

Unveiling ALMA Band 2 Workshop 2026

Tuesday 24th - Thursday 26th February 2026

Congress Centre of the CNR Bologna (Italy)

<https://arc.ira.inaf.it/events/b2-workshop-2026/>

2'-Hydroxyacetophenone: Lab data and ALMA archive screening

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Department of Chemistry G. Ciamician

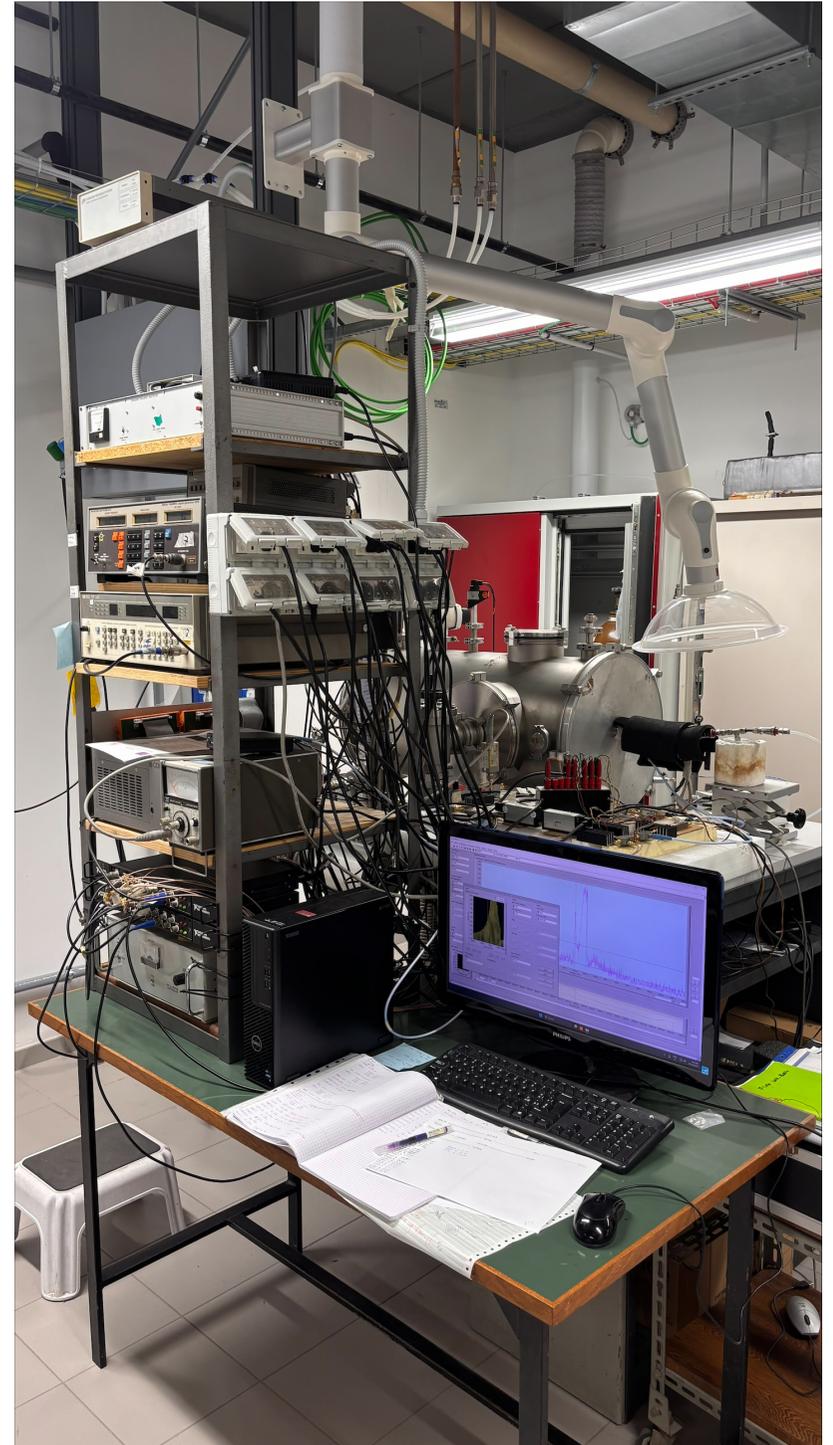
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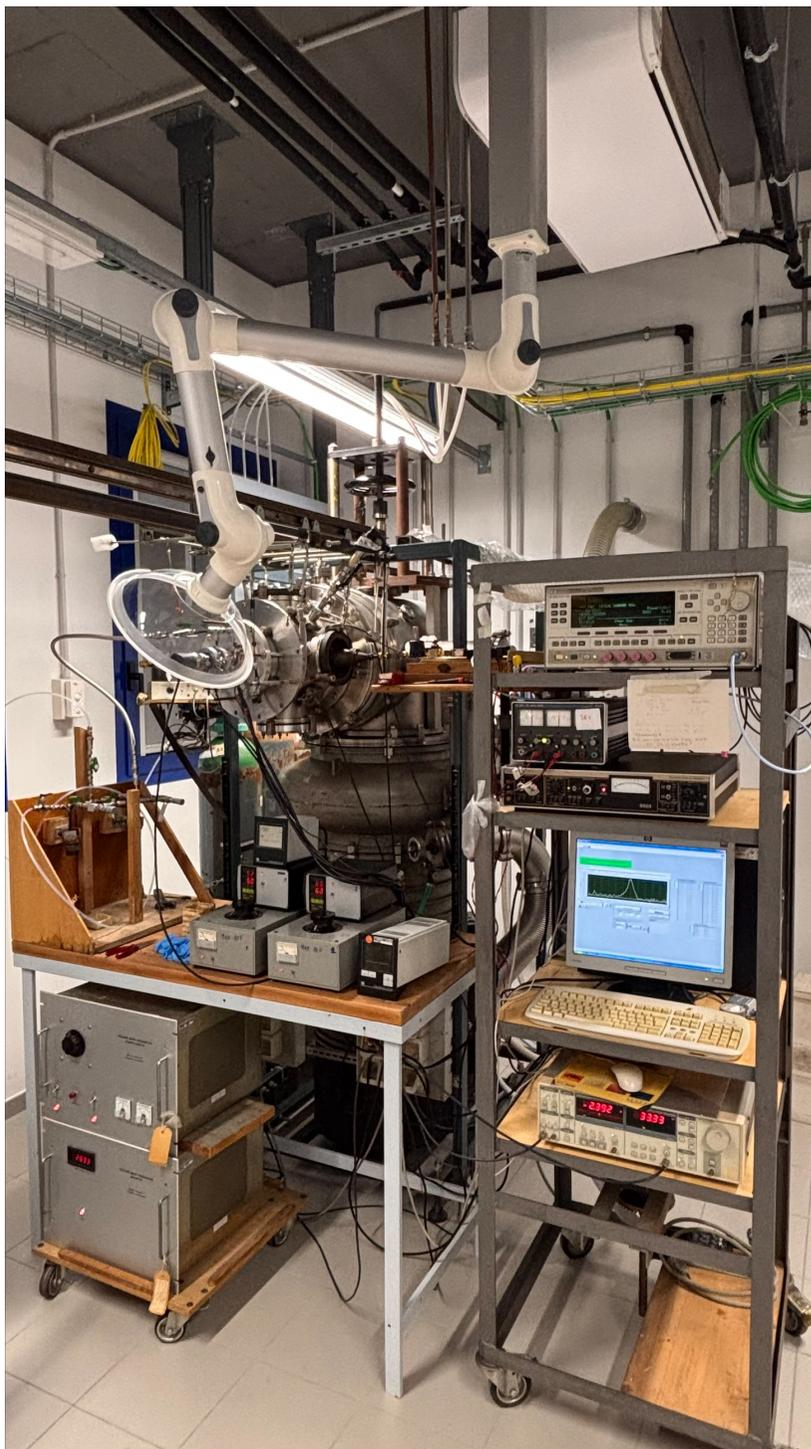
Supersonic expansion Fourier transform microwave spectrometer

**Frequency range 6-18 GHz
Resolution 10 kHz
Accuracy 5 kHz**

Rotational temperature ≈ 1 K

Sample temperature up to 80 °C





Millimeter wave free-jet absorption Stark modulated spectrometer

**Frequency range 59.6-74.4 → 110 GHz
Resolution 300 kHz
Accuracy 50 kHz**

Rotational temperature ≈ 10 K

Sample temperature up to 150 °C



GIER - RSRG

Grupo de Investigación en
Espectroscopía Molecular - Rotational
Spectroscopy Research Group

UIC-293 Junta de Castilla y León

Welcome to the website of the RSRG of the University of
Valladolid, Spain.

