Laboratory Investigations of Carbonaceous Molecules

Sandra Brünken

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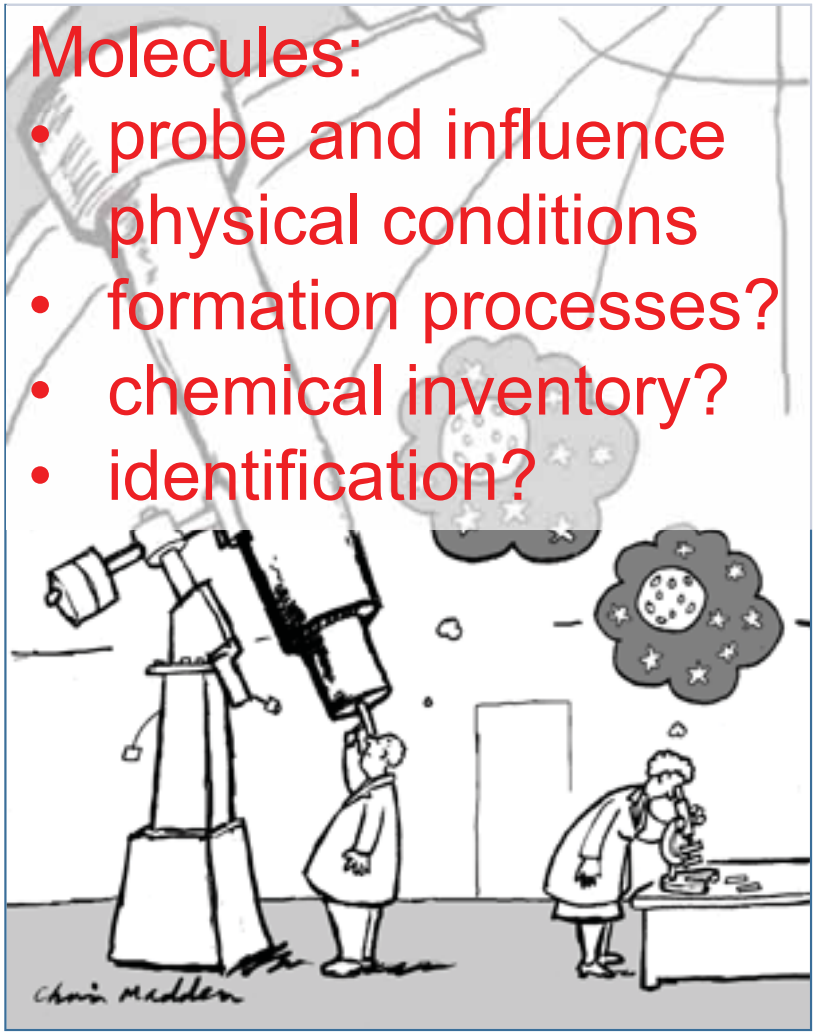
Laboratory Spectroscopy & Astrochemistry

Molecules:
- probe and influence physical conditions
- formation processes?
- chemical inventory?
- identification?



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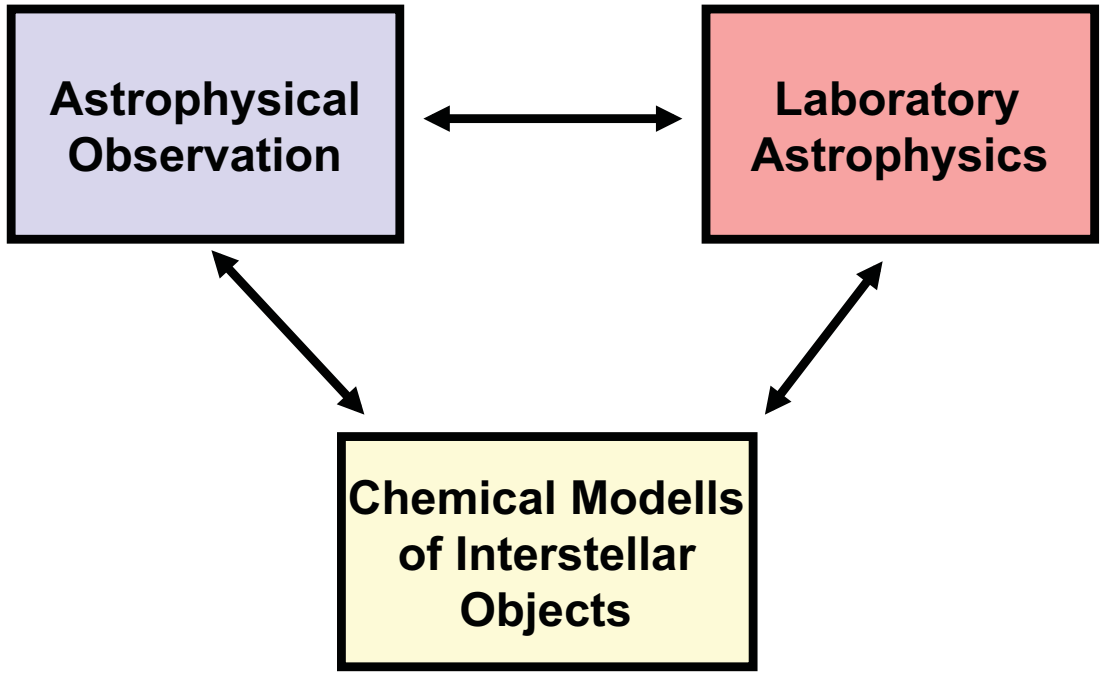


Astronomical needs:

transition frequency accuracies $\Delta\nu/\nu = 10^{-6}$

➔ high resolution gas phase spectroscopy

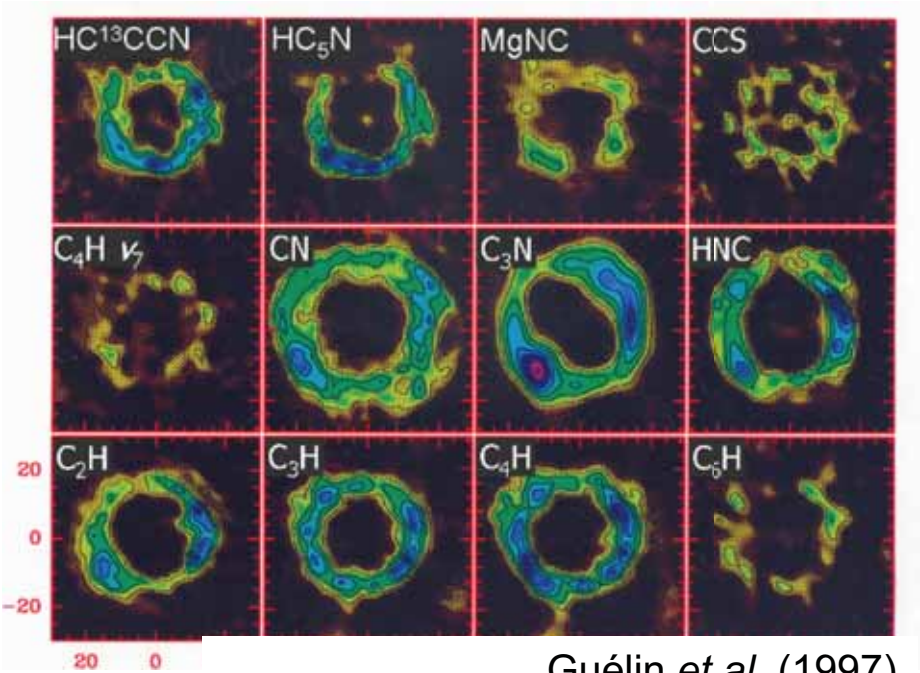
B1377: An unidentified sequence of astronomical lines

Line survey of **IRC+10216**

(Kawaguchi *et al.*, PASJ, 1995)

7 lines (Nobeyama 45m)

- circumstellar envelope around carbon rich star
- extremely rich chemistry: > 50 molecules



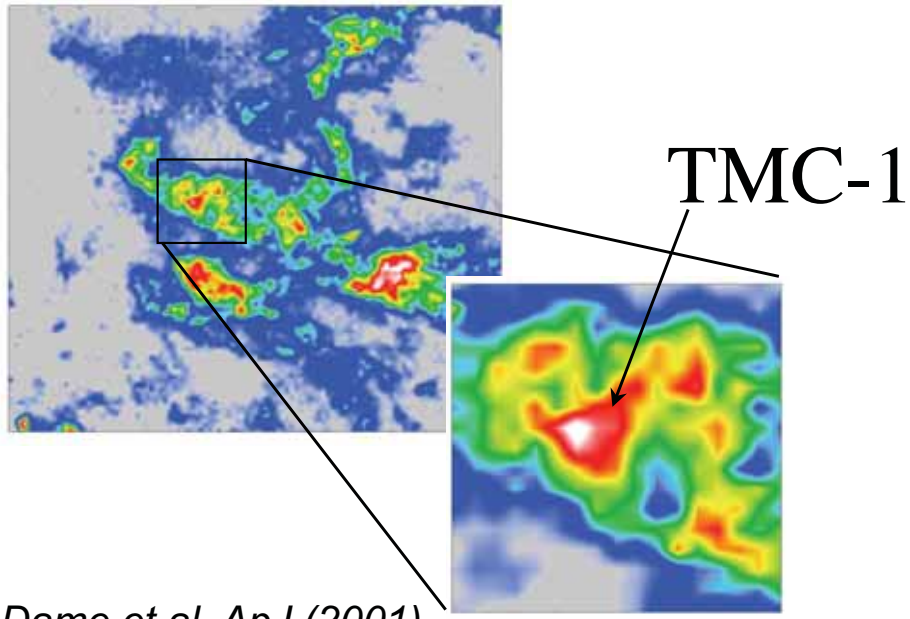
Guélin *et al.* (1997)

TMC-1 (Taurus-Auriga Molecular Cloud)

(McCarthy *et al.*, ApJL, 2006)

2 lines (GBT 100m)

