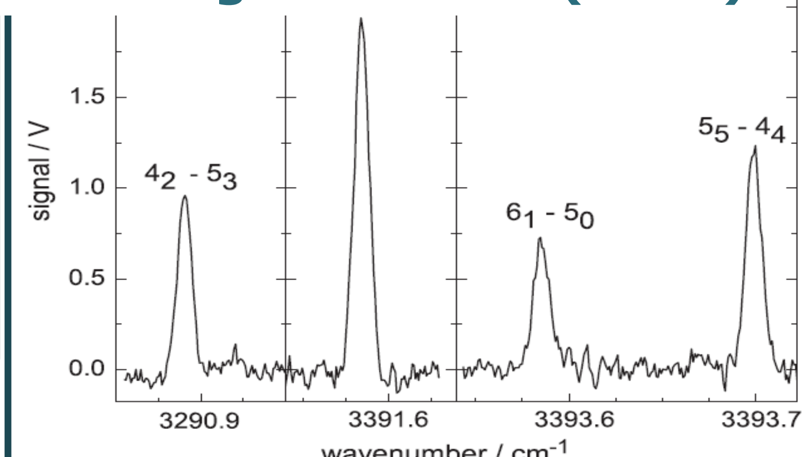
MEASUREMENTS





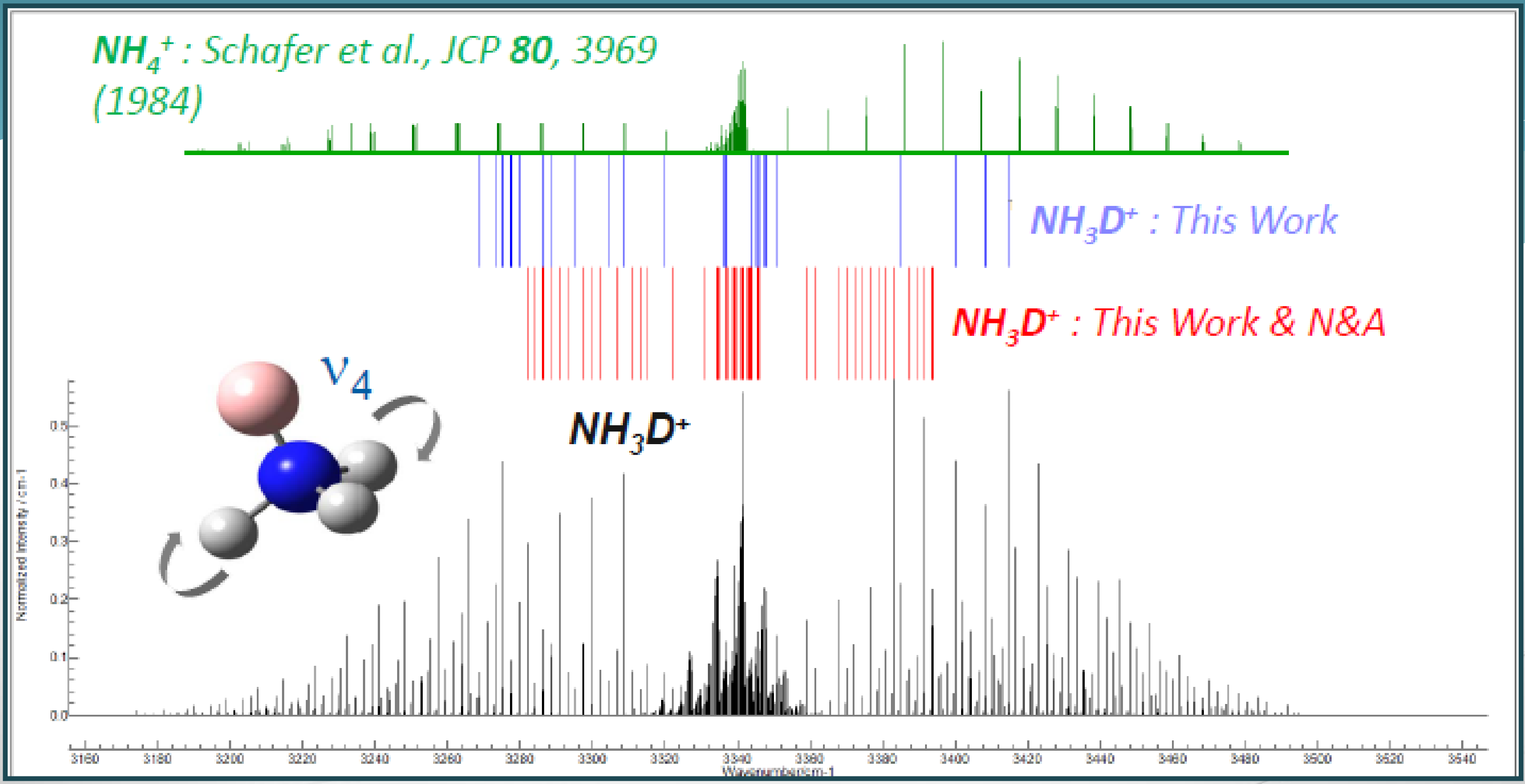
This work **Nakanaga & Amano (1986)**





Ion concentration ~10^{10} cm^{-3} ~10^{-9} bar

RESULTS



Simulations and fits have been done with PGOPHER . (Colin Western, University of Bristol, http://pgopher.chm.bris.ac.uk)