Grupo de Investigación en Espectroscopía de Rotación



Chirped pulsed supersonic expansion Fourier transform microwave spectrometer

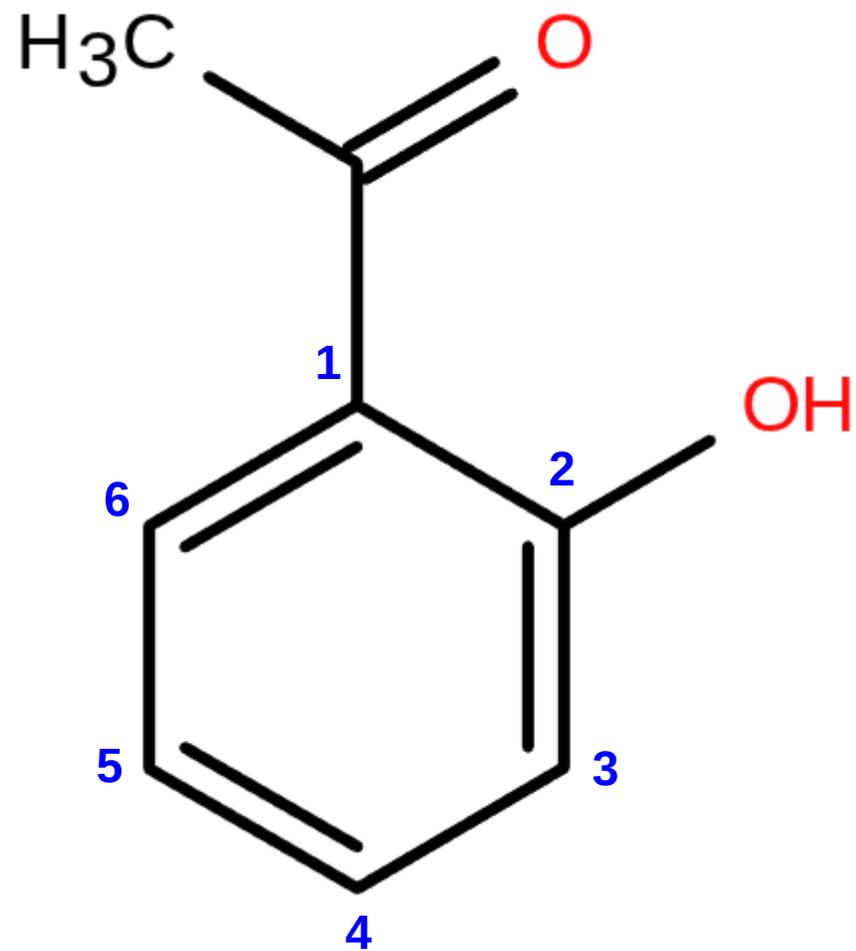
Frequency range 2-8 GHz

Resolution 30 kHz

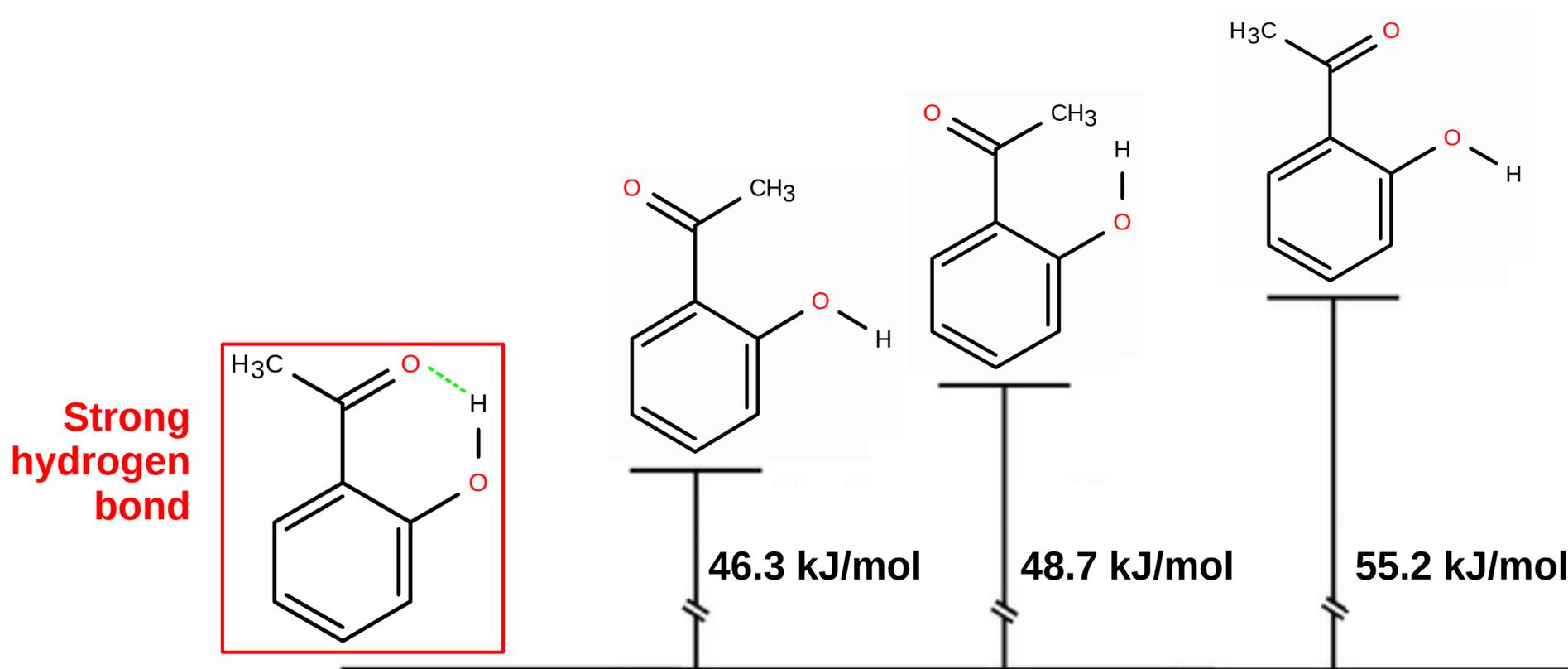
Accuracy 10 kHz

Rotational temperature ≈ 7 K

2'-hydroxyacetophenone C₈H₈O₂



Under equilibrium conditions, up to 1000 K only one conformer is populated



B3LYP-D3(BJ)/Def2-TZVP [Boi+ 2024]