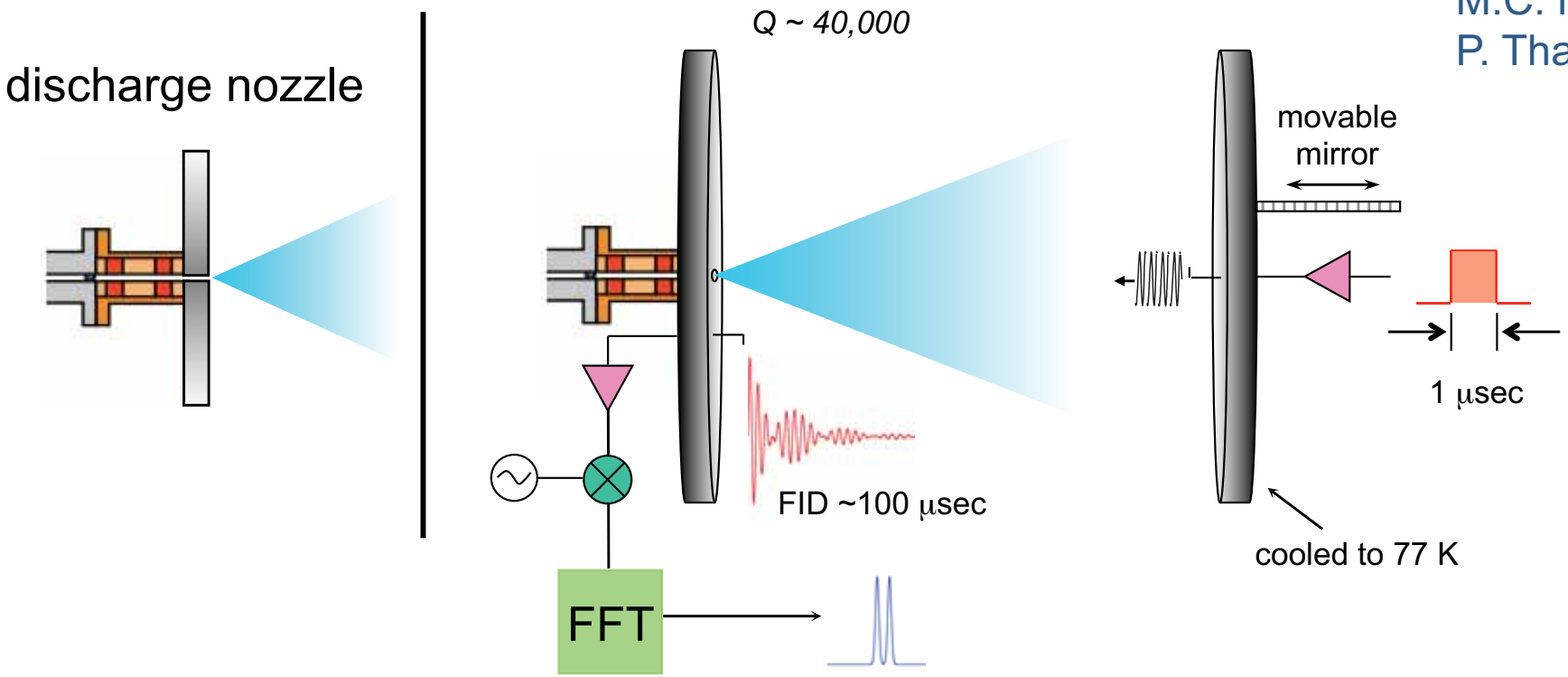
- cold (10 K), dense (10^4 cm^{-3})
- rich in carbon-chains
- no metal-bearing molecules



Dame et al. ApJ (2001)

Experimental setup – Fourier Transform Microwave Spectrometer (FTM)

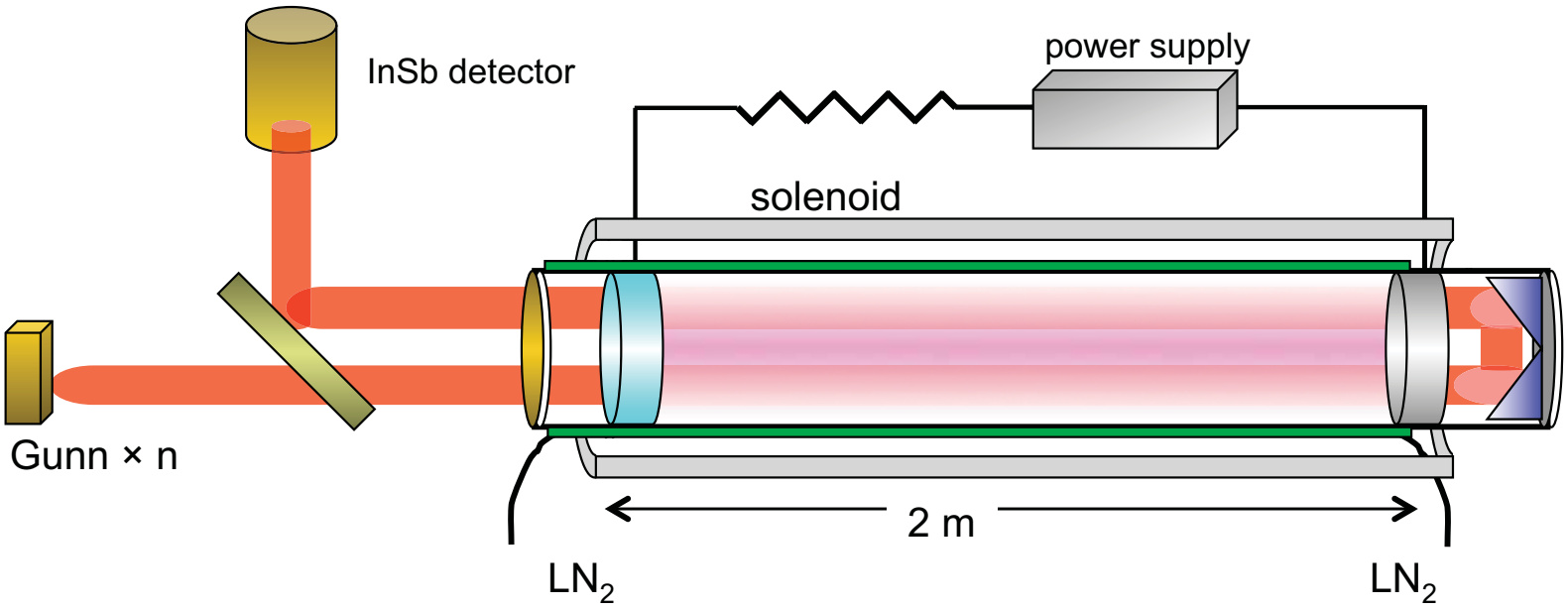
supersonic nozzle coupled to a high-Q Fabry-Perot cavity



M.C. McCarthy
P. Thaddeus

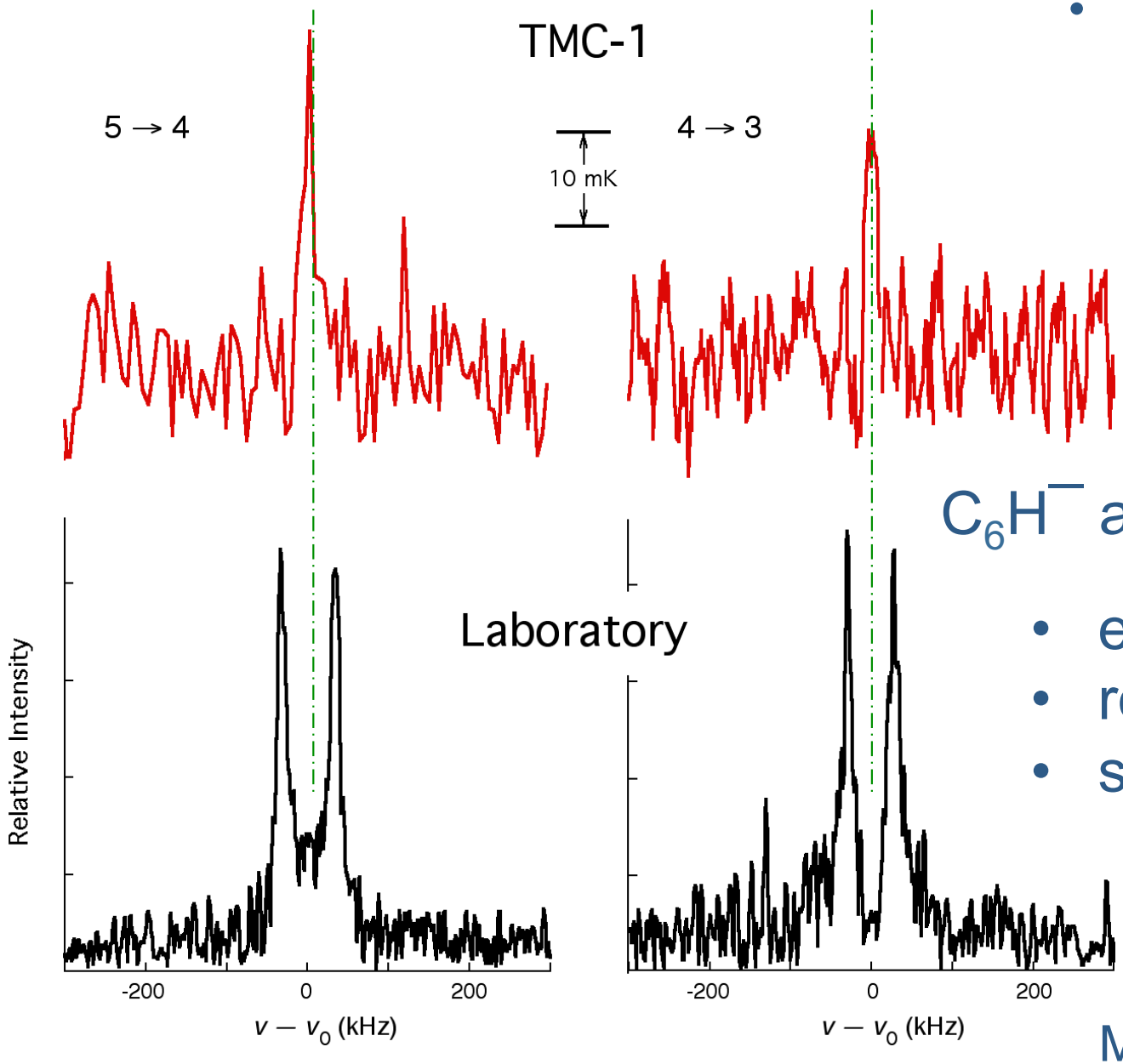
- frequency range: 5 – 42 GHz resolution: 20 kHz accuracy: 1-2 kHz
- low current (~20 mA) discharge of C_4H_2 or C_2H_2 (0.1 %) in Ne (He, H_2)

Experimental setup – mm-wave absorption spectrometer



- low current dc glow discharge of C_2H_2 (85 %) + Ar (15 %)
- frequency coverage: 68 – 600 GHz
- frequency accuracy: 10 – 50 kHz
- cell walls cooled by IN_2

Identification of C_6H^- as the carrier of B1377



- 15+ lines detected over two decades of frequency

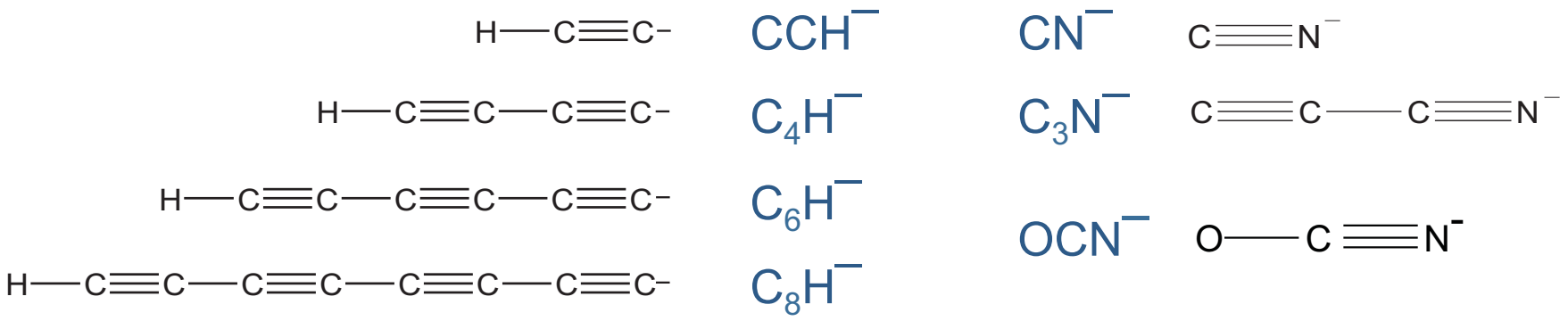
C_6H^- as carrier confirmed by

- elemental composition
- rotational constant
- symmetry, charge state

McCarthy *et al.*, ApJL (2006)

