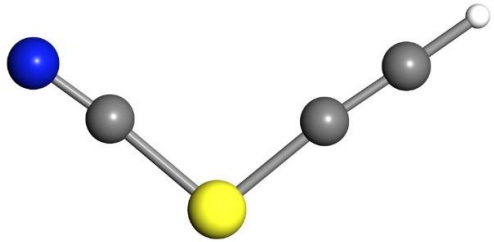
Universidad de Valladolid

76th International Symposium on Molecular Spectroscopy

SYNTHESIS AND SPECTROSCOPIC CHARACTERIZATION OF INTERSTELLAR CANDIDATE ALKYNYL THIOCYANATE: HCCSCN.

Elena R. Alonso*[a], Aran Insausti[b], Lucie Kolesniková[c], Iker León[a] and Jean Claude Guillemin[d]



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June 2023

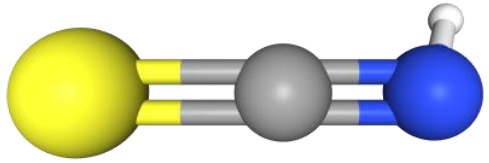
BACKGROUND

JOURNAL OF MOLECULAR SPECTROSCOPY **10,** 418–441 (1963)

The Millimeter Wave Spectra of Isocyanic and Isothiocyanic Acids*

ROGER KEWLEY, K. V. L. N. SASTRY, AND MANFRED WINNEWISSER

Department of Physics, Duke University, Durham, North Carolina



isothiocyanic acid

THE ASTROPHYSICAL JOURNAL, 706:1588–1593, 2009 December 1 doi:10.1088/0004-637X/706/2/1588

LABORATORY DETECTION OF THIOCYANIC ACID HSCN

S. BRÜNKEN[1,2,3], Z. YU[1,2,4], C. A. GOTTLIEB[1,2], M. C. MCCARTHY[1,2], AND P. THADDEUS[1,2]
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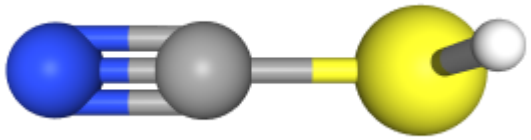
Received 2009 May 18; accepted 2009 October 8; published 2009 November 16



thiocyanic acid

THE ASTROPHYSICAL JOURNAL, 234:L143–L145, 1979 December 1

INTERSTELLAR ISOTHIOCYANIC ACI

M. A. FRERKING AND R. A. LINKE
Bell Telephone Laboratories, Crawford Hill Laboratory, Holmdel, New J
AND
P. THADDEUS
Goddard Institute for Space Studies, New York City
Received 1979 June 14; accepted 1979 July 18

ABSTRACT

Isothiocyanic acid (HNCS) has been identified in Sgr B2 from millimeter-wave spectral line observations. We have definitely detected three rotational lines, and have probably detected two others. The rotational temperature of HNCS in Sgr B2 is 14 ± 5 K, its column density is 2.5 ± 1.0 × 10^{13} cm^{-2}, and its abundance relative to HNCO is consistent with the cosmic S/O ratio, 1/42.
Subject headings: interstellar: molecules

THE ASTROPHYSICAL JOURNAL, 702:L124–L127, 2009 September 10 doi:10.1088/0004-637X/702/2/L124

DETECTION OF A NEW INTERSTELLAR MOLECULE: THIOCYANIC ACID HSCN

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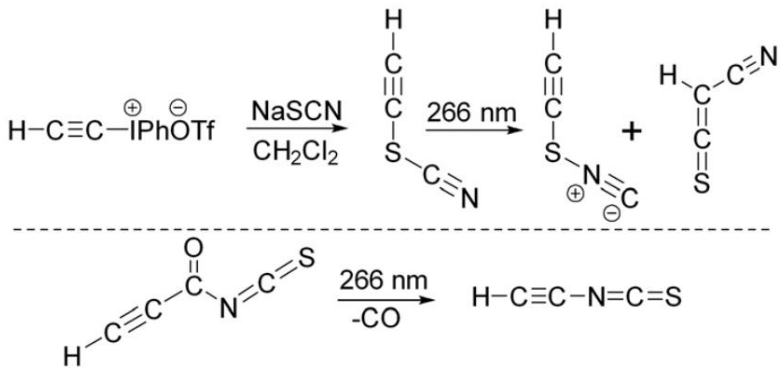
The simplest alkynyl thiocyanate HCCSCN and its isomers†‡

Bo Lu,[a] Zhuang Wu,[a] Lina Wang,[a] Bifeng Zhu,[a] Guntram Rauhut[b] and Xiaoqing Zeng*[a]

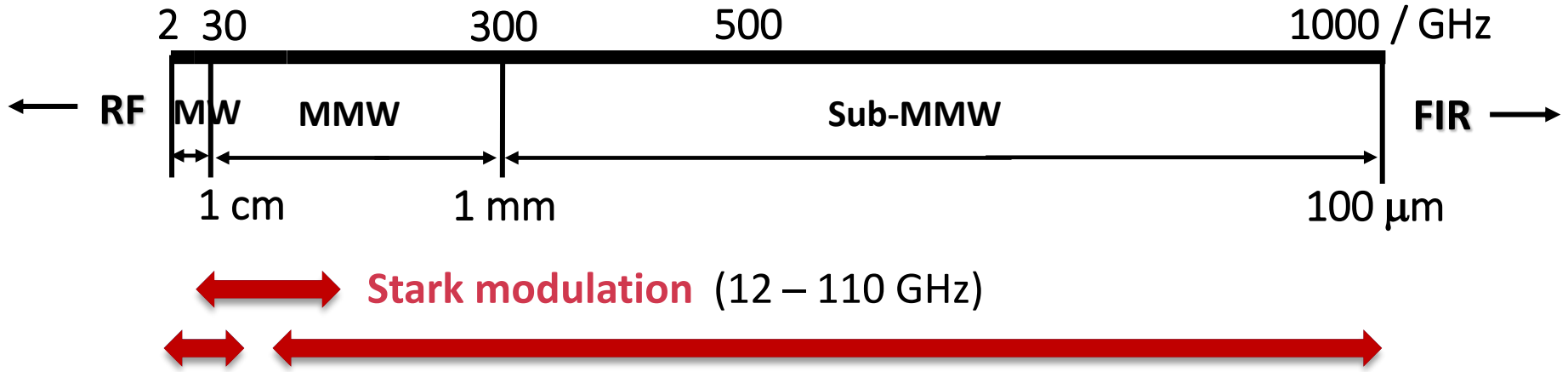


Scheme 1 Generation of HCCSCN and its isomers.

GOOD CANDIDATE TO BE STUDY BY ROTATIONAL SPECTROSCOPY TO ENABLE ITS SEARCH IN THE ISM.

EXPERIMENTAL METHODOLOGY FOR ASTROCHEMISTRY

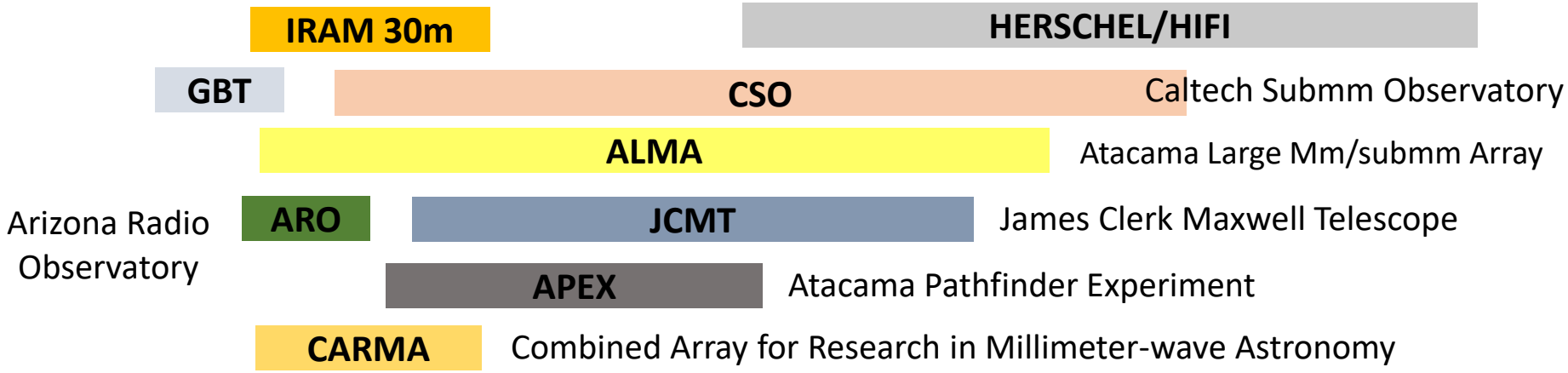
EXPERIMENTAL METHODOLOGY AT THE SERVICE OF ASTROCHEMISTRY



Stark modulation (12 – 110 GHz)