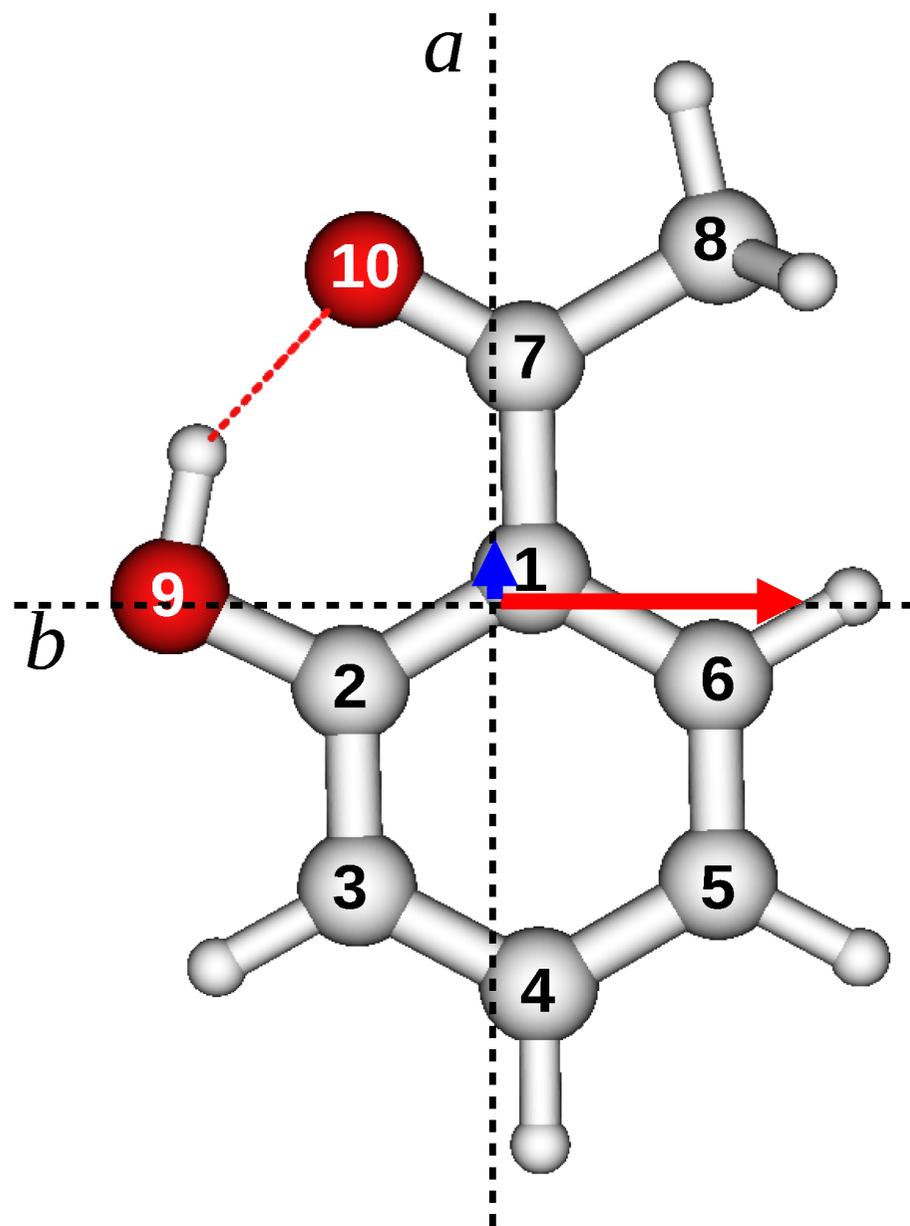
Electric dipole moment

$$\mu_{\text{tot}}=3.24 \text{ D}$$

$$\mu_a=0.77 \text{ D}$$

$$\mu_b=3.15 \text{ D}$$

MP2/aug-cc-pVTZ



Benzene derivatives in TMC-1

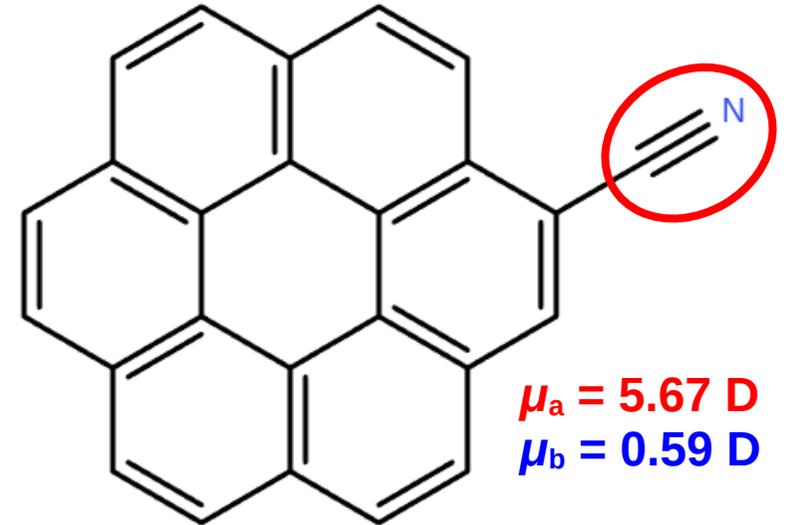
Yebees 40m and GBT 100m

- **Substituted benzene**

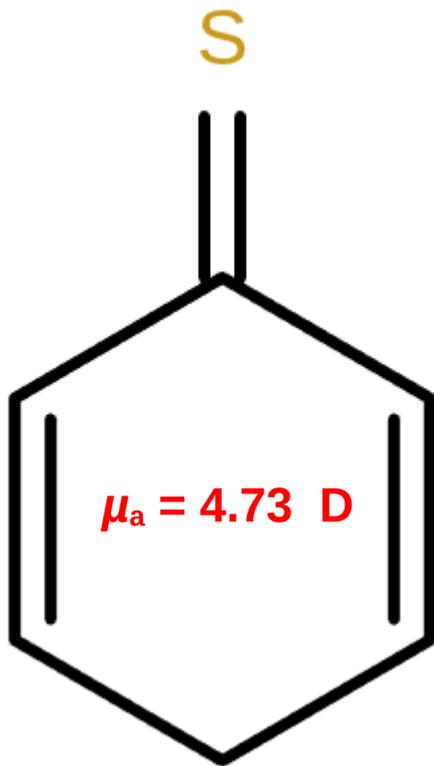
- ethynylbenzene (c-C₆H₅CCH) Loru+ 2023
- indene (C₉H₈) Cernicharo +2021
- phenalene (C₁₃H₁₀) Cabezas +2025

- **Cyano-PAHs**

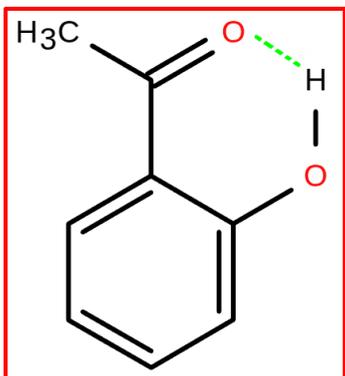
- benzonitrile (c-C₆H₅CN) McGuire+ 2018
- 2-cyanoindene (C₉H₉CN) Madelyn+ 2022
- 1- and 2-cyanonaphthalene (C₁₀H₇CN) McGuire+ 2021
- cyanoacenaphthylenes (C₁₂H₇CN) Cernicharo+ 2021, Cernicharo+ 2026
- cyanopyrenes (C₁₆H₉CN) Wenzel+ 2024, Wenzel+ 2025
- cyanocoronene (C₂₄H₁₁CN) McGuire+ 2025