Carbon chain anions – laboratory measurements

- **seven molecular carbon chain anions detected so far**

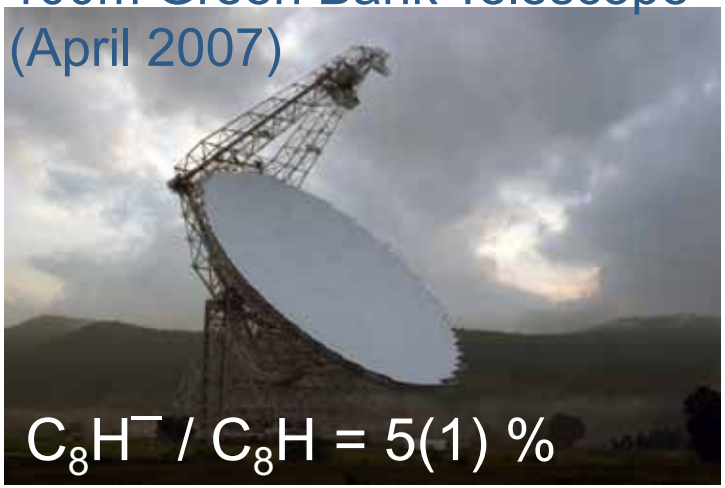


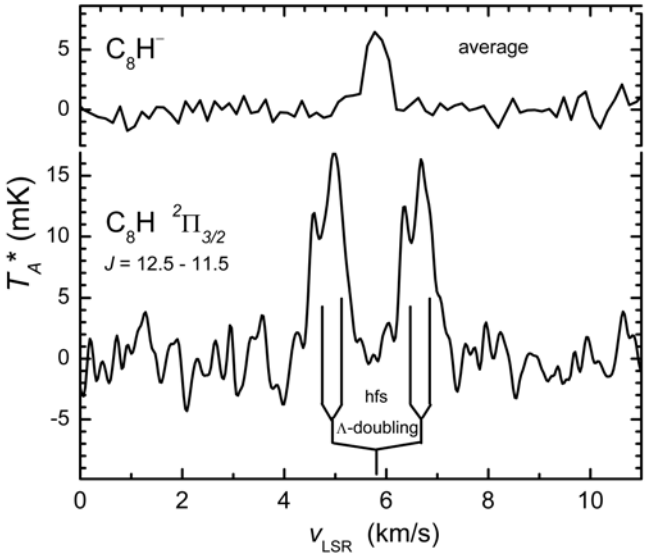
- detections secured by:

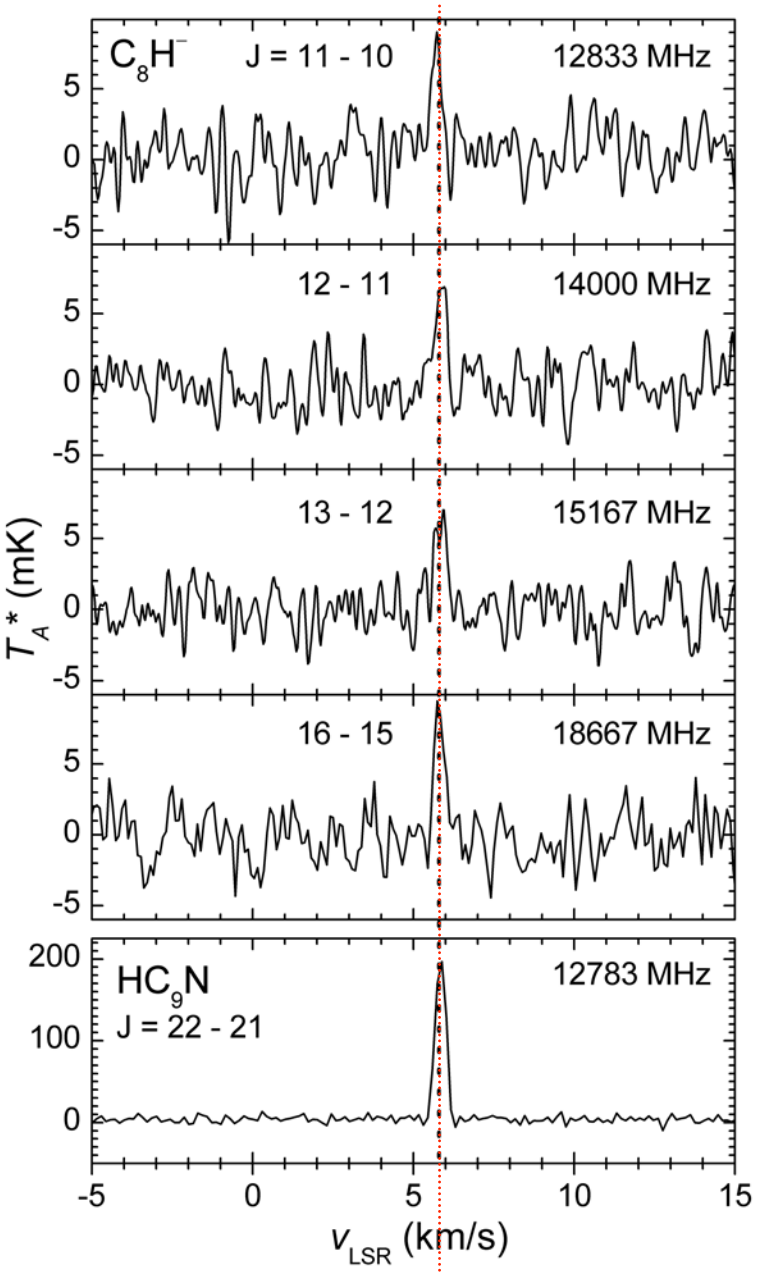
✓ elemental composition
✓ harmonicity
✓ close agreement with calculations
✓ isotopic shift
✓ determination of charge state

Detection of C_8H^- in TMC-1

100m Green Bank Telescope (April 2007)







Brünken *et al.*, ApJL, 2007

Carbon chain anions in space

- C_6H^- and C_8H^- detected in TMC-1

- C_4H^-, C_6H^- , C_8H^-, CN^-, C_3N^- and C_5N^- detected in IRC+10216

  (Cernicharo *et al*. ApJL, 2007; Remijan *et al*., ApJL, 2007, Kawaguchi *et al*., PASJ, 2007, Thaddeus et al., ApJ 2008, Cernicharo *et al*., ApJL 2008)

  C_8H^- anion to neutral ratio 28-37% !

- detection of C_6H^- in additional sources – prestellar, star-forming:

  ✓ IRAS 04368+2557 in L1527 (Sakai et al. ApJL, 2007; Agundez et al. A&A, 2008) (C_4H^- also detected)

  ✓ L1544
  ✓ L1521F (Gupta *et al*., ApJ 2009)

  ✓ L1251A
  ✓ L1512 (Cordiner *et al*., ApJ 2011)

Influence of anions on chemistry

- new formation (but also destruction) pathways for neutral carbon chains:

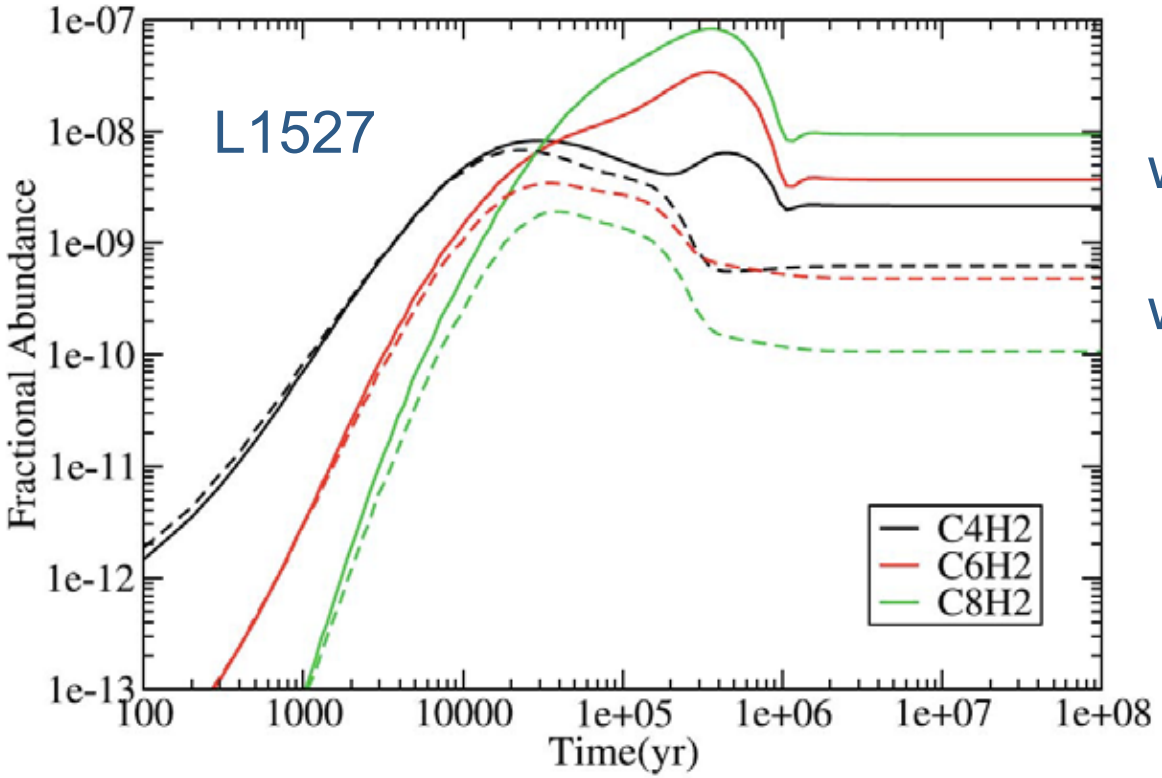
$C_n^- + H \rightarrow C_nH + e^-$

$C_{n-1}H^- + C \rightarrow C_nH + e^-$

$C_{2n}H^- + H \rightarrow C_{2n}H_2 + e^-$

$C_nH^- + N \rightarrow HC_nN + e^-$

Millar et al., ApJL, 2007;
Herbst & Osamura, ApJ, 2008;
Harada & Herbst, ApJ, 2008;
Walsh et al., ApJ, 2009
Cordiner et al., ApJ, 2009