FTMW techniques
(2 – 40 GHz)

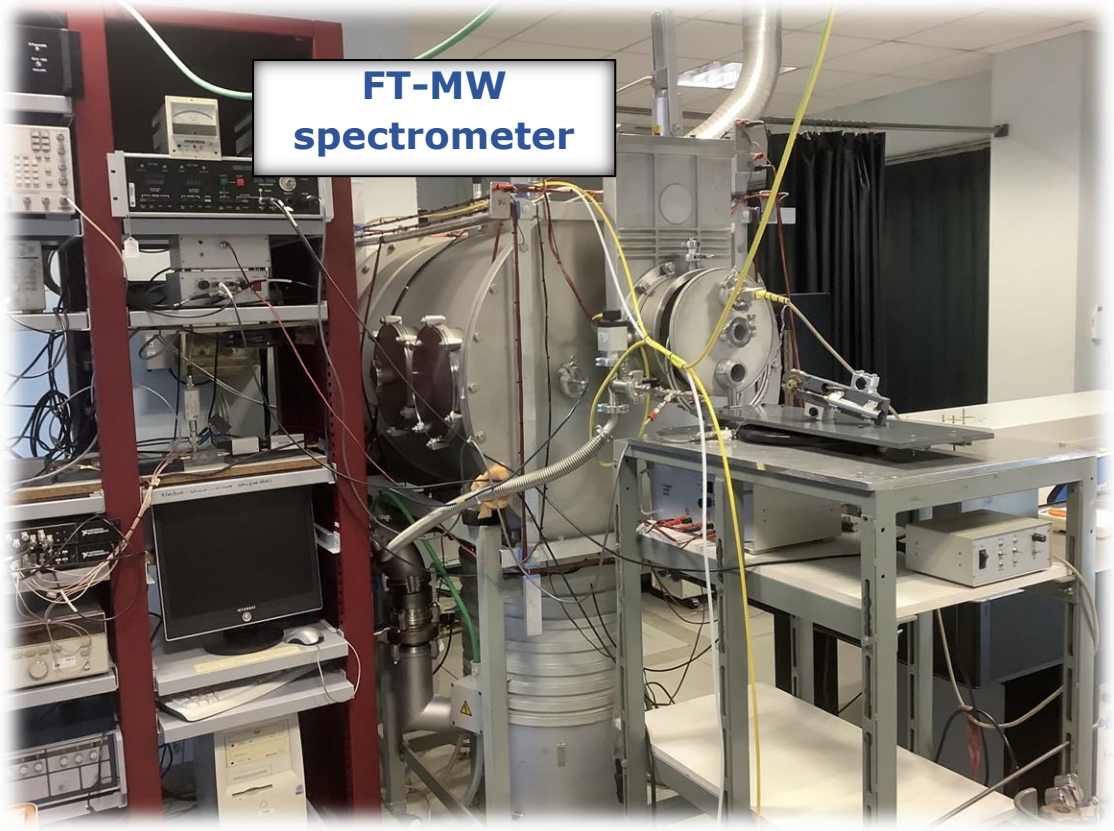
Frequency modulation mmw and sub-mmw spectroscopy (50 – 1000 GHz)

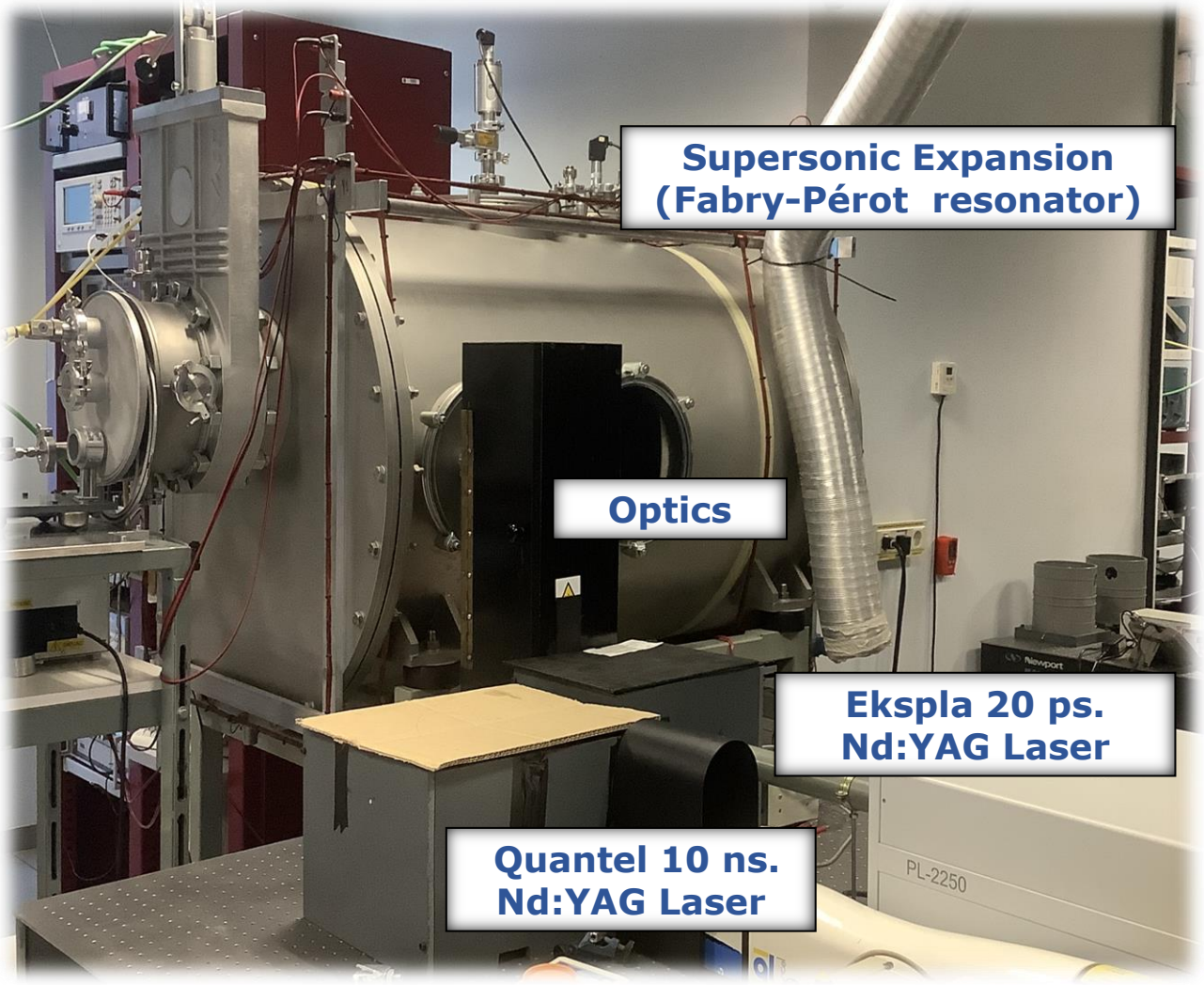


EXPERIMENTAL METHODOLOGY FOR ASTROCHEMISTRY

Time domain techniques (2 – 40 GHz)

LA-MB-FTMW Spectrometer (2 – 14 GHz)