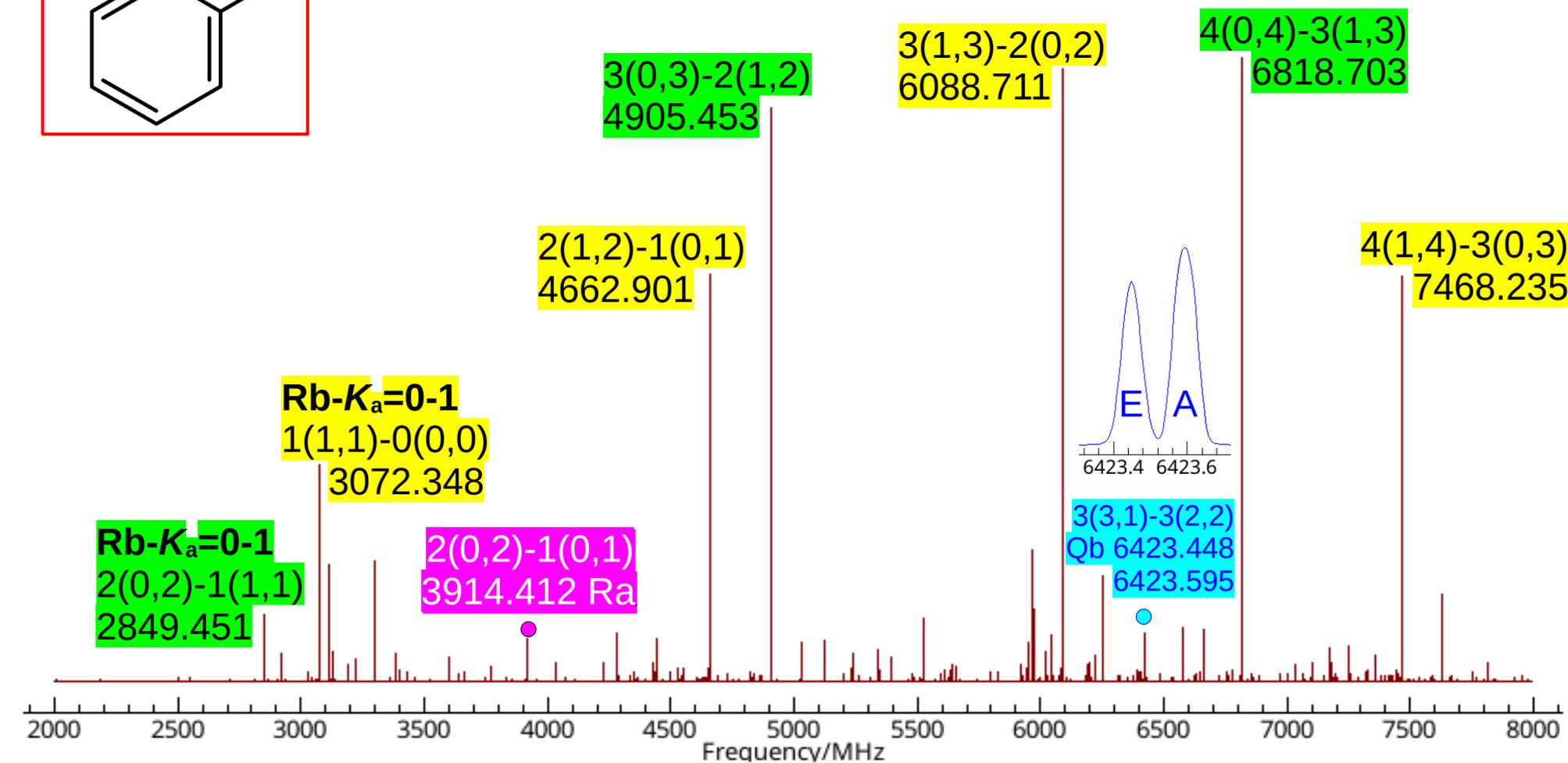
Other ring molecules toward the Galactic Center molecular cloud G+0.693-0.027



- 2,5-cyclohexadien-1-thione
- c-C₆H₆S
- IRAM 30-m and Yebes 40-m
- Araki+ 2026



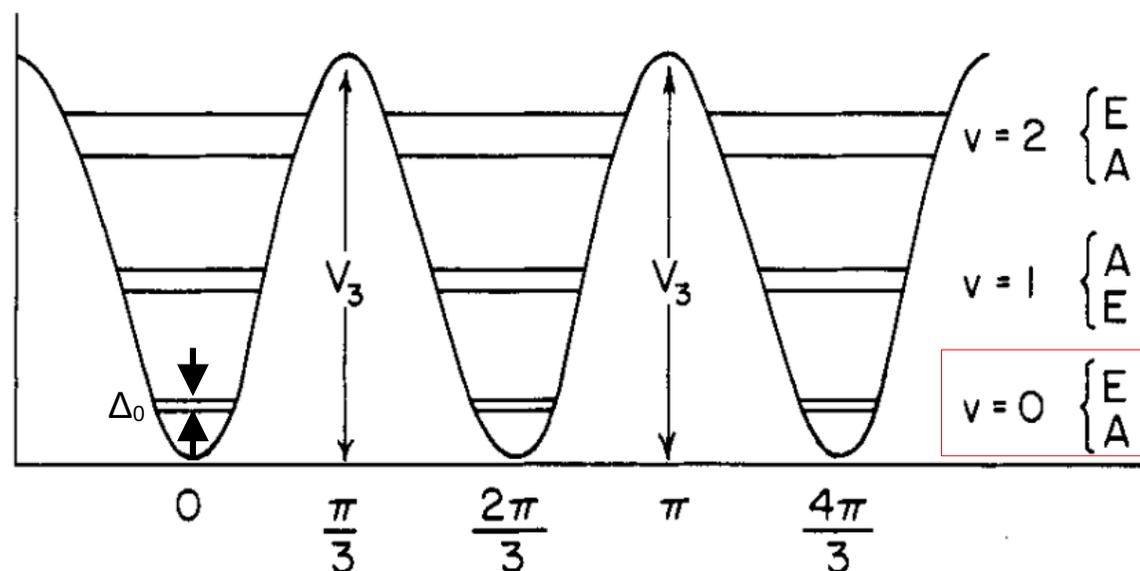
Why not?