We have been guided by Nakanaga & Amano previous work

RESULTS

- We have recorded **114** transitions between 3268.4 and 3414.7 cm^{-1}. Finally **76** have been included in the fit (vs. 61 in N&A). Lines not included: J,K >8; or show interference from NH_3; or are too broad.

$$\nu(1_0 - 0_0) = 2B'' - 4D''$$

New Predicted J_k (1_0-0_0) =

262817 ± 6 MHz (±3σ)

- A', A'', D_K', D_K'', ζ cannot be determined independently. Constraining A'', D_K'' affects ν_0, ζ, A', D_K'

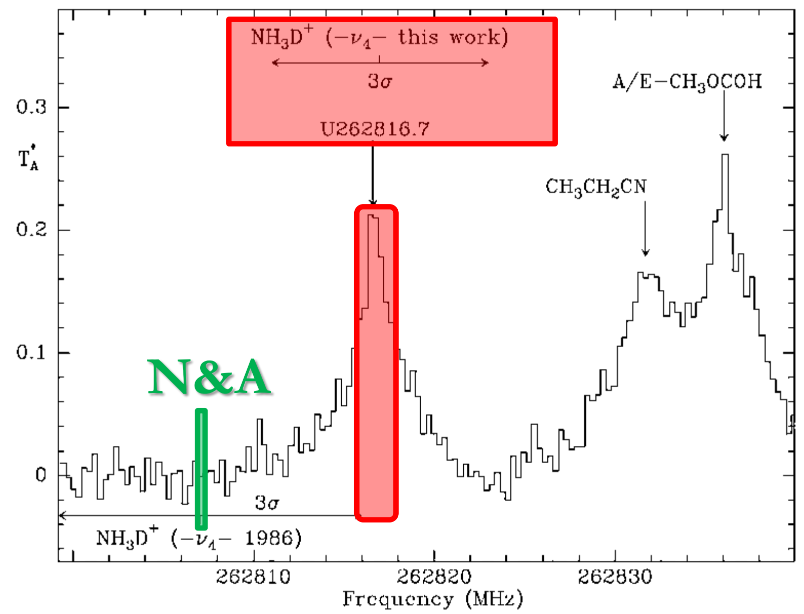
- s.d. of the fit: 5×10^{-4} cm^{-1}

Table 2. Constants derived from the fit

Constants /cm^{-1}	This work	N&A (1986)
A''	5.852[a]	5.852[a]
B''	4.3834351(294)	4.38327(5)
D''_J	$6.1363(373)\times10^{-5}$	$5.87(9)\times10^{-5}$
D''_{JK}	$1.4689(293)\times10^{-4}$	$1.52(6)\times10^{-4}$
D''_K	0.0[a]	0.0[a]
ν_0	3341.07498(17)	3341.0764(3)
A'	5.818834(37)	5.81871(9)
B'	4.3640729(278)	4.36391(5)
D'_J	$5.4024(339)\times10^{-5}$	$5.13(10)\times10^{-5}$
D'_{JK}	$9.705(296)\times10^{-5}$	$1.02(7)\times10^{-4}$
D'_K	$3.801(91)\times10^{-5}$	$3.1(3)\times10^{-5}$
ζ	0.0582020(76)	0.058191(14)[b]
η_J	$-4.2581(686)\times10^{-4}$	$-4.23(13)\times10^{-4}$
η_K	$1.744(74)\times10^{-4}$	$1.76(18)\times10^{-4}$
q_+	$-3.393(98)\times10^{-4}$[c]	$2.93(19)\times10^{-4}$

CONCLUSIONS

- We believe our frequencies are good to 10 MHz (3σ)
- Our Ar+ laser is locked to an I_2 line known with 0.1 MHz accuracy
- We have measured some more lines than in N&A work
- All statistical parameters are somewhat better
- We propose 262817±6 MHz (±3σ) as the frequency of the 1_0-0_0 rotational transition of NH_3D^+, supporting the assignment of emissions in Orion IRc2 and Perseo B1-bS to NH_3D^+



CONCLUSIONS

2013	NH_3D^+	**Detection of the Ammonium Ion in Space** J. Cernicharo, B. Tercero, A. Fuente, J. L. Domenech, M. Cueto, E. Carrasco, V. J. Herrero, I. Tanarro, N. Marcelino, E. Roeff, M. Gerin, and J. Pearson. ApJ 771:L10 (2013) **Improved Determinination of the 1_0-0_0 Rotational Frequency of NH_3D^+ from the High-Resolution Spectrum of the v_4 Infrared Band** J. L. Doménech, M. Cueto, V. J. Herrero, I. Tanarro, B. Tercero, A. Fuente, and J. Cernicharo. ApJ 771:L11 (2013)	Orion-IRc2, B1-bS 1_0-0_0(262816.73 MHz)

http://www.astrochymist.org/astrochymist_mole.html

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AND YOU, FOR YOUR ATTENTION!!!