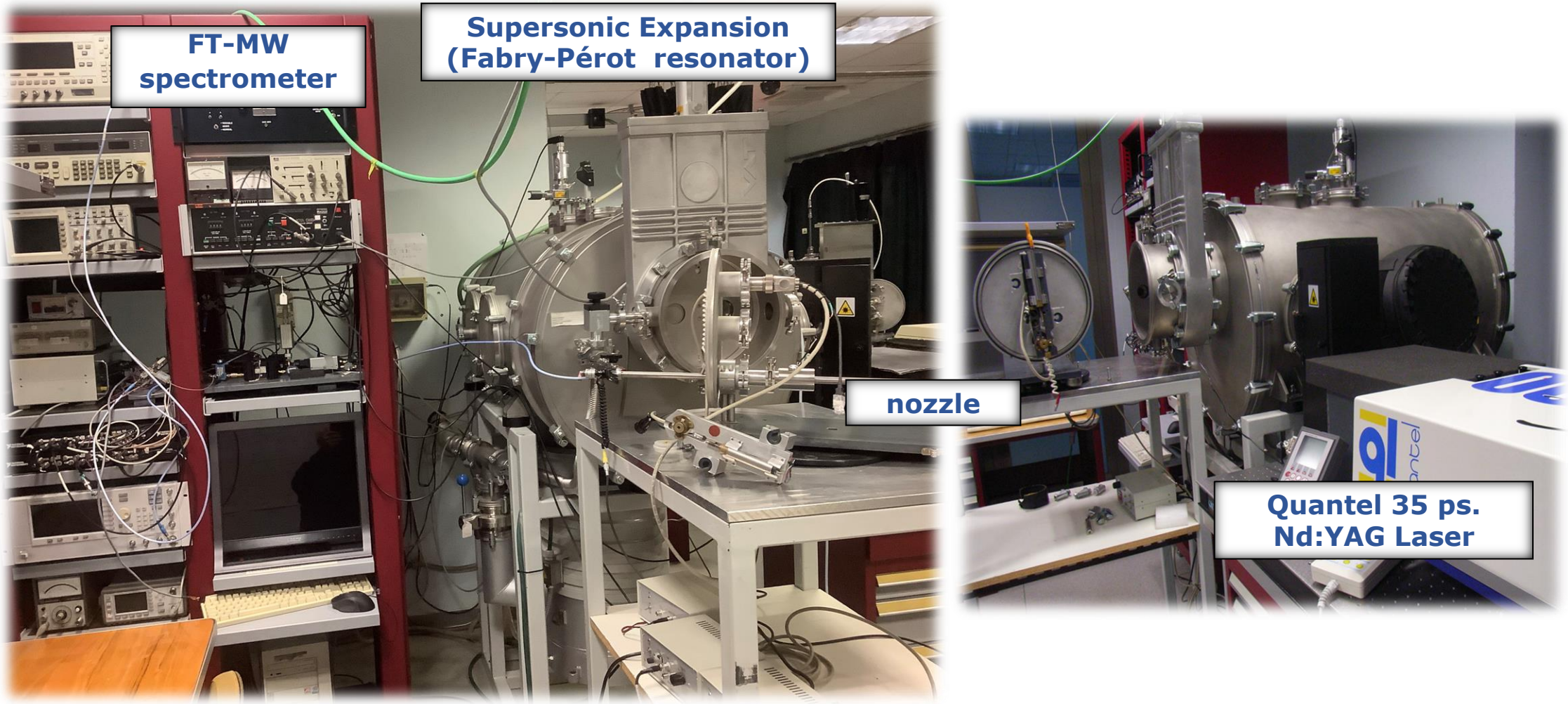




EXPERIMENTAL METHODOLOGY FOR ASTROCHEMISTRY

Time domain techniques (2 – 40 GHz)

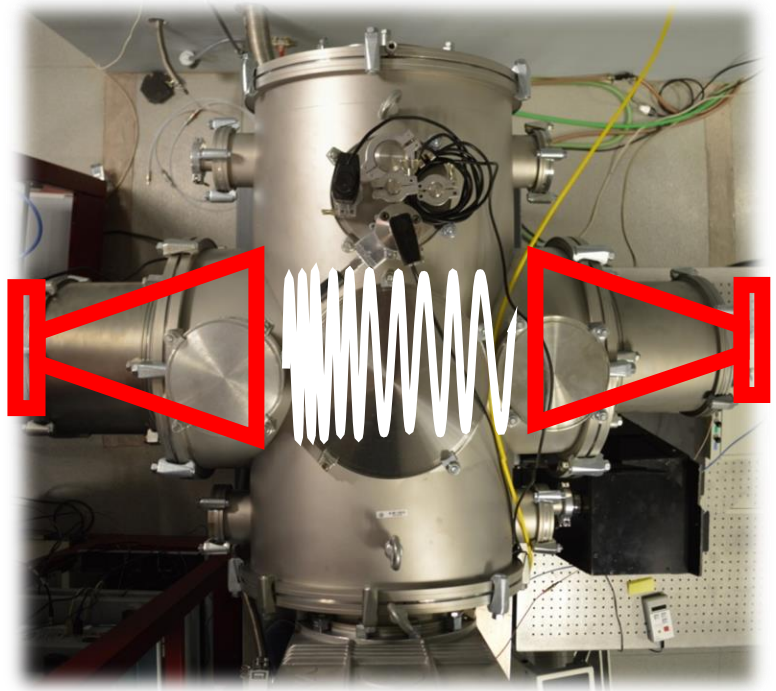
LA-MB-FTMW Spectrometer (6 – 26 GHz)

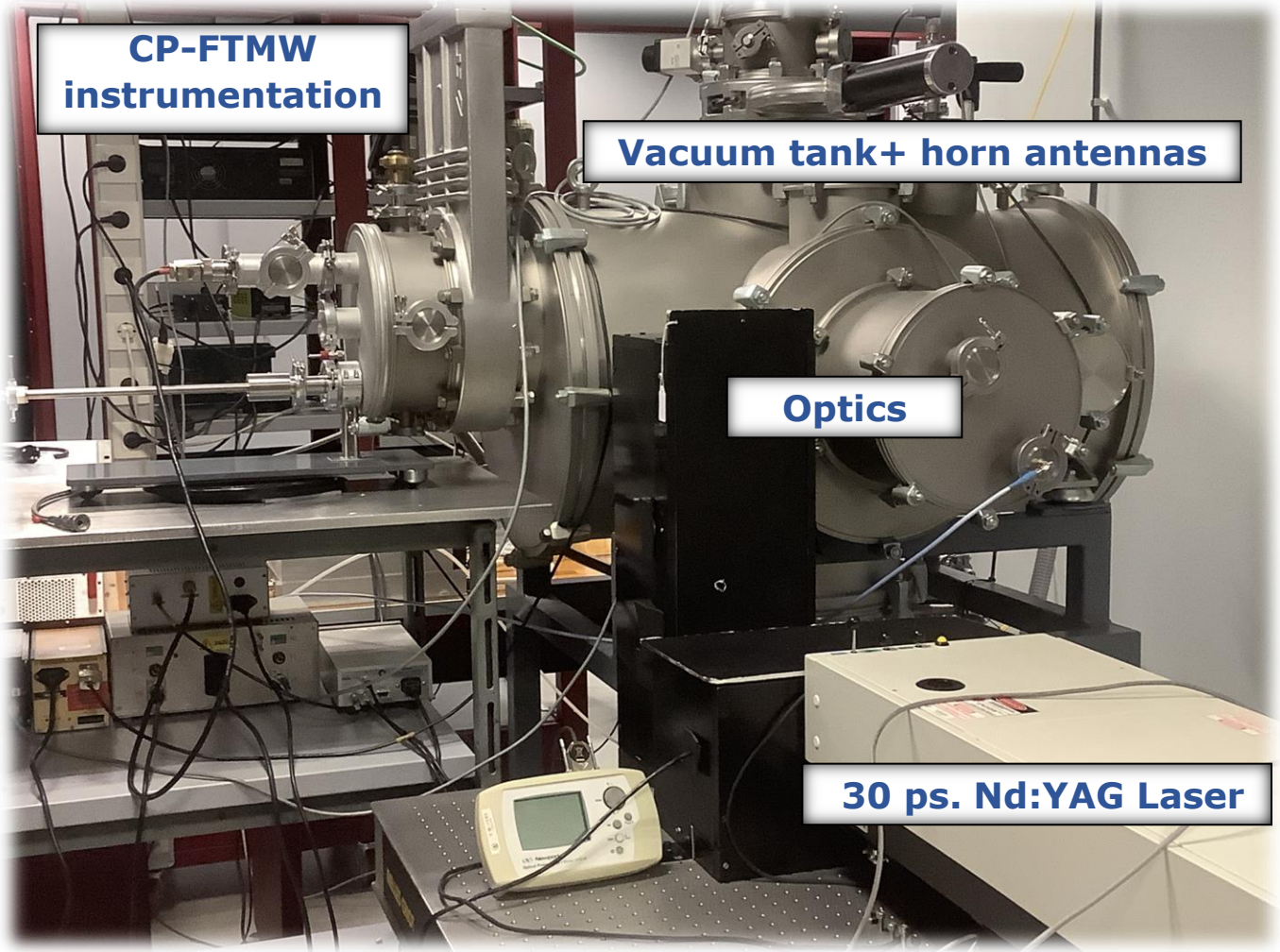


EXPERIMENTAL METHODOLOGY FOR ASTROCHEMISTRY

Time domain techniques (2 – 40 GHz)