CP-FTMW spectrum
 23/09/2024 P_2O_5 $\text{P}_0(\text{Ne})=2$ bar 680 kAv

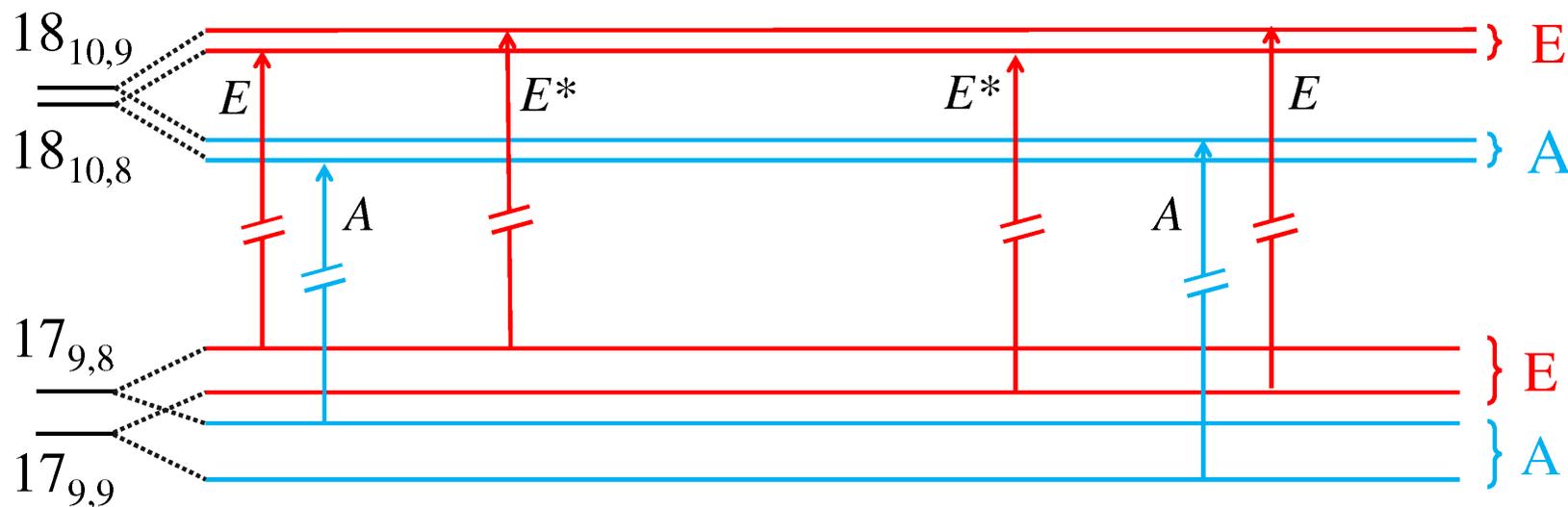
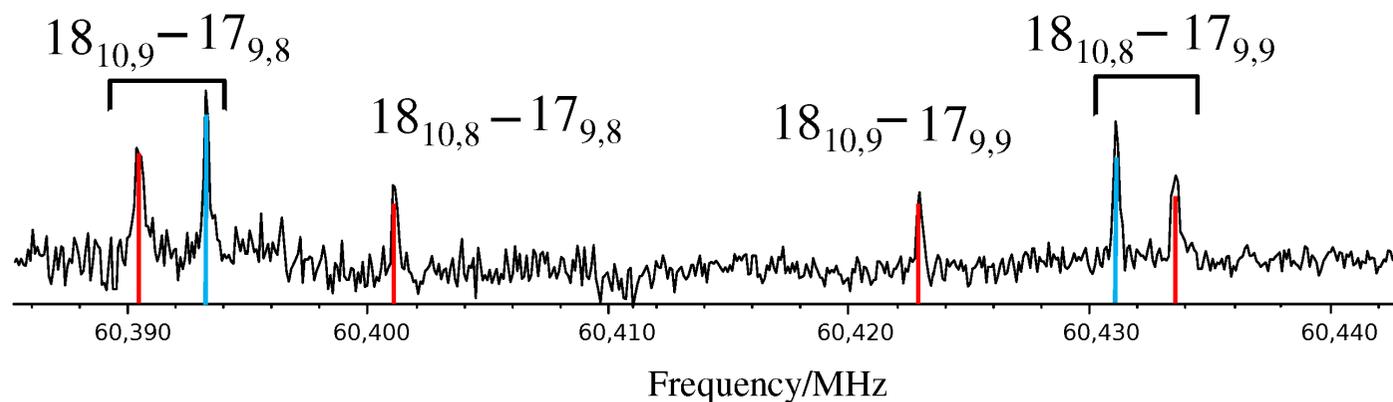
Fit: S-reduction, I' representation

B_J	1.0036926(2)	GHz
B_K	1.2733804(3)	GHz
$B.$	0.2084173(1)	GHz
D_J	24.2(7)	Hz
D_{JK}	24(2)	Hz
D_K	118(2)	Hz
d_1	-7(2)	Hz
d_2	-3.1(8)	Hz
V_3	16946(12)	GHz
F_0	[161.74]	GHz
δ	[31°]	
RMS	20	kHz
N	216	
k	-0.43739	
s	46.135985	
$w^{(1)}$	-0.000094	
F	163.248547	GHz
Δ_0	0.052	GHz

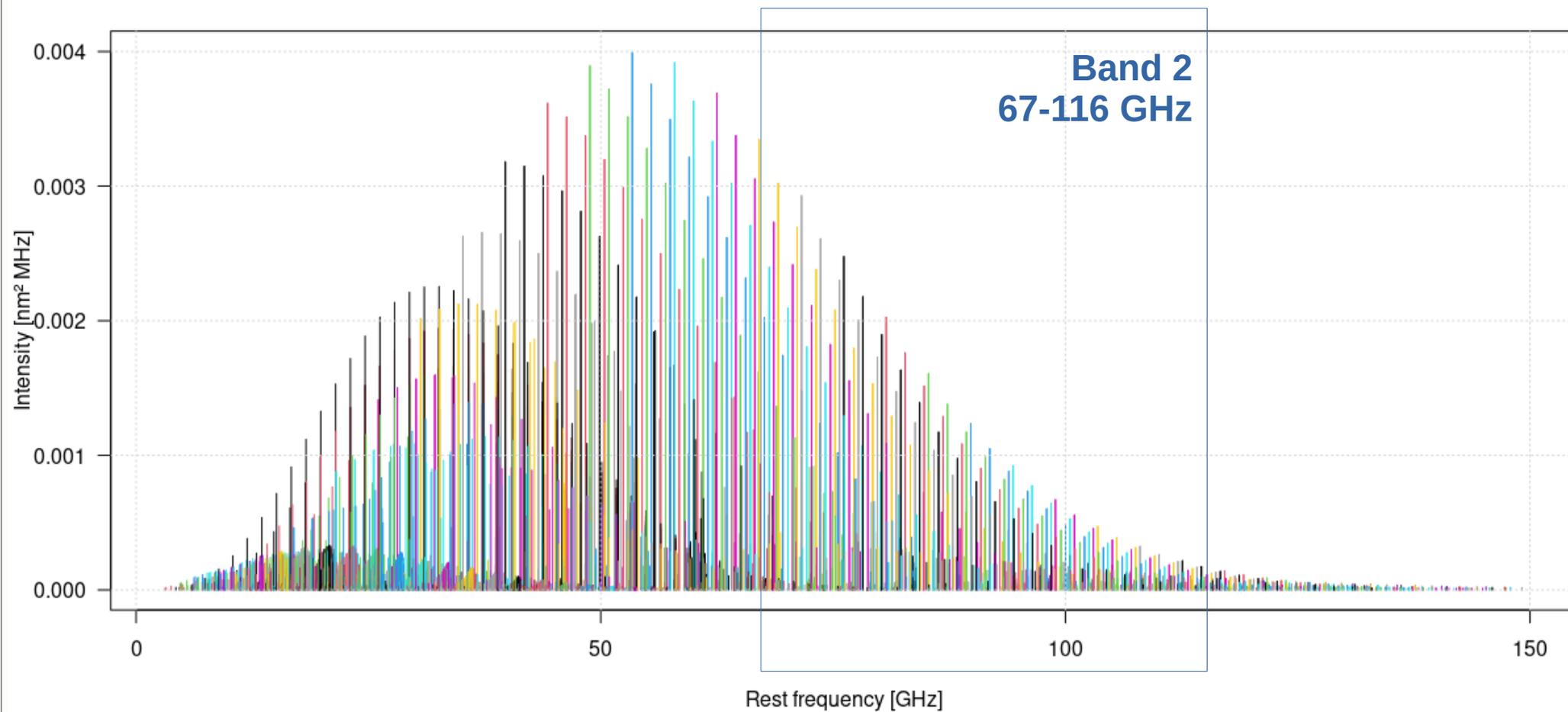


Methyl internal rotation

An issue or a boost?