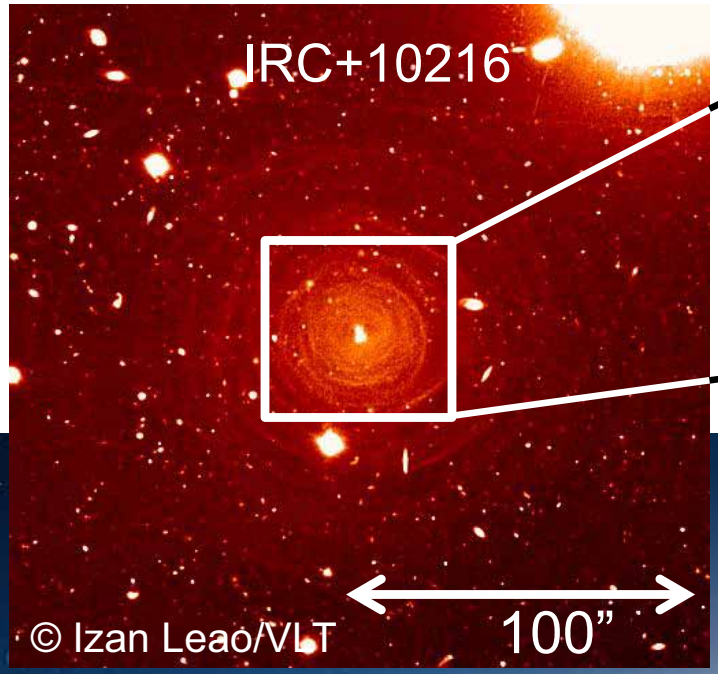


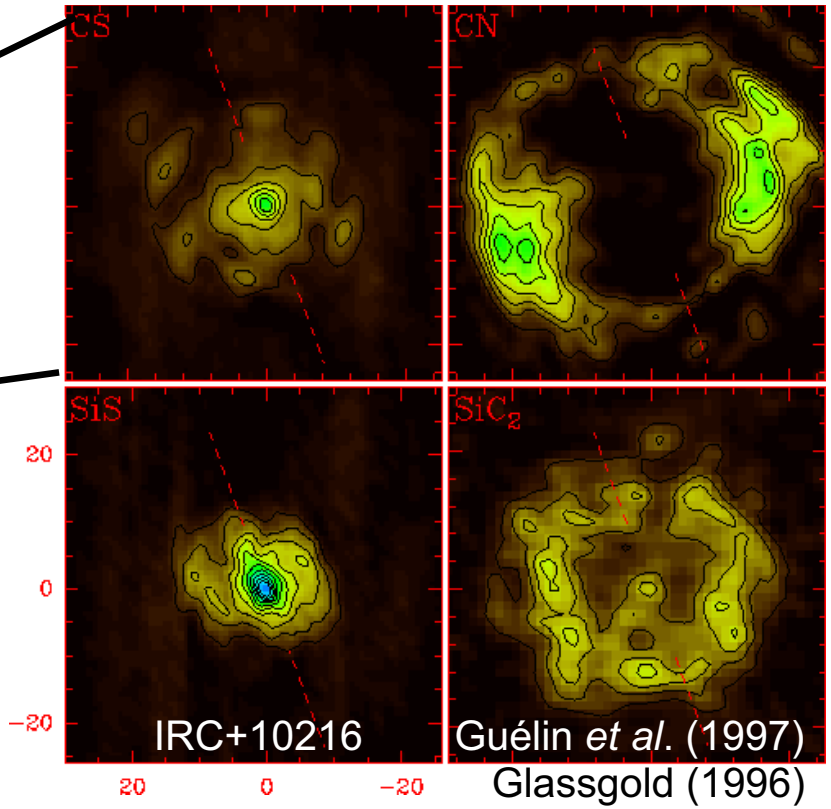
with anions

without anions

Harada & Herbst, ApJ, 2008;

The need for data on isotopic and excited species
IRC+10216 spectral line survey in the 345 GHz band



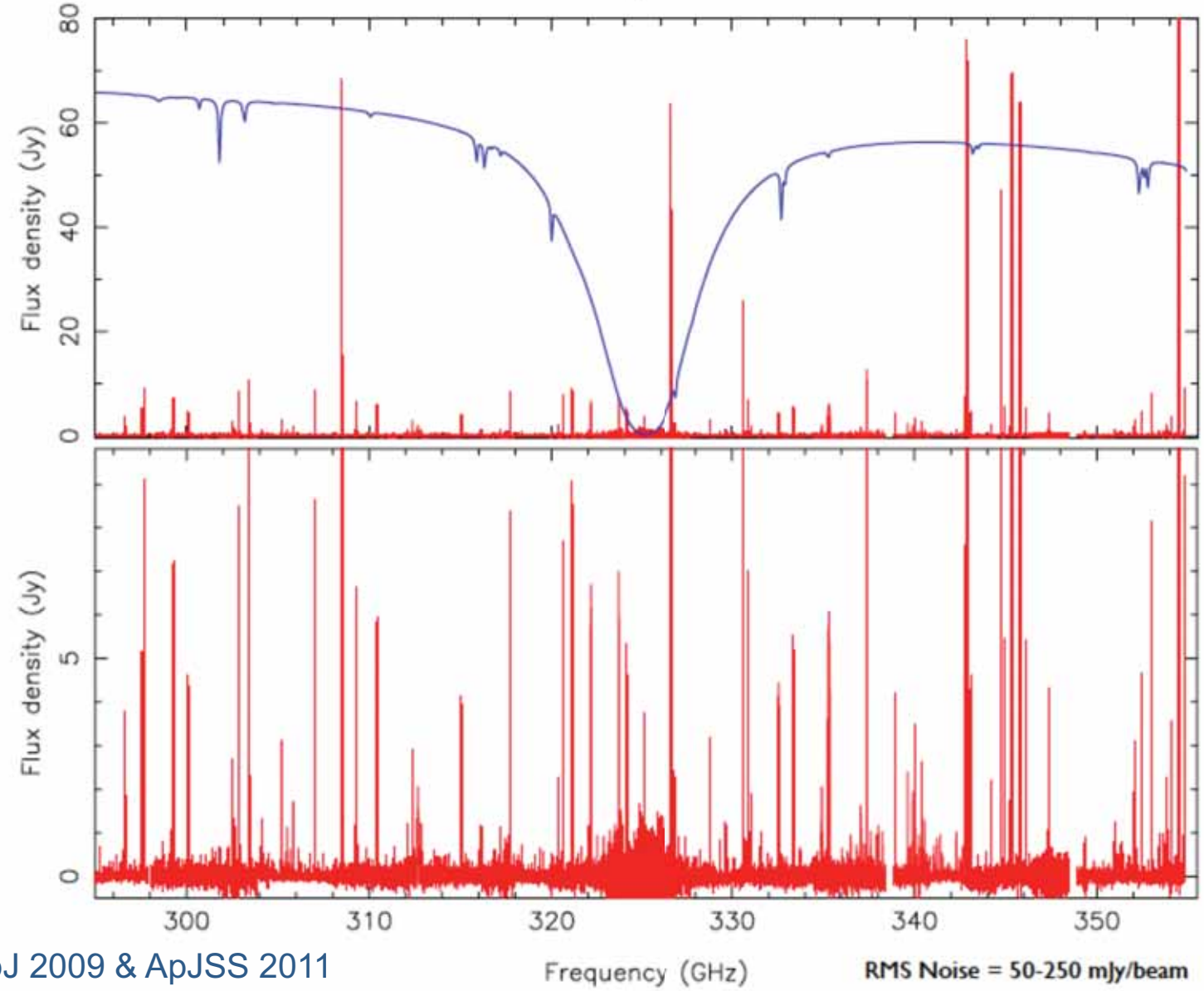


SMA: spatial resolution 3”

Patel et al., ApJ 2009 & ApJSS 2011

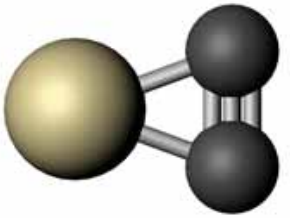
SMA IRC+10216 overview spectrum

442 lines detected, > 200 first detections, still 150 U-lines
vibrational excited states, isotopic species