LA-CP-FTMW Spectrometer (2 – 8 GHz)

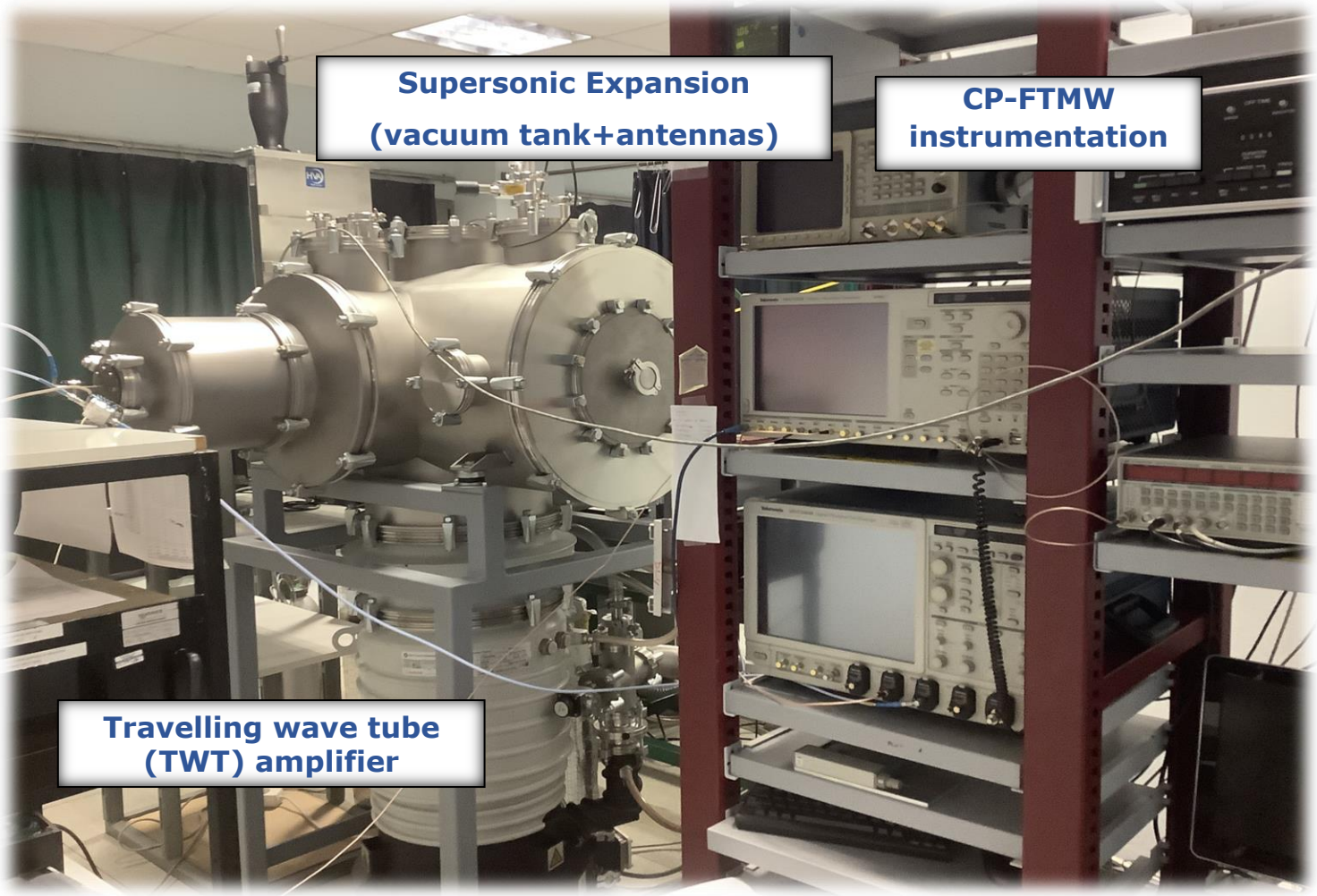


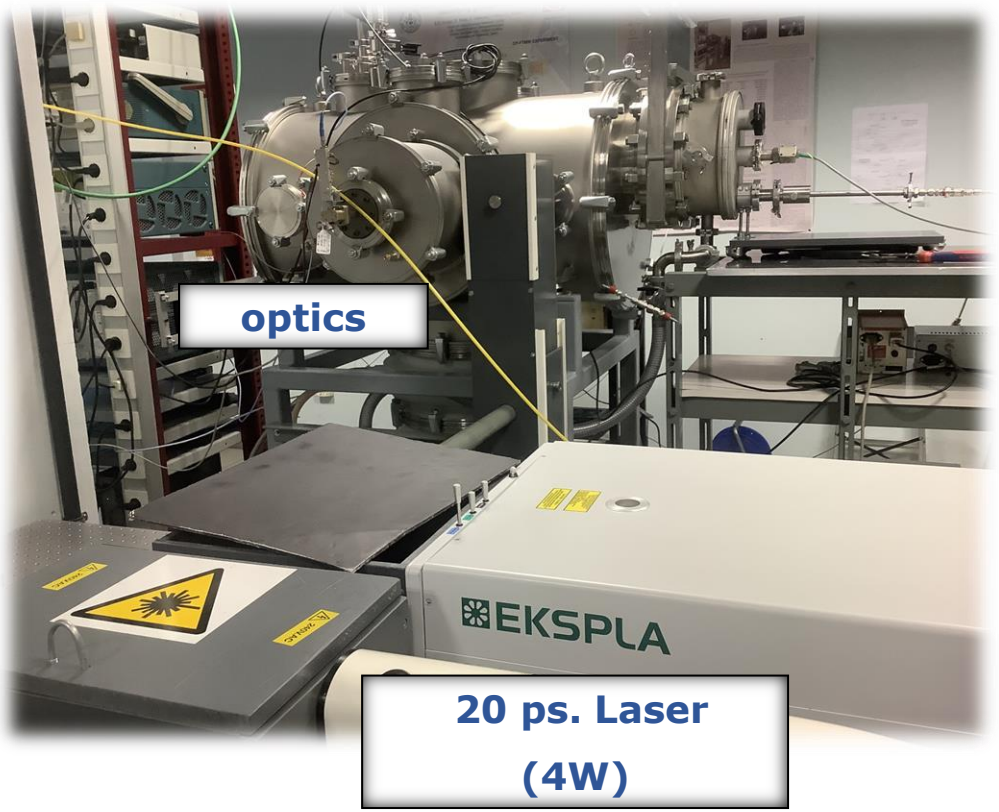


EXPERIMENTAL METHODOLOGY FOR ASTROCHEMISTRY

Time domain techniques (2 – 40 GHz)

LA-CP-FTMW Spectrometer (6.5 – 18 GHz)





EXPERIMENTAL METHODOLOGY FOR ASTROCHEMISTRY

Time domain techniques (2 – 40 GHz)