2'-hydroxyacetophenone / simulated absorption spectrum / b-type / T=10 K



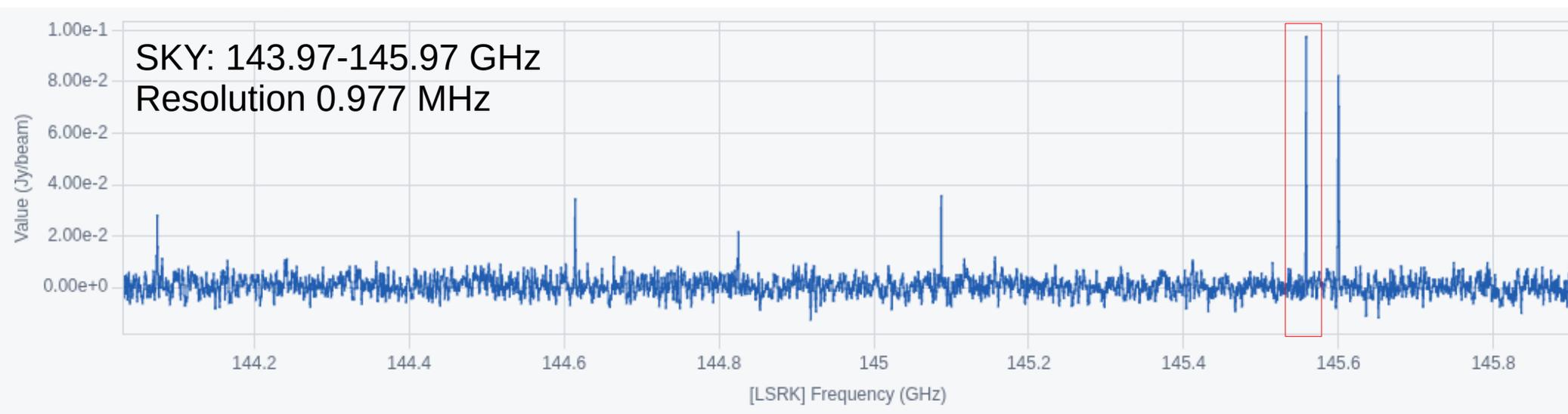
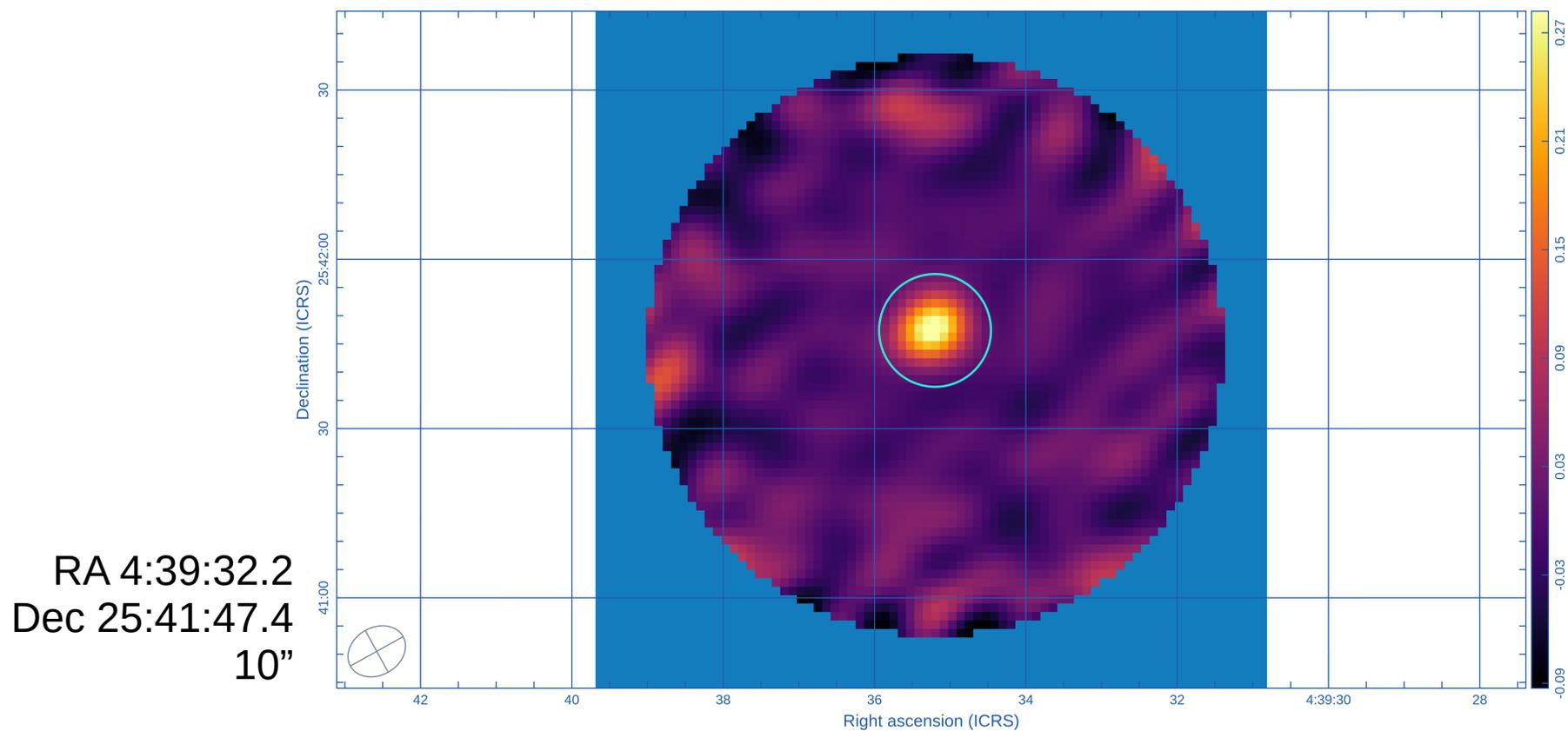
ALMA Archive