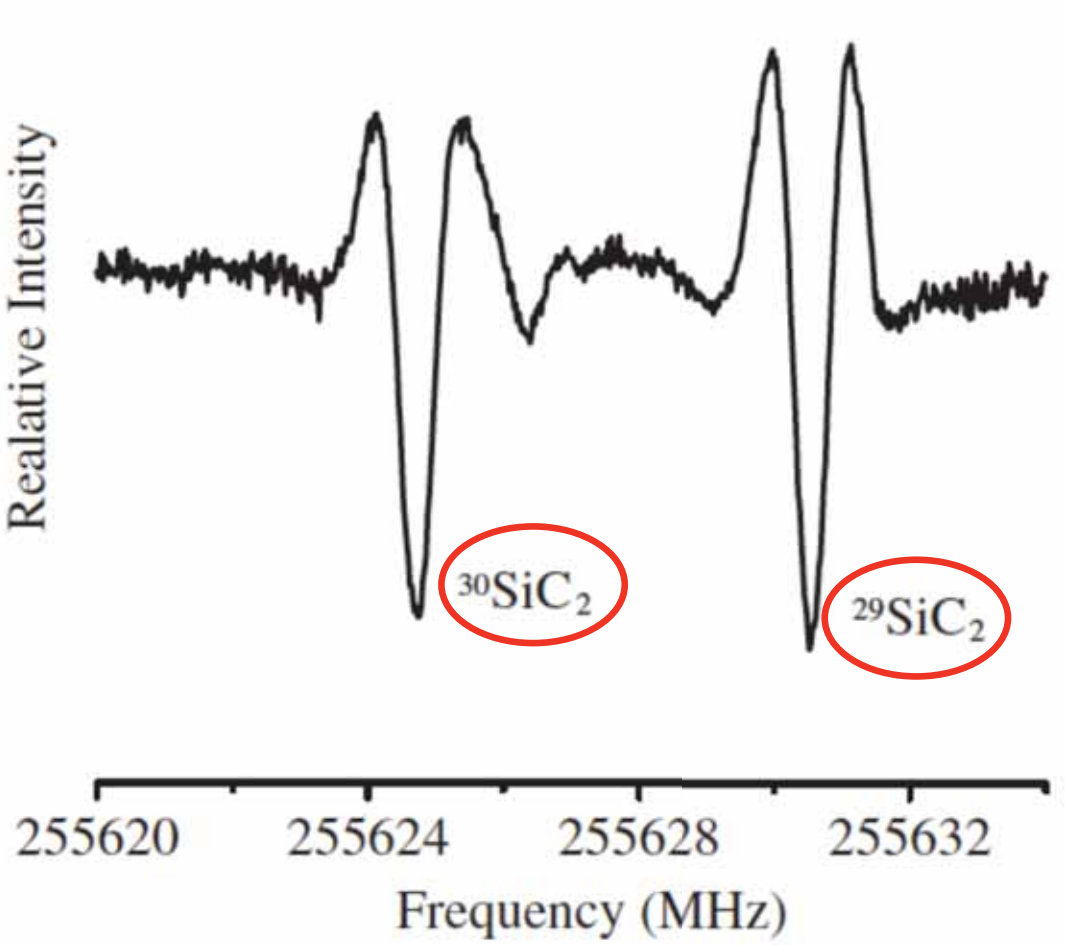


Patel et al., ApJ 2009 & ApJSS 2011

Isotopic Species – SiC_2



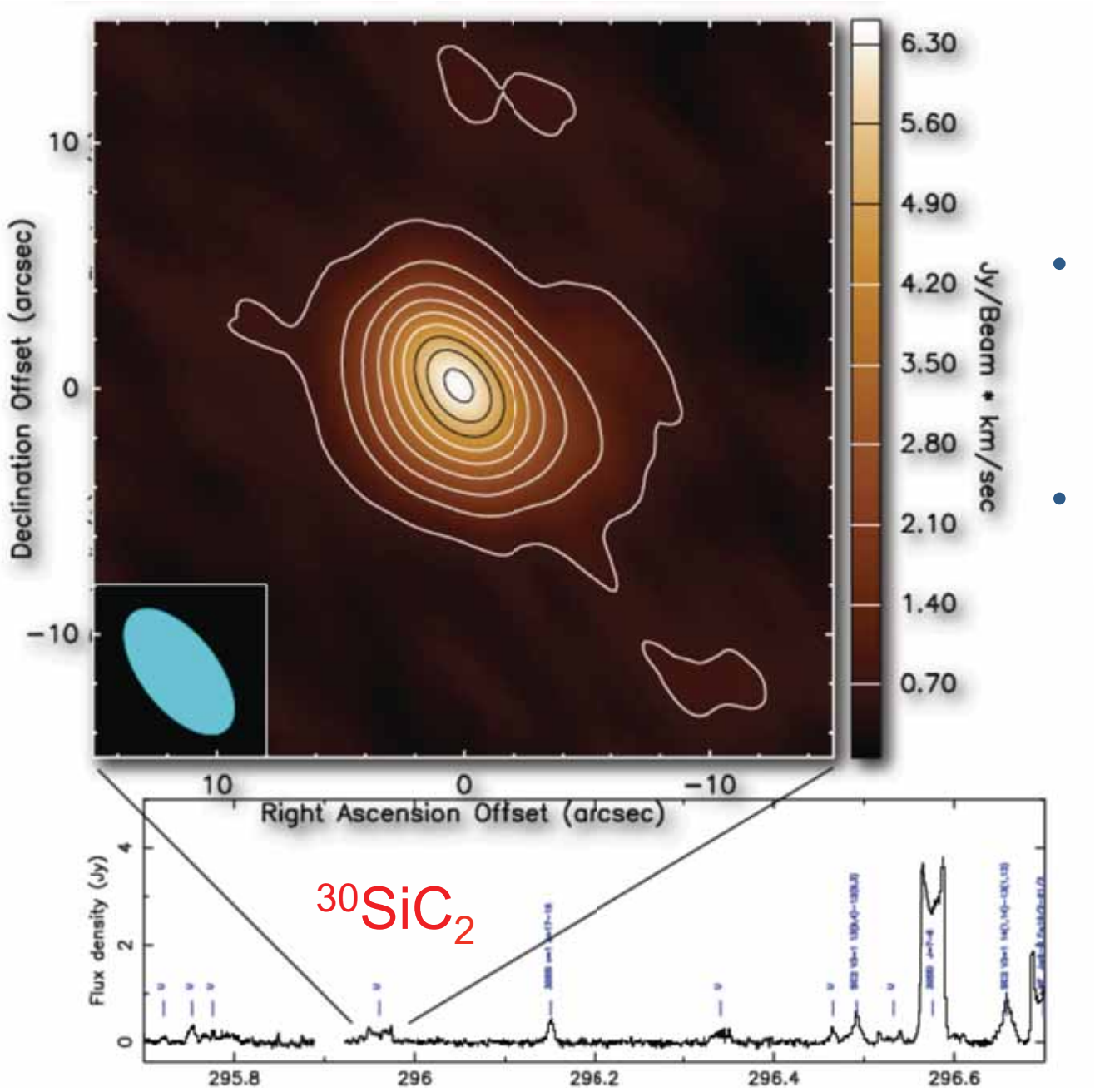
- 35 lines measured in the laboratory between 140 – 360 GHz
- high rotational quantum numbers
- predictions < 500 GHz to better than 1 km/s now possible



discharge of SiH_4, C_2H_2 & Ar

Kokkin et al., ApJSS 196 (2011)

Isotopic SiC_2 in IRC+10216

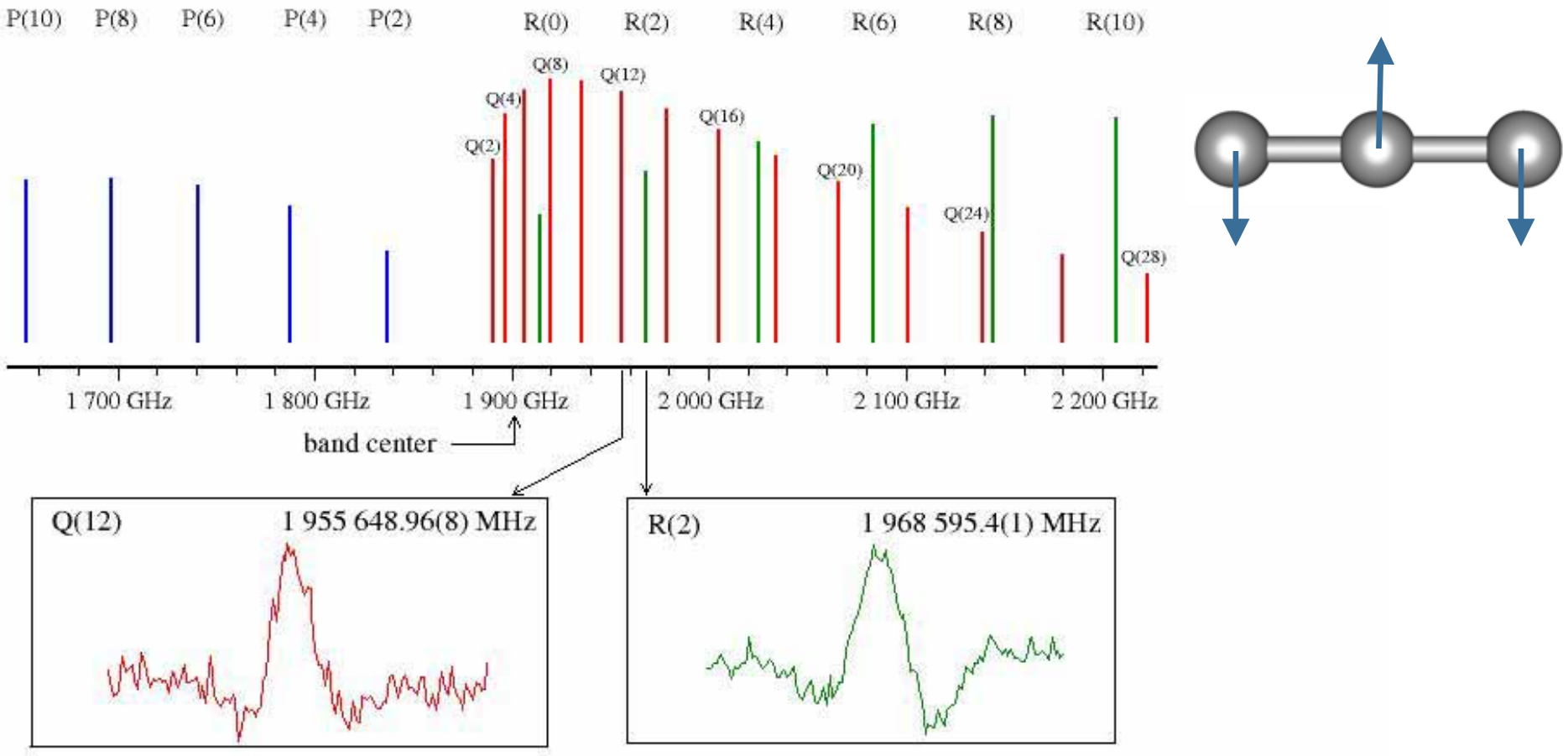


- 25 lines of isotopic $^{29}SiC_2$ & $^{30}SiC_2$ assigned in SMA data
- Still missing data on many vibrationally excited states

Patel et al., ApJSS 193 (2011)
Kokkin et al., ApJSS 196 (2011)

Low bending vibrations in the THz region – C_3

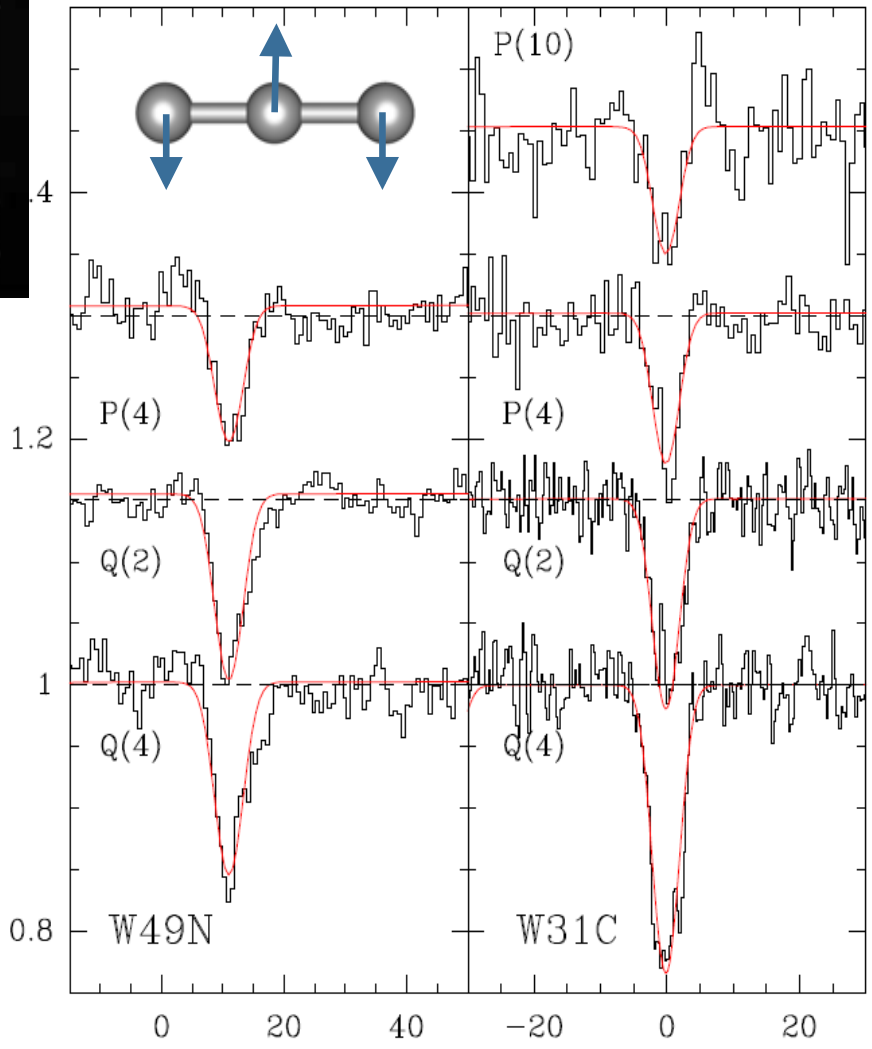
Cologne **S**ideband **S**pectrometer for **T**erahertz **A**pplications– COSSTA