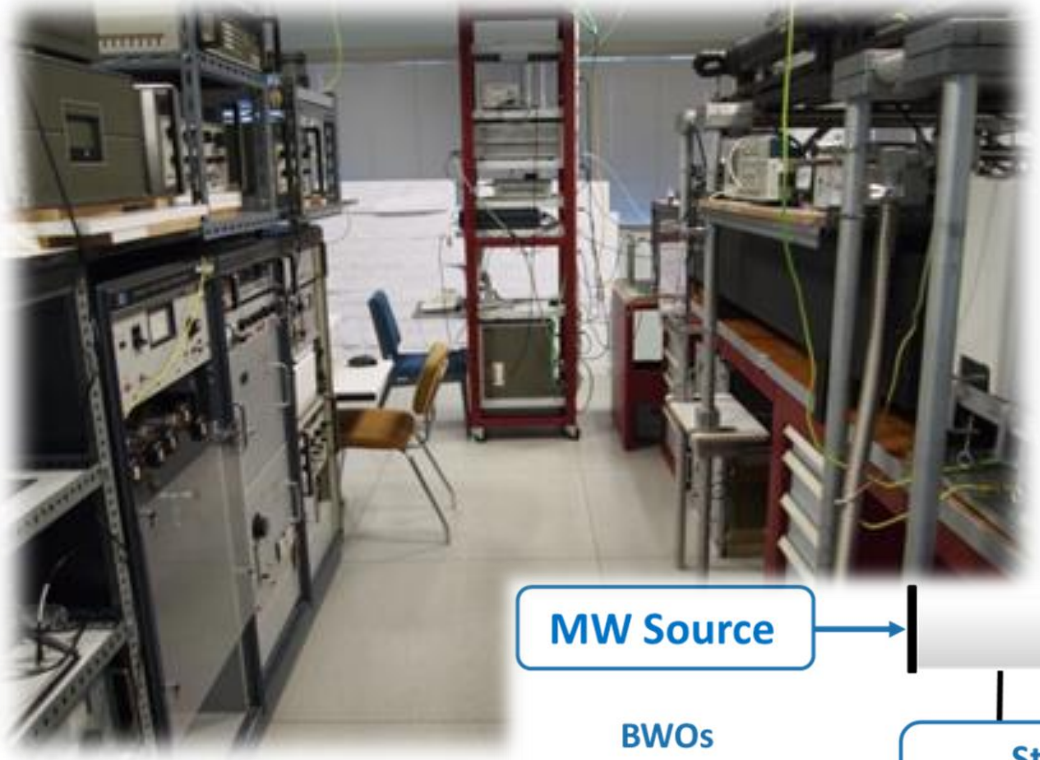
Multinozzle CP-FTMW Spectrometer (2 – 18 GHz)

EXPERIMENTAL METHODOLOGY FOR ASTROCHEMISTRY

Frequency domain techniques (12 – 1000 GHz)

Room temperature

Stark Spectrometer (12.5 – 110 GHz)



MW Source → **Stark Cell** → **Detector**

BWOs
12.5 – 40 GHz
+ V-2X (Spacek Labs)

Stark Modulation
(10 – 3000 V at 33.333 kHz)

12.5 – 110 GHz

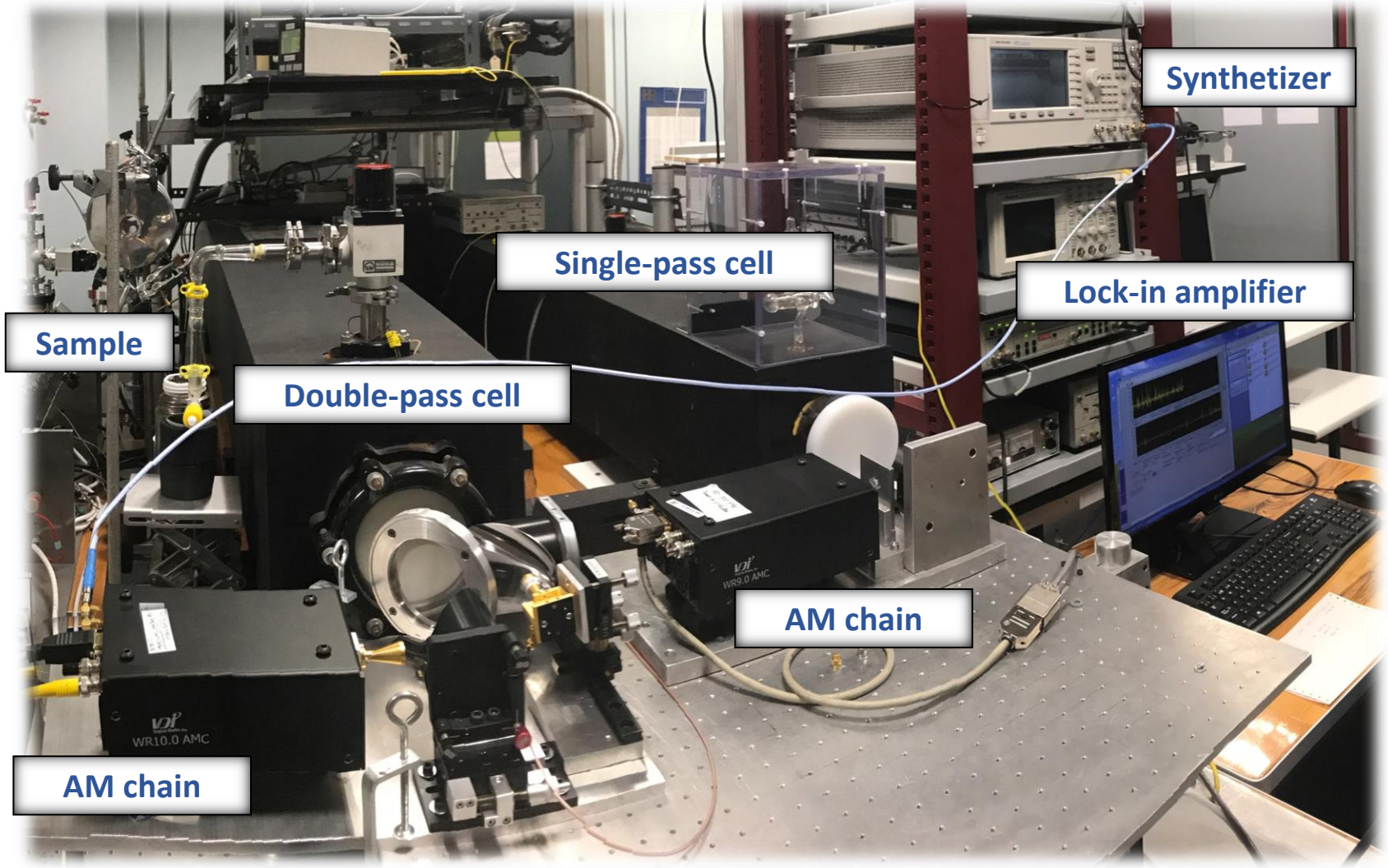
Agilent Synthesizer
250 kHz – 20 GHz + WR15 (4x), WR10 (6x) AMC (VDI, Inc.)
or Ka-2X, Q-3X, V-4X (Spacek Labs)

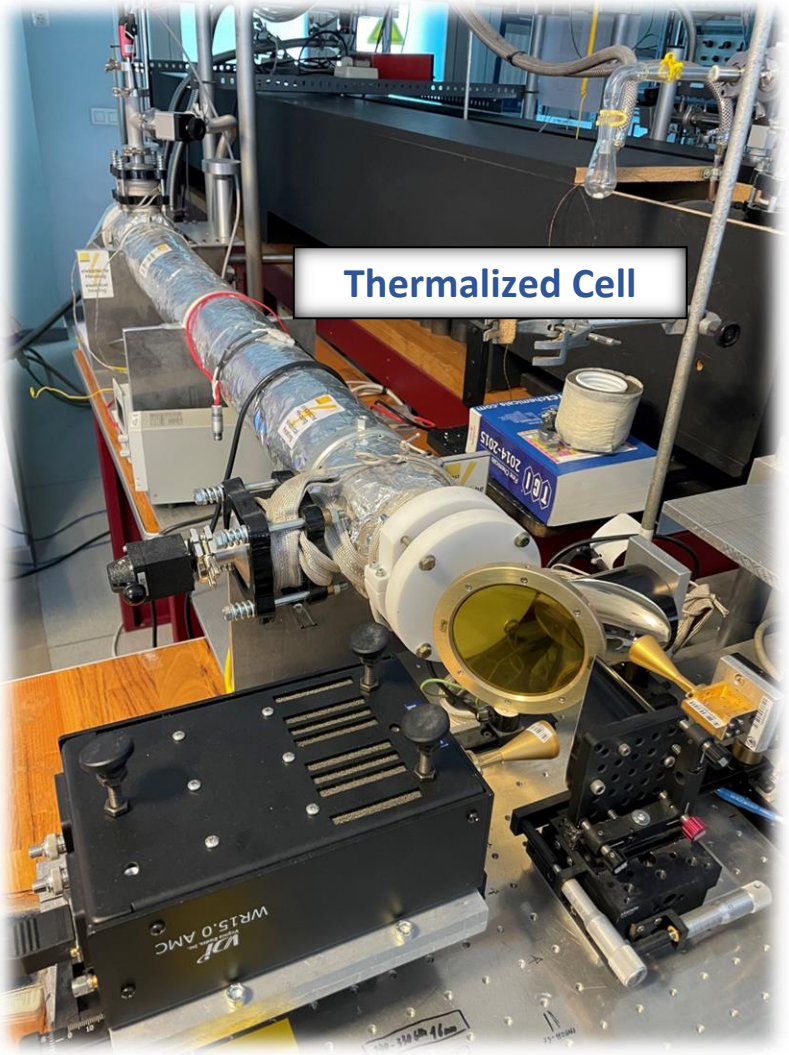
EXPERIMENTAL METHODOLOGY FOR ASTROCHEMISTRY