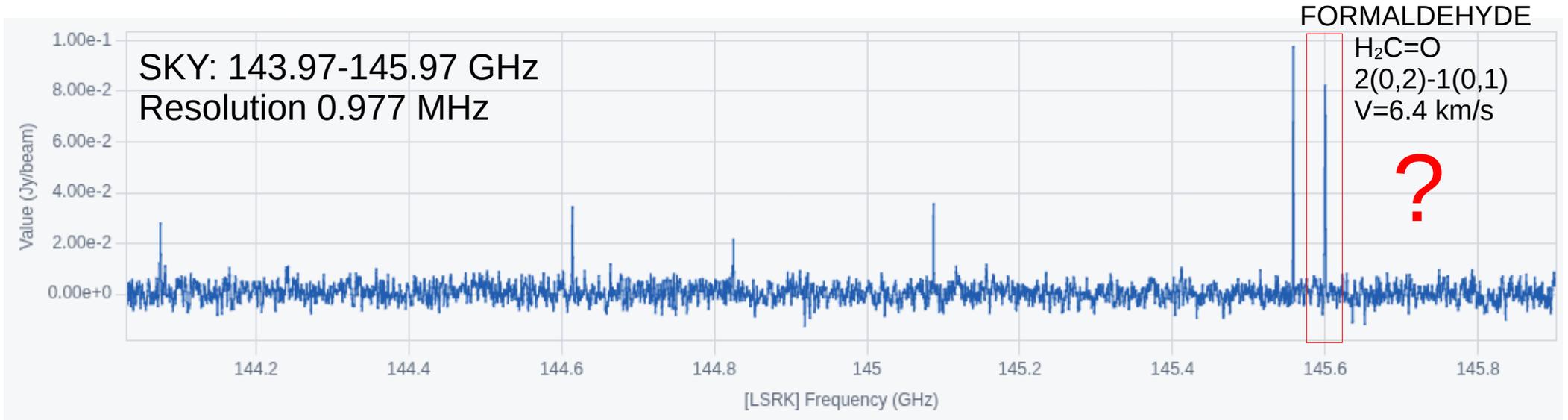
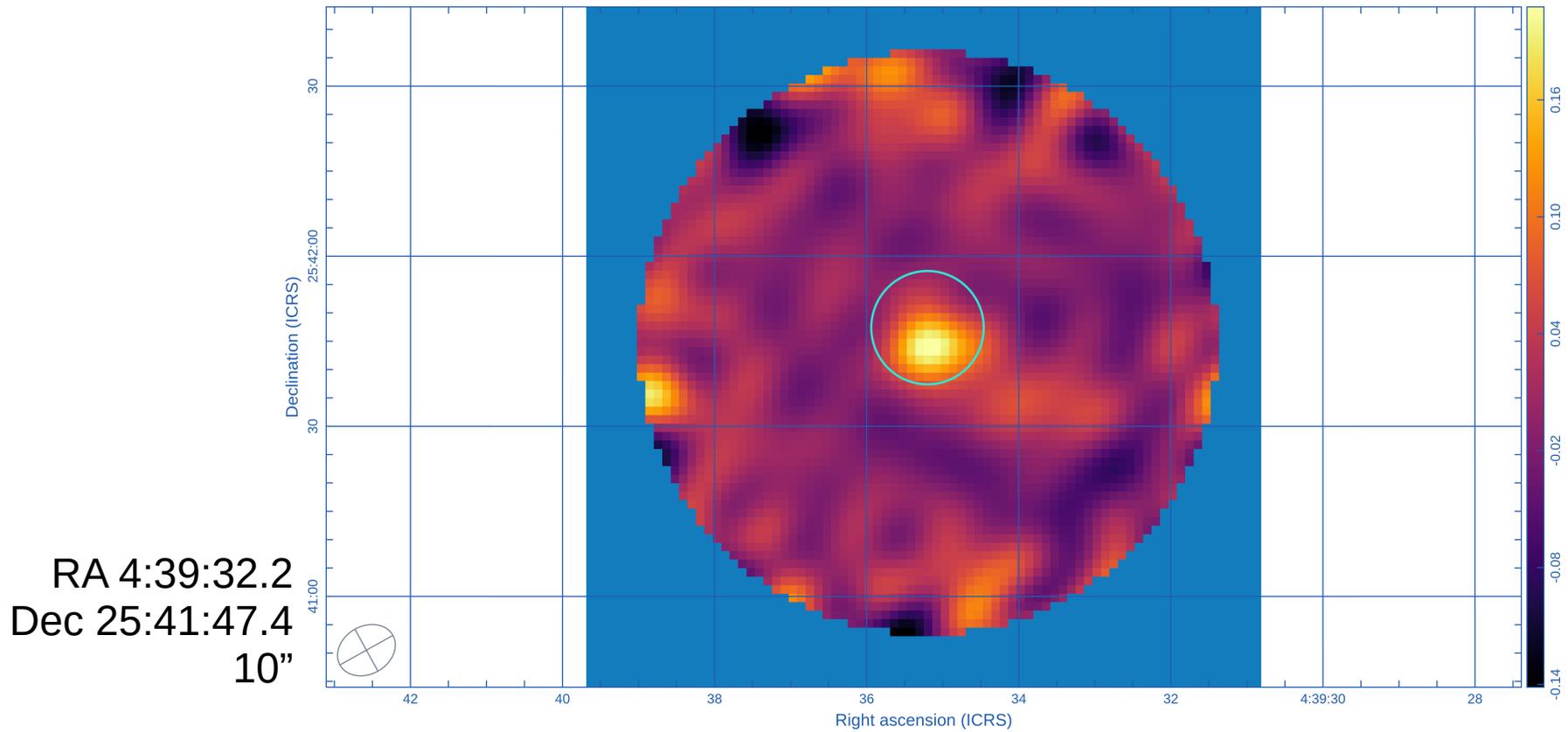
<https://almascience.eso.org/aq/>

ALMA source name: tmc Band: 3|4 x

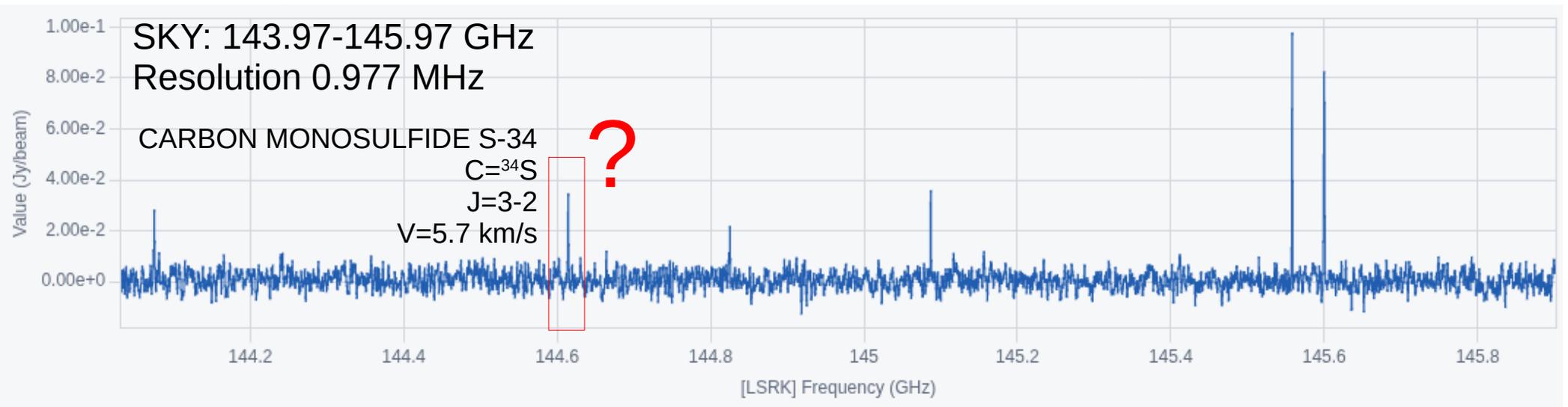
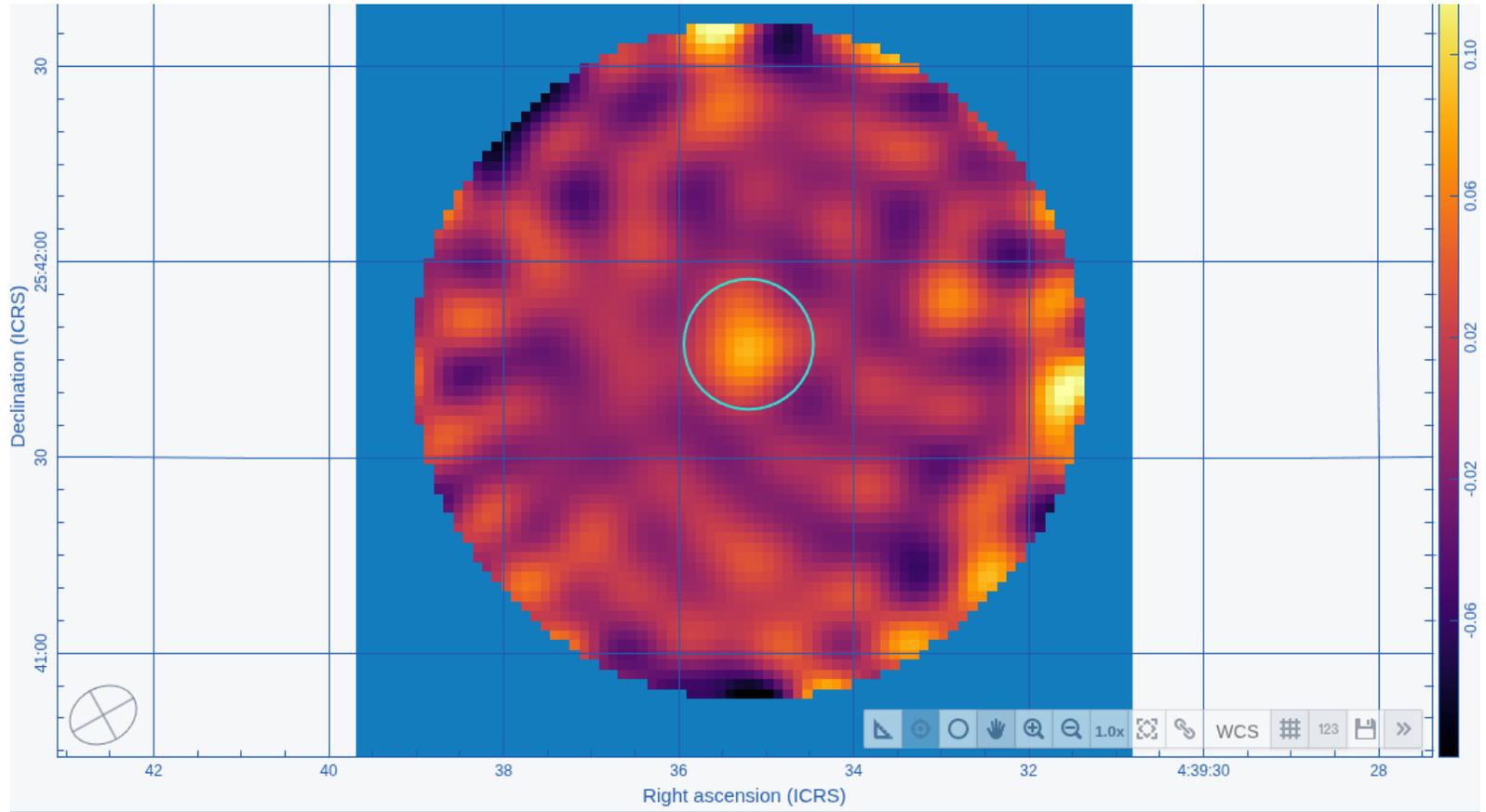
	Project code	ALMA source name	RA	h:m:s -	Dec	d:m:s -	Band	Cont.sens. mJy/beam	Frequency support	Release date
<input type="checkbox"/>  	<input type="text"/>	<input type="text" value="tmc"/>	<input type="text"/>		<input type="text"/>		<input type="text" value="3 4"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="checkbox"/>    	<input type="text" value="2017.1.00765.S"/>	TMC1	04:41:45.900		+25:41:27.000		4	0.3263	<input type="text" value="143.967..158.01 GHz"/>	2019-11-25
<input type="checkbox"/>    	<input type="text" value="2017.1.00765.S"/>	TMC1A	04:39:35.194		+25:41:44.730		4	0.3263	<input type="text" value="143.967..158.01 GHz"/>	2019-11-25
<input type="checkbox"/>    	<input type="text" value="2021.1.01099.S"/>	TMC1	04:41:41.900		+25:41:27.094		3	0.4597	<input type="text" value="93.142..96.769 GHz"/>	2023-03-30
<input type="checkbox"/>    	<input type="text" value="2021.1.01099.S"/>	TMC1	04:41:41.900		+25:41:27.100		3	1.6755	<input type="text" value="93.14..96.771 GHz"/>	2023-12-13
<input type="checkbox"/>    	<input type="text" value="2021.1.01099.S"/>	TMC1_OFF_0	04:42:31.000		+23:32:33.468		3	2.2899	<input type="text" value="93.141..96.771 GHz"/>	2023-12-13
<input type="checkbox"/>    	<input type="text" value="2021.1.01099.S"/>	TMC1	04:41:42.021		+25:41:28.469		3	3.7832	<input type="text" value="93.14..96.771 GHz"/>	2023-12-20
<input type="checkbox"/>    	<input type="text" value="2022.1.00131.S"/>	TMC-1A	04:39:35.000		+25:41:45.000		3	0.0934	<input type="text" value="99.969..115.591 GHz"/>	2024-05-03
<input type="checkbox"/>    	<input type="text" value="2022.1.01357.S"/>	TMC1A	04:39:35.200		+25:41:44.230		3	0.0241	<input type="text" value="89.581..105.413 GHz"/>	2024-08-29
<input type="checkbox"/>    	<input type="text" value="2022.1.00131.S"/>	TMC_1A	04:39:34.806		+25:41:44.199		3	0.8006	<input type="text" value="99.965..115.593 GHz"/>	2025-01-25
<input type="checkbox"/>    	<input type="text" value="2024.1.00117.S"/>	tmc1a	04:39:35.200		+25:41:44.230		3	0.7838	<input type="text" value="99.065..113.722 GHz"/>	2026-01-05