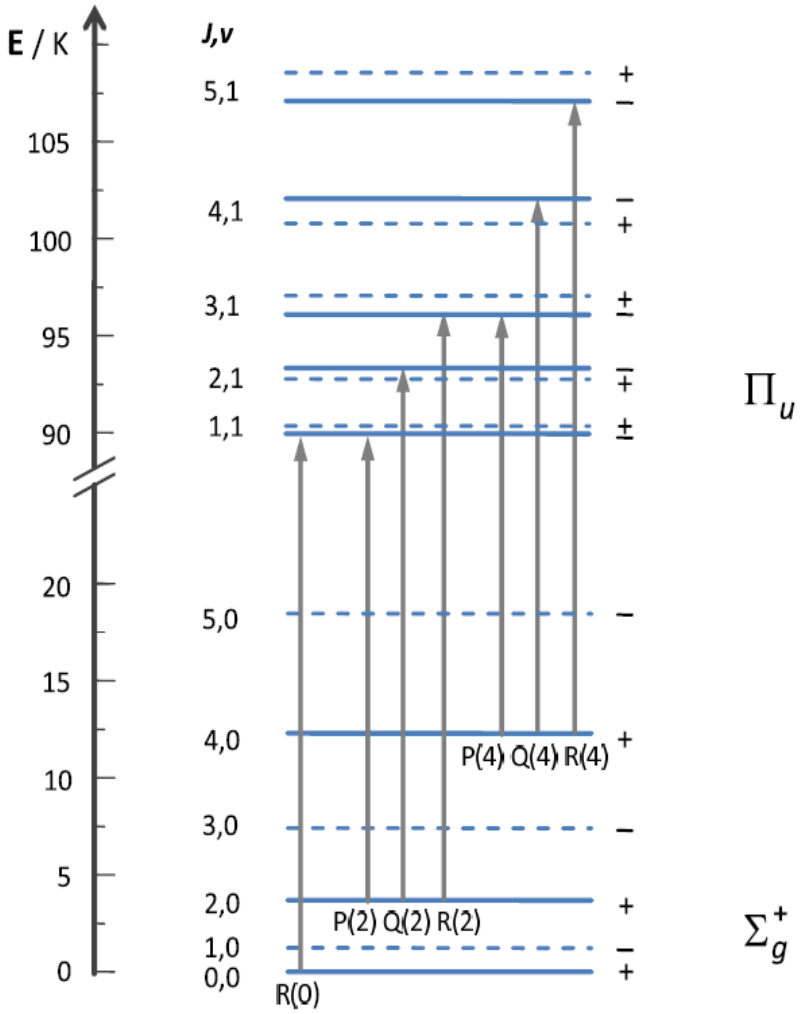


T.F. Giesen, A. O. Van Orden, J.D. Cruzan, R.A. Provencal, R.J. Saykally, R. Gendriesch, F. Lewen, G. Winnewisser, *Astrophys. J.* 551, L181, (2001)

Excitation and Abundance of C_3 in star forming cores

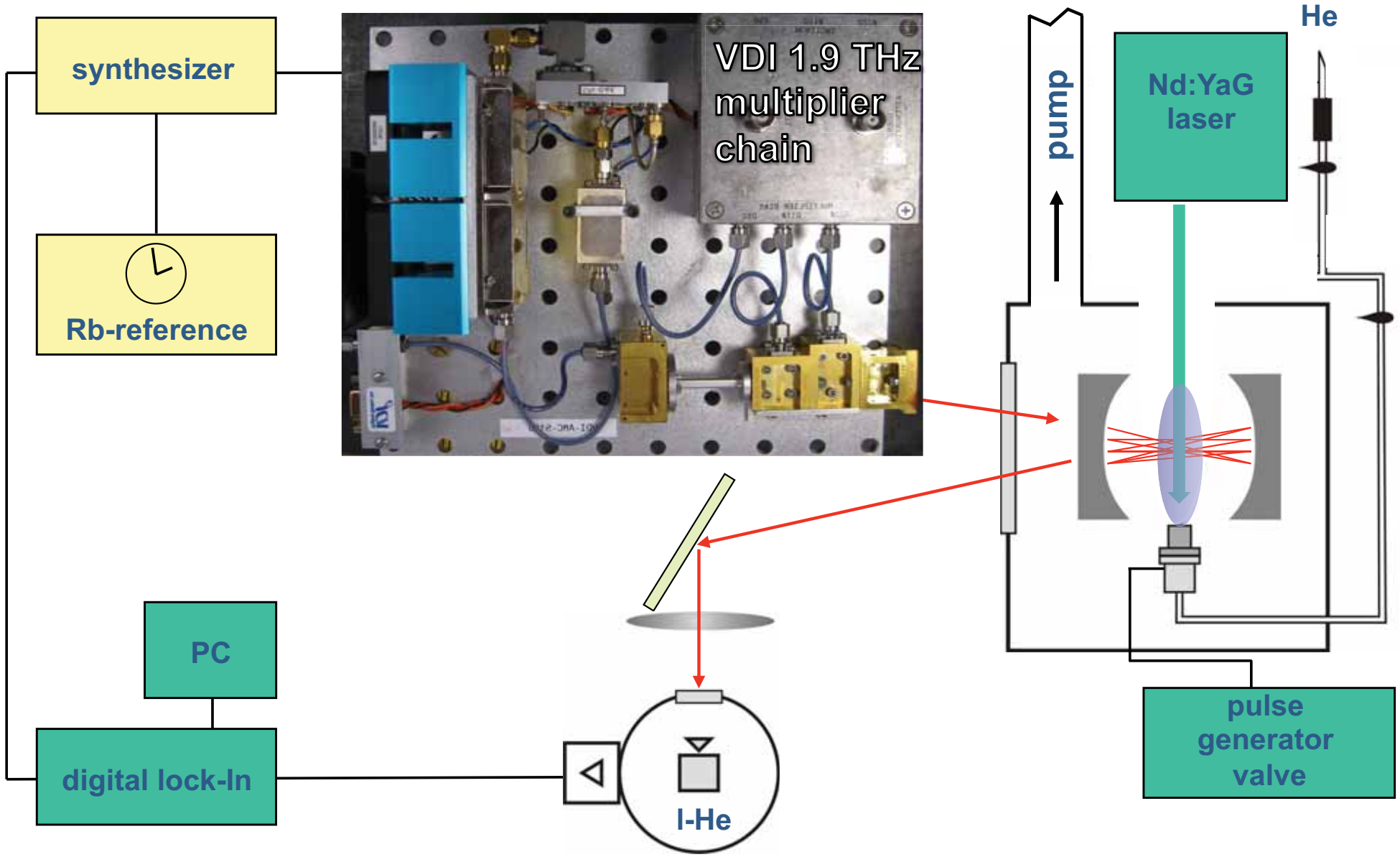
Herschel/HIFI observations towards W31C and W49N



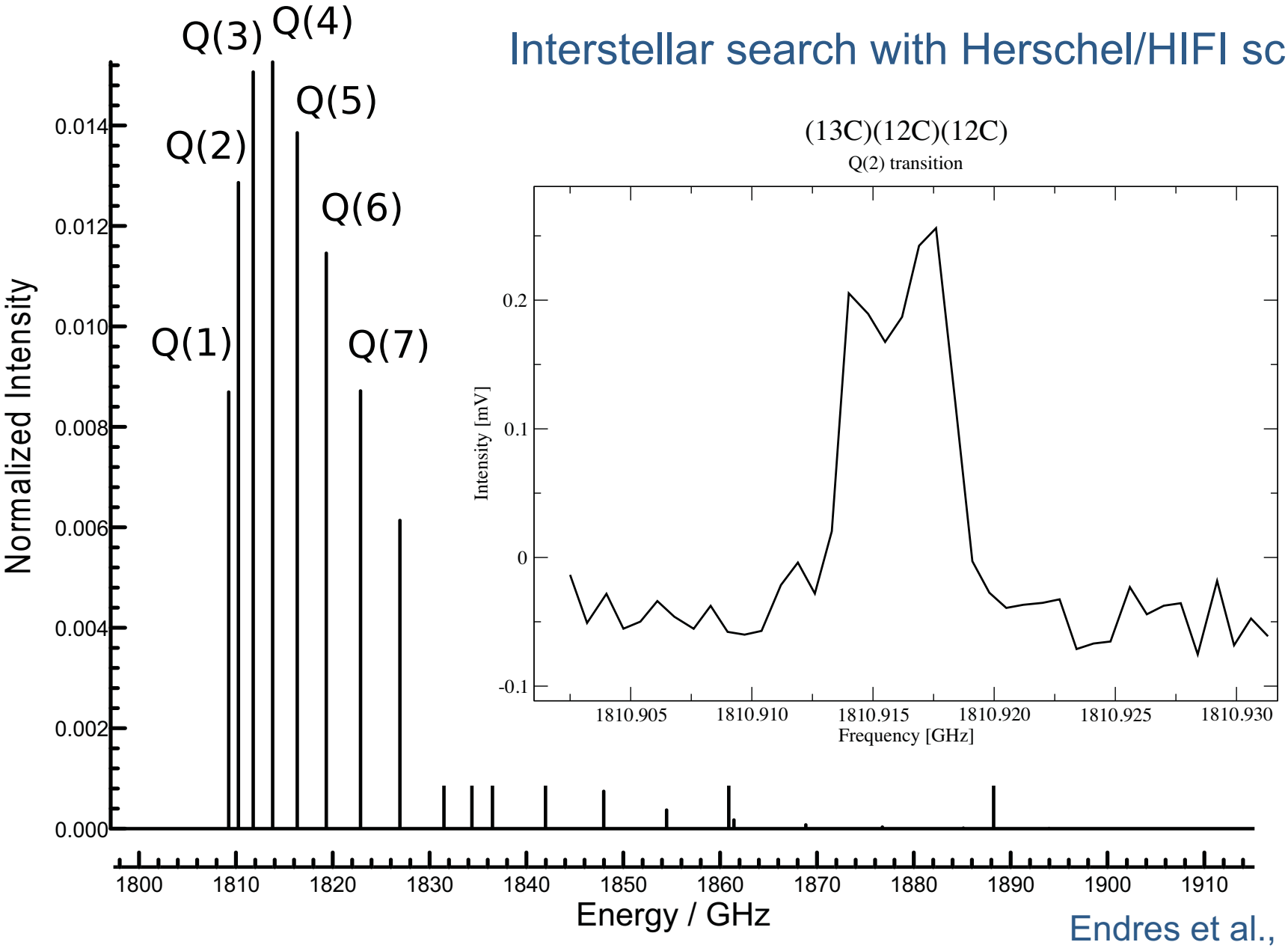


B. Mookerjea, T. Giesen, J. Stutzki, et al. A&A 2010

Supersonic **Je**t **S**pectrometer for **T**Hz **A**pplications (SuJeSTA)