Room temperature

Frequency domain techniques (12 – 1000 GHz)

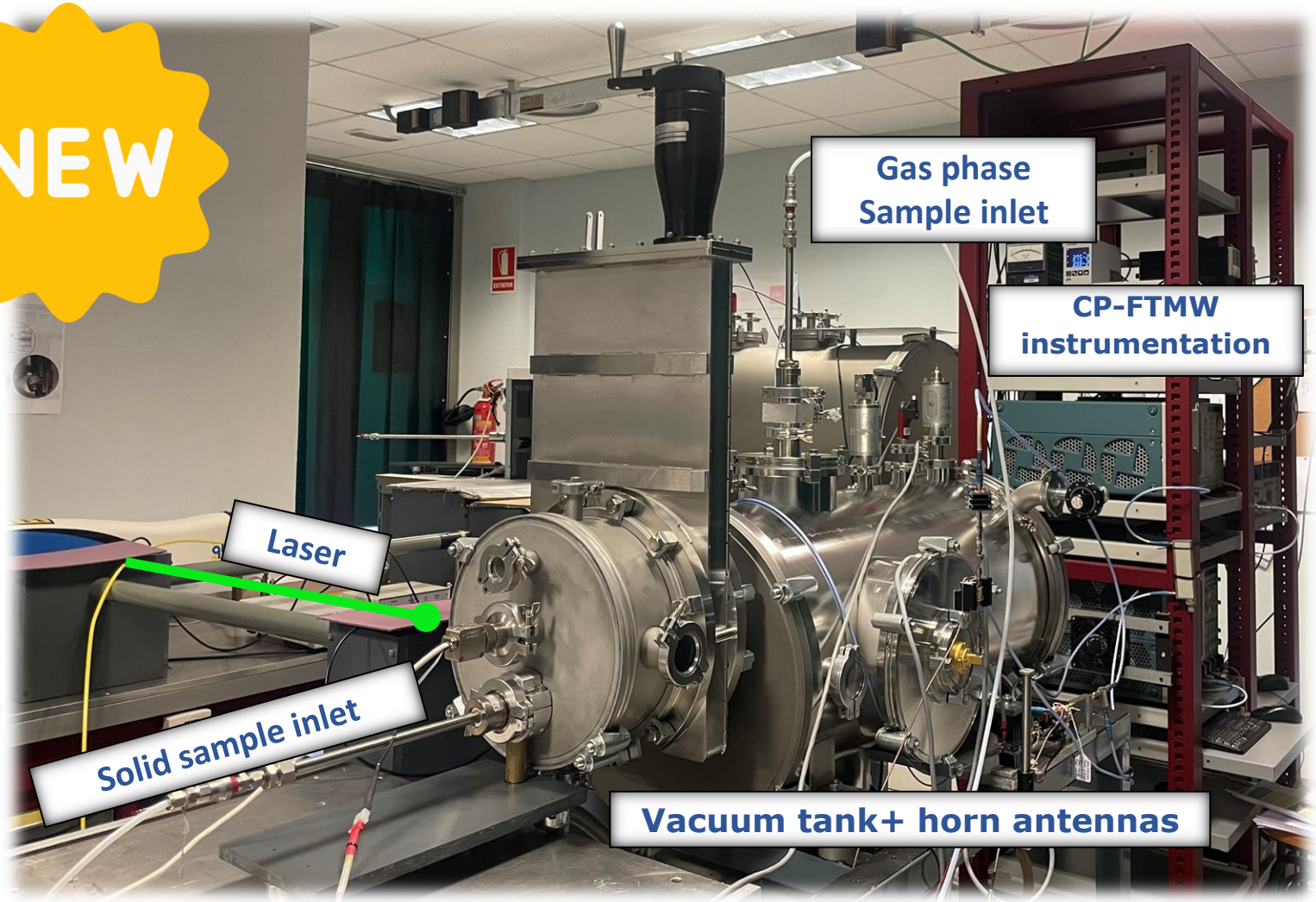
Millimeter and sub-millimeterwave Spectrometer (50 – 1000 GHz)





EXPERIMENTAL METHODOLOGY FOR ASTROCHEMISTRY

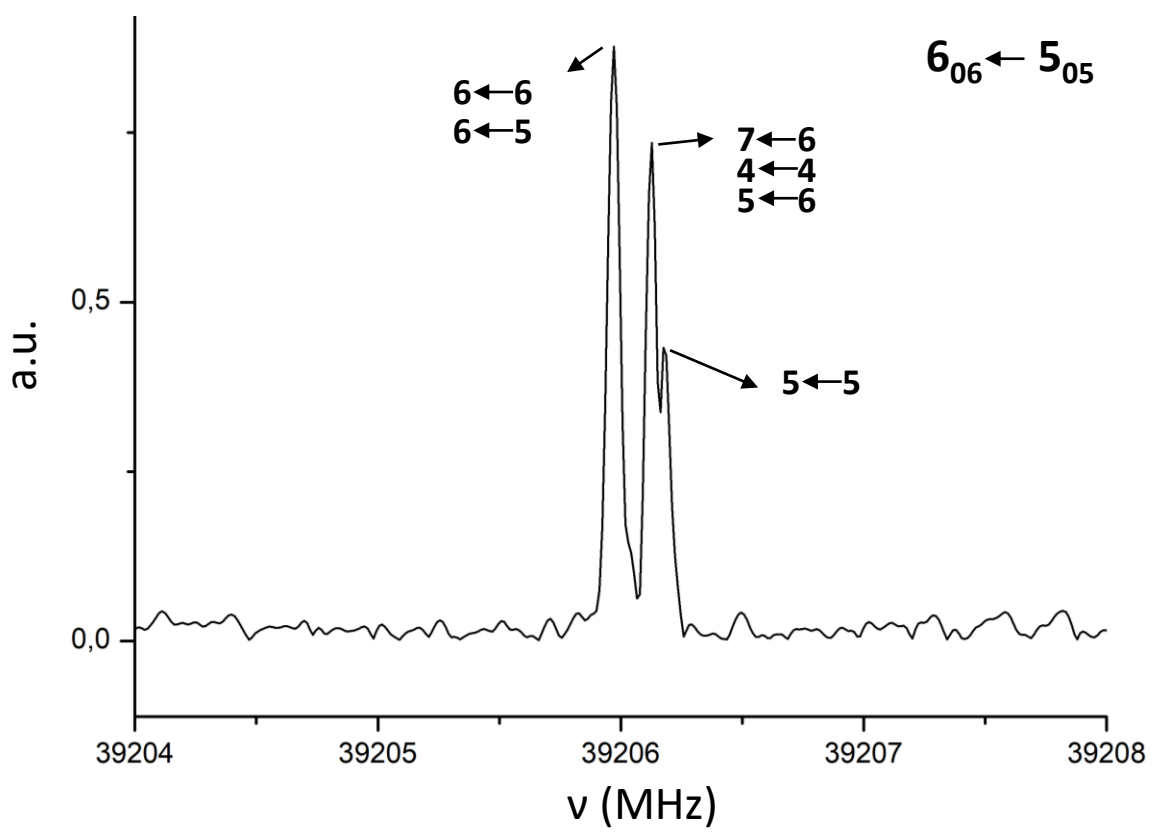
Laser Ablation Millimeter-wave CP-FTMW Spectrometer (33 – 125 GHz)