- 2017.1.00765.S TMC-1 Band 4 CARTA WINDOW DOES NOT OPEN
- 2021.1.01099.S TMC-1 Band 3 SMALL RANGE
- 2022.1.00131.S TMC-1A Band 3 SMALL RANGE
- 2022.1.01357.S TMC-1A Band 3 NO IMAGE
- 2024.1.00117.S TMC-1A Band 3 NO CARTA





RA 4:39:32.2
Dec 25:41:47.4
10"



In conclusion, we have not found 2'-hydroxyacetophenone yet, but I am sure we could...

...with your expertise!

Acknowledgments

- Riccardo Stanganini (BSc thesis)
- Filippo Baroncelli (poster on methylurea)
- Martino Napoli (working on automatic fit methods)
- Andrea Maggio & Jinxi Huang (working on sulfur compounds)

Free-jet Rotational Spectra of Urea Analogues: Laboratory Data for Future ALMA Band 2 Searches
 Filippo Baroncelli, Luca Evangelisti, Sonia Melandri, Assimo Maris
 Free Jet Microwave Spectroscopy Group, Department of Chemistry G. Ciamician, University of Bologna

Key results

- Measurements and assignments of the rotational spectrum of N-methylurea under supersonic expansion in the 8–18 GHz and 55.6–79.3 GHz ranges.
- Modelling methyl internal rotation and ¹⁴N nuclear quadrupole coupling splittings.
- Providing a Band 2-ready spectral prediction for searches in astronomical surveys.

Urea and derivatives in space

The detection of urea in the ISM ($2.7 \times 10^{10} \text{ cm}^{-1}$ toward Sgr 82(N), $6.3 \times 10^{11} \text{ cm}^{-1}$ toward G+0.093-0.027) raises the question of whether larger urea analogues could also be present.

Free-jet absorption millimeter wave rotational spectrometer

- Use of Free-jet Expansion: $T_{\text{rot}} = 200\text{--}400 \text{ K}$, $T_{\text{trans}} = 10 \text{ K}$, $P = 100\text{--}200 \text{ Torr}$, $Q = 20\text{--}30 \text{ Torr}$. Coating of vibrational and rotational levels enabling high-resolution rotational spectroscopy of complex organic molecules (COMs).
- Overlap with ALMA Band 2 Frequency Region: Free jet Frequency Range 55.6–79.3 GHz, Resolution 300 MHz, Error: 50 kHz. Precise experimental reference data.

N-Methylurea: a complex rotational pattern

Methyl Internal Rotation Tumbling Line Structure, Nuclear Quadrupole Coupling Hyperfine Structure, Determination of Nitrogen NDC Constants from Line Spectral Moments Analysis, Determination of Methyl Internal Rotation Parameters.

Parameter	A-State	E-State
A / MHz	10569.801(2)	10451.270(4)
B / MHz	4078.3718(7)	4072.259(8)
C / MHz	2005.1602(7)	2003.269(8)
N lines	273	350
Q / MHz		22
N ₁ / MHz	28	N
N ₂ / MHz	Y	Y
N ₃ / MHz	Y	Y
N ₄ / MHz	122.4160(2)	122.013(8)
M ₁ / kHz	45.91793(2)	46.275(5)
M ₂ / kHz	1.48119(2)	2.000(3)

Predicted absorption spectrum for N-methylurea (T=10 K)

Predicted rotational transitions highlighting in bold the top high-intensity lines with low frequency uncertainty as candidate target for astronomical surveys.

We thank and acknowledge:
 Daniel Kallen for recording the FJ-AMMW spectrum
 Dr. Charlette N. Cummings, and Dr. Nick Walker of Newcastle University for recording the CP-FTMW experimental spectra

... and thank you for your attention