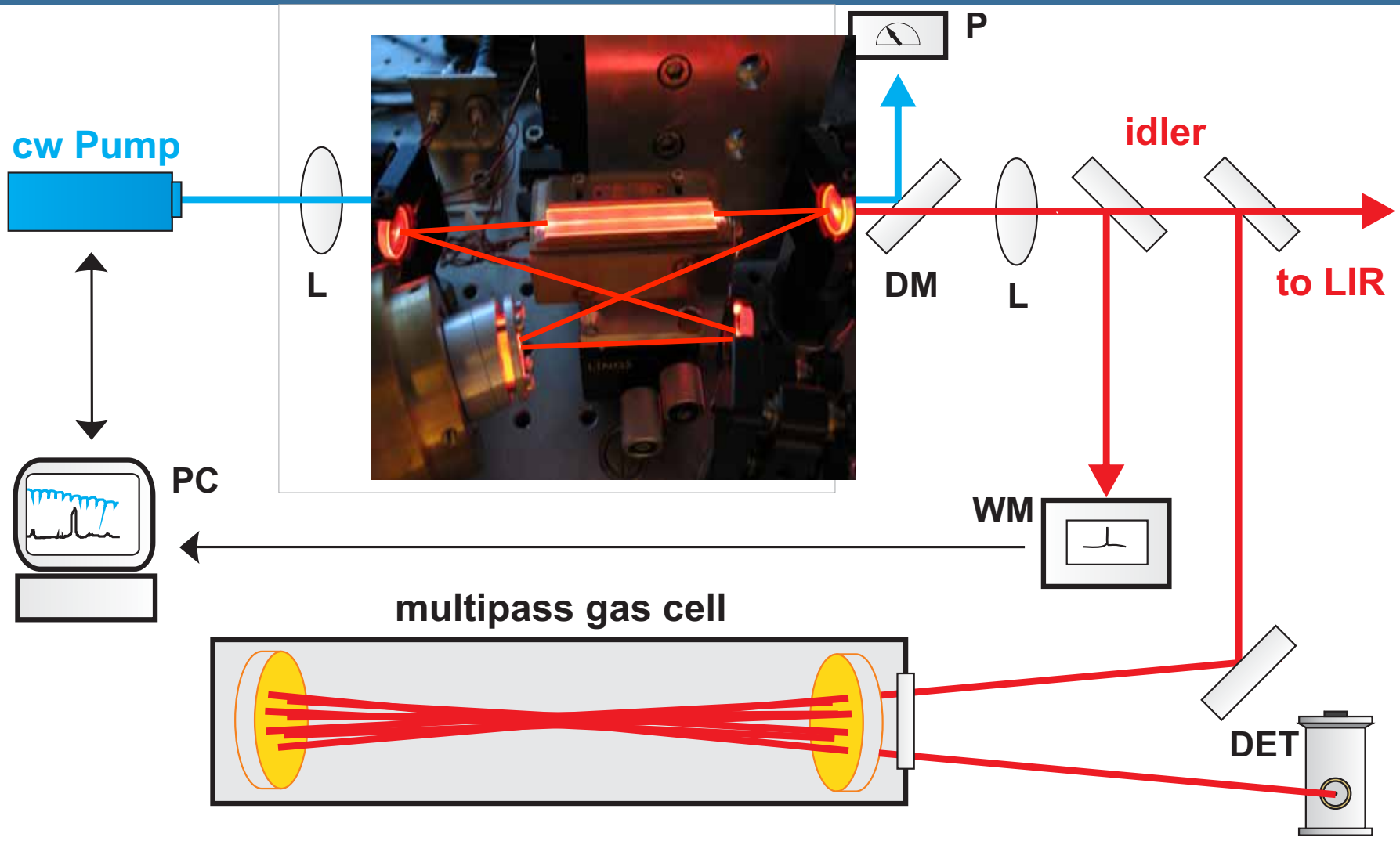
Isotopic C_3 – $^{13}C^{12}C^{12}C$



Interstellar search with Herschel/HIFI scheduled

Endres et al., in preparation

High resolution IR spectroscopy – cw-OPO system

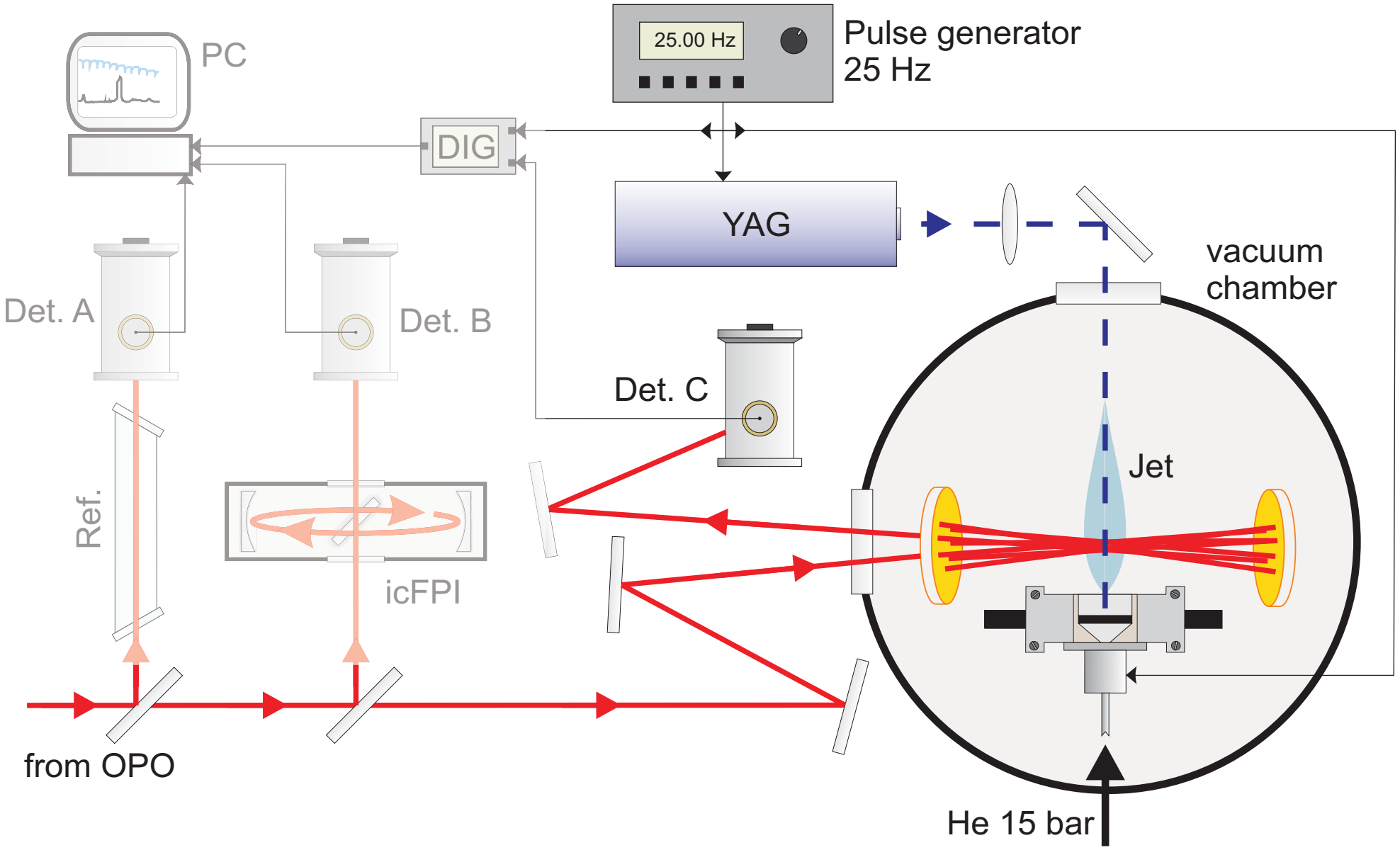


Range: 3 – 5 μm Power: 1 W
Tuning: 15 GHz mode-hop free

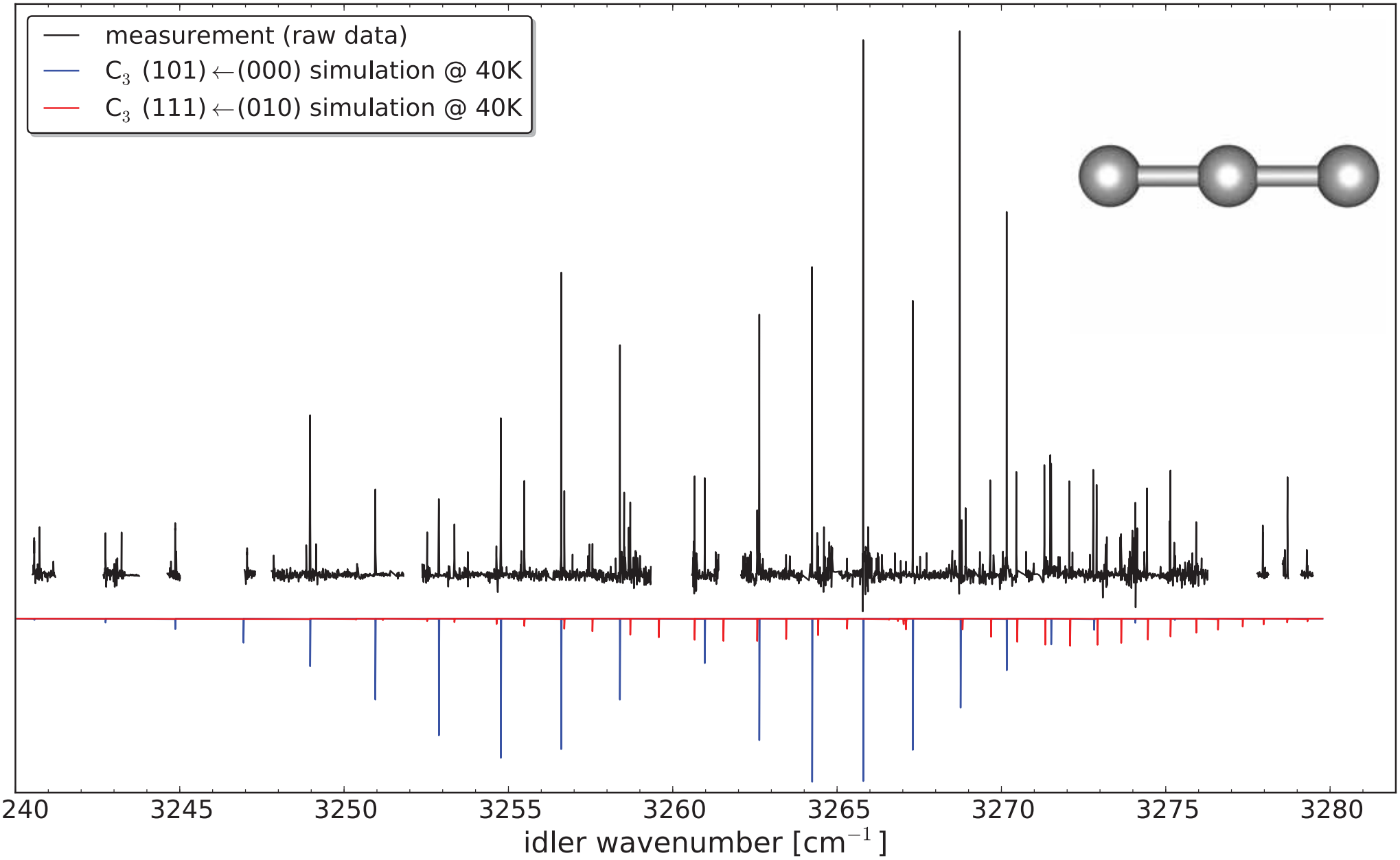
Linewidth: 0.1-0.3 MHz
Calibration: wavemeter & reference gas

Krieg et al., Rev. Sci. Instrum. 82 (2011)