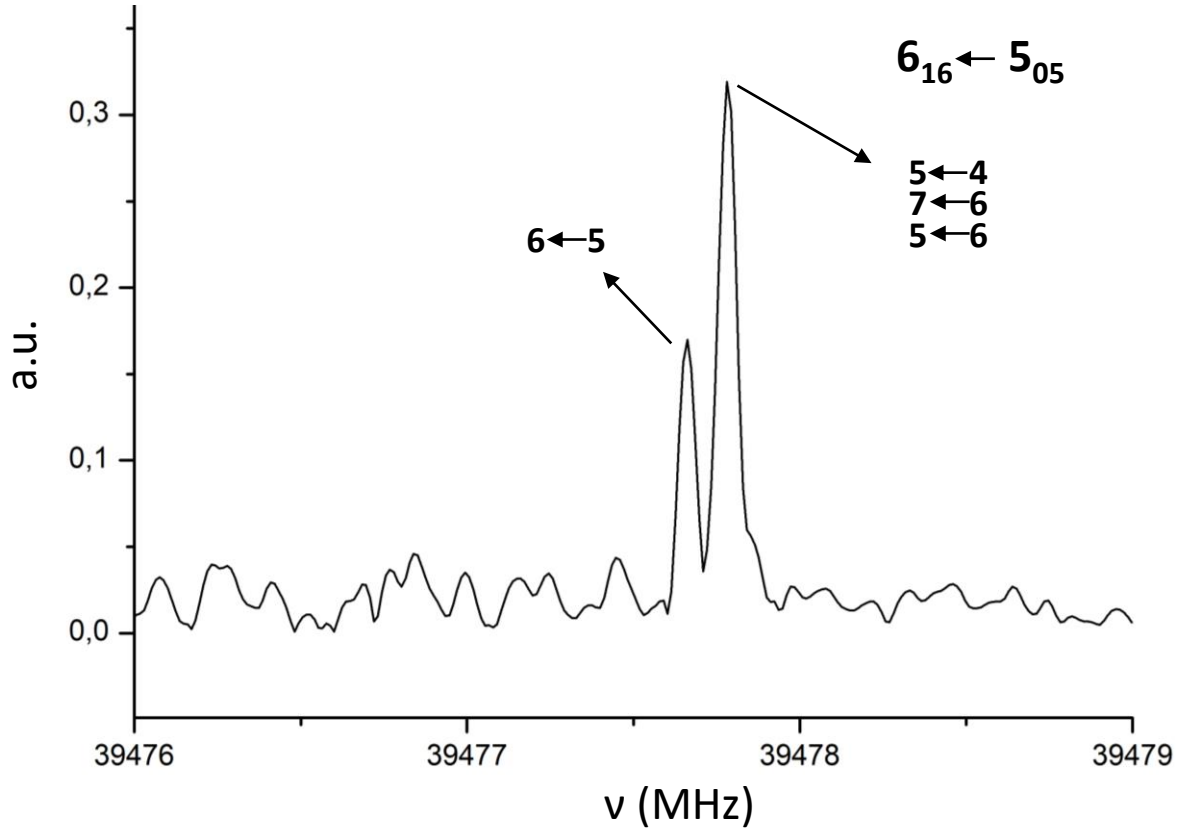


EXPERIMENTAL METHODOLOGY FOR ASTROCHEMISTRY

Laser Ablation Millimeter-wave CP-FTMW Spectrometer (33 – 125 GHz)

10000 acqs





EXPERIMENTAL METHODOLOGY FOR ASTROCHEMISTRY

Laser Ablation Millimeter-wave CP-FTMW Spectrometer (33 – 125 GHz)

NEW

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An Innovative Approach for the Generation of Species of the Interstellar Medium

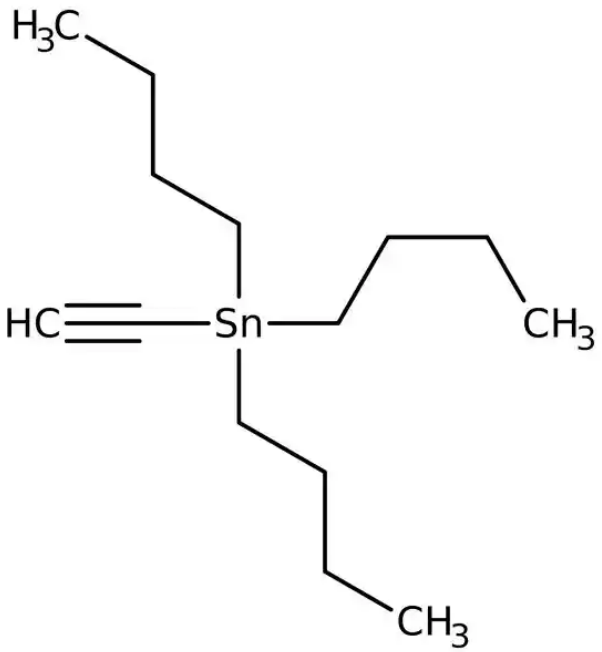
Dr. Lucie Kolesniková, Dr. Iker León, Dr. Elena R. Alonso, Santiago Mata, Prof. Jose Luis Alonso

First published: 08 September 2021 | https://doi.org/10.1002/anie.202110325 | Citations: 7

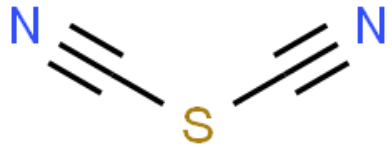
EXPERIMENTAL APPROACH FOR HCCSCN

Prof. Jean-Claude Guillemin

CHEMICAL SYNTHESIS

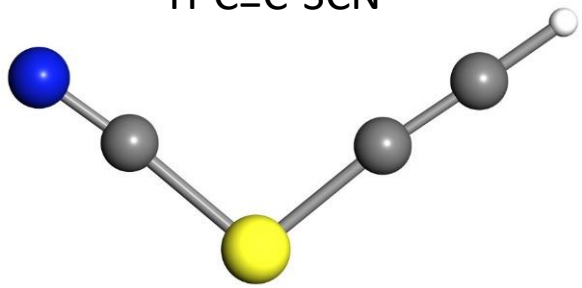


tributylethynylstannane



sulfur cyanide

H-C≡C-SCN



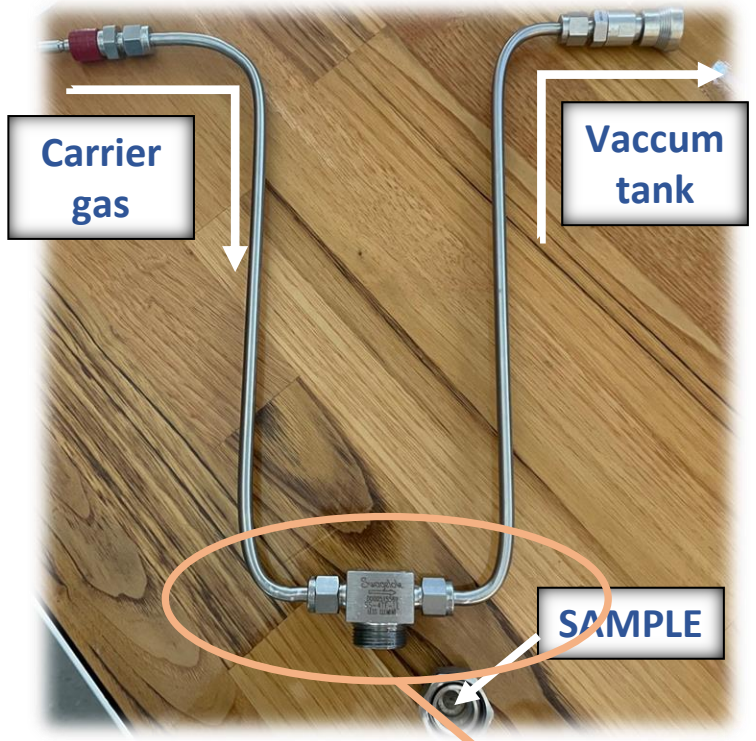
Yield: 71%

HCCSCN is a very volatile liquid
at room temperature (m.p. = -30.7 °C)

quick decomposition

EXPERIMENTAL APPROACH FOR HCCSCN

EXPERIMENTAL SYSTEM



Swagelok filter

submerged
dry ice container

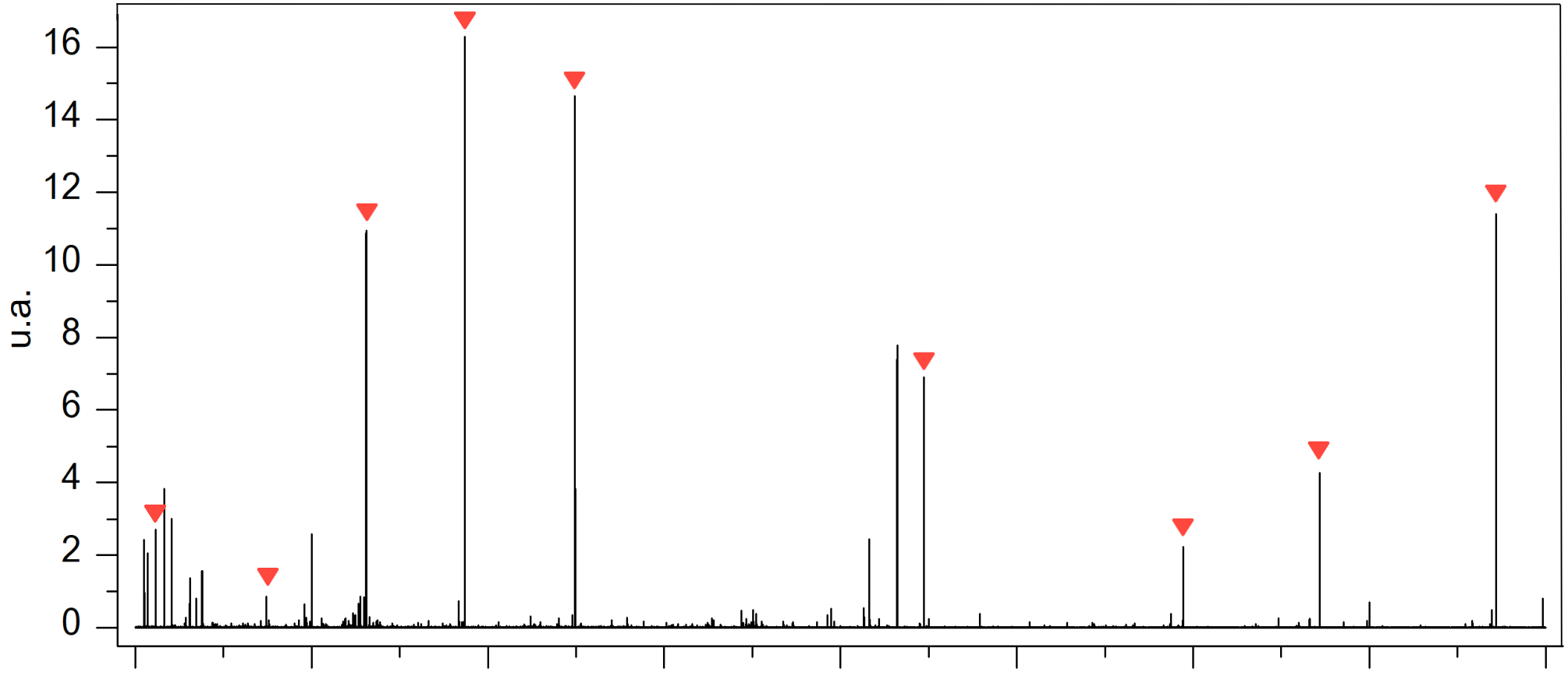
Multinozzle CP-FTMW Spectrometer (2 – 18 GHz)

Dr. Aran Insausti

RESULTS

CP-FTMW Spectra (8 – 16 GHz)

70000 acqs

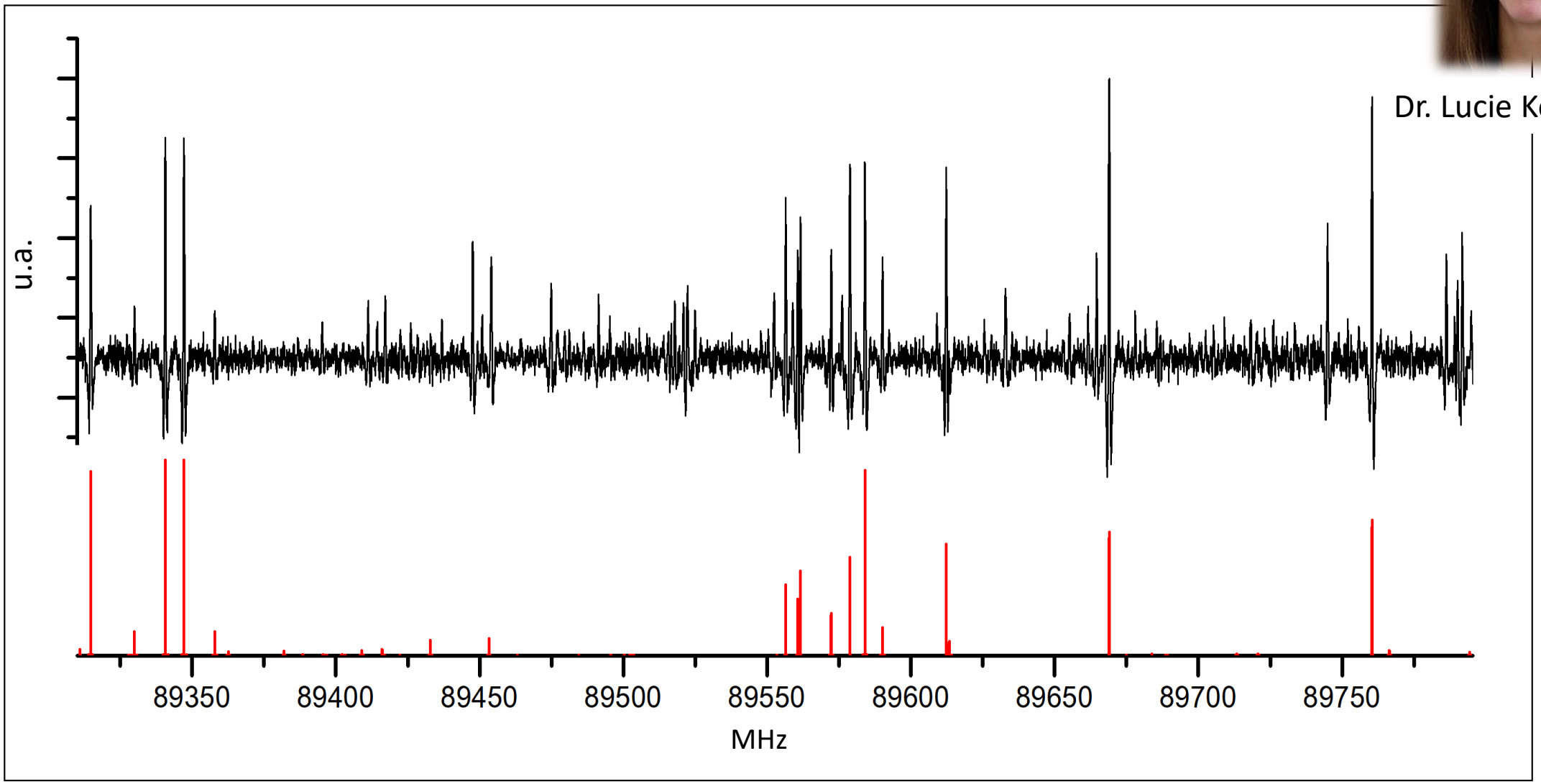


RESULTS

Millimeter wave Spectra (50 – 120 GHz)

Room temperature conditions
SUPER QUICK DECOMPOSITION!

Dr. Lucie Kolesniková



WHAT'S NEXT?

ACKNOWLEDGMENTS

http://www.gem.uva.es/

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