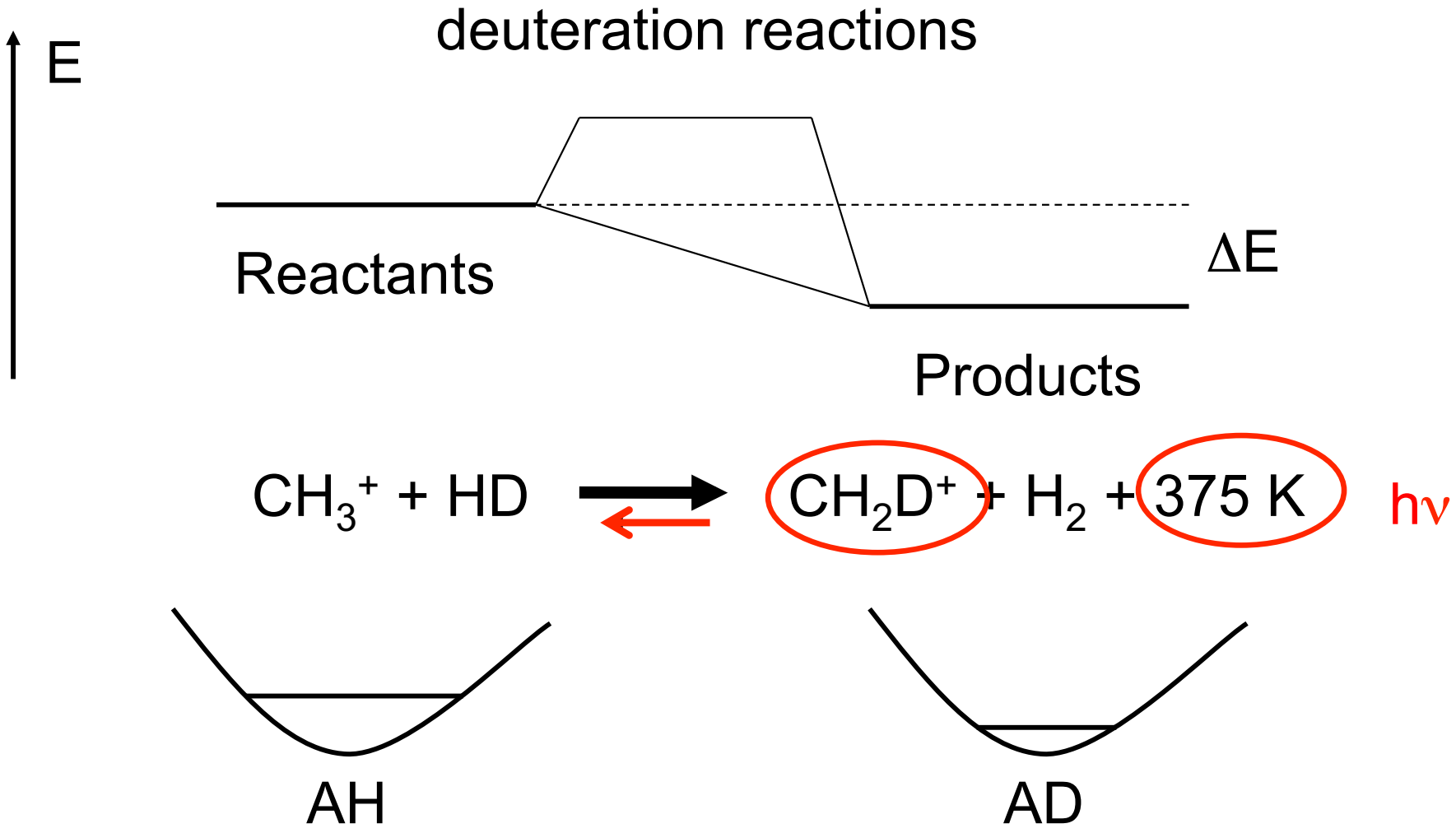
IR spectroscopy in a molecular jet – experimental setup



IR spectra of C_3

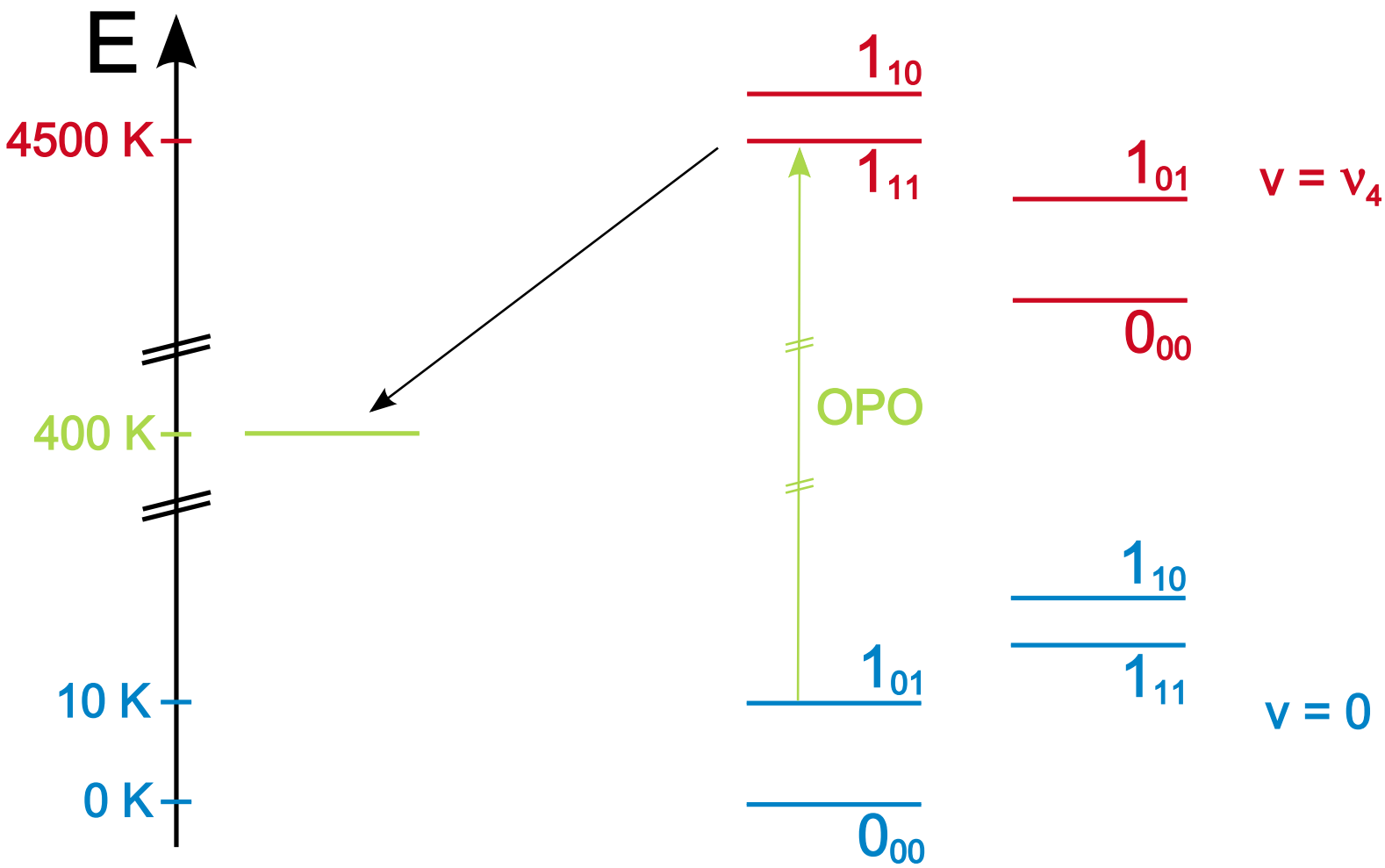


Laser Induced Reactions (LIR) – action spectroscopy principle



CH_3^+ plays important role in deuterium fractionation in warmer (50 K) ISM

LIR scheme of CH_2D^+



$$CH_3^+ + HD \longleftarrow CH_2D^+ + H_2$$

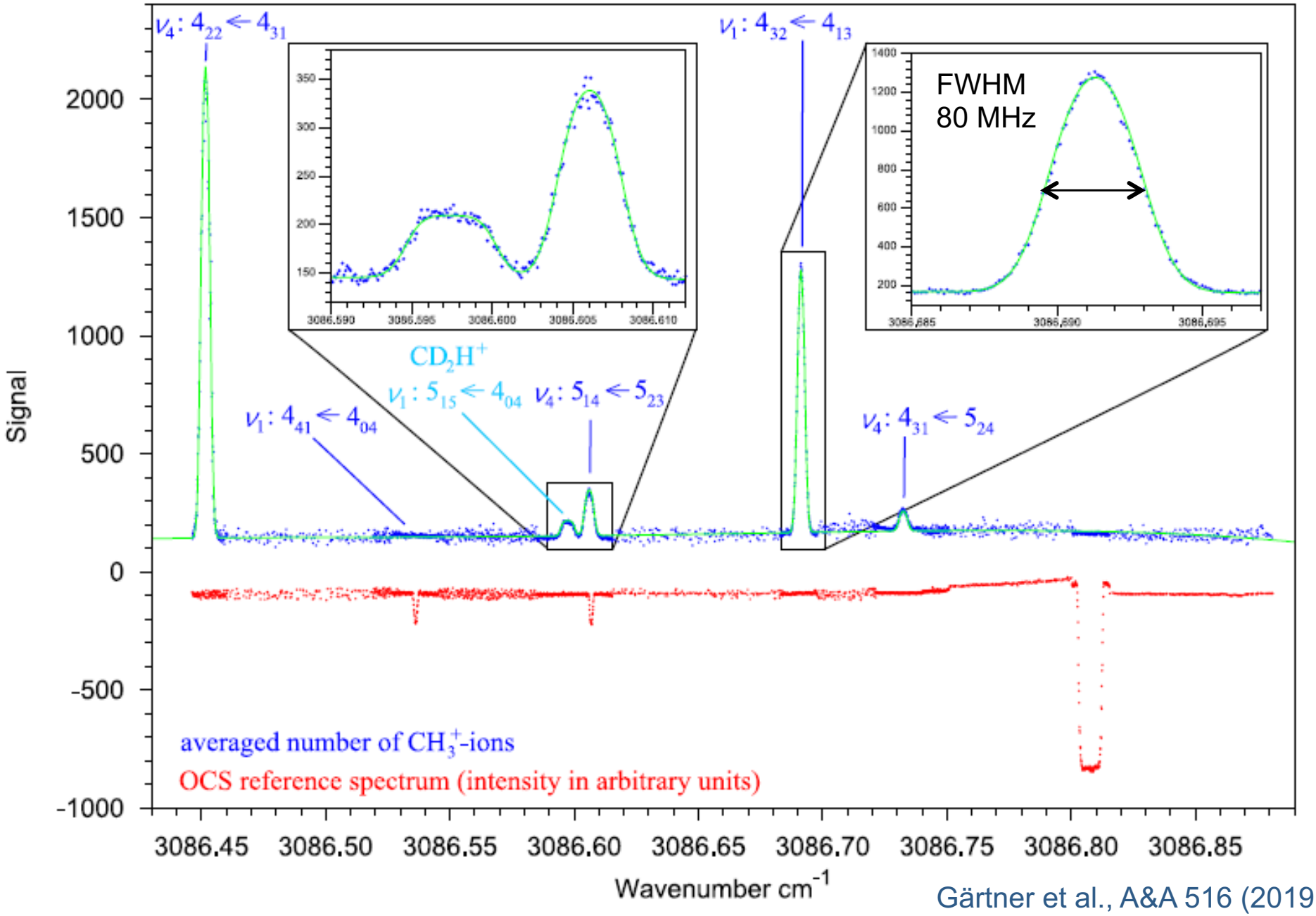
LIR – 22-pole ion trap apparatus

O. Asvany, S. Schlemmer et al., Rev. Sci. Instrum. 81, 076102 (2010)

Mass selected I	
Number of Ions	
Temperature	
Density	
Reaction Rates	10^{-8} – 10^{-17} cm^3s^{-1}

$$CH_2D^+ + H_2 + h\nu \rightarrow CH_3^+ + HD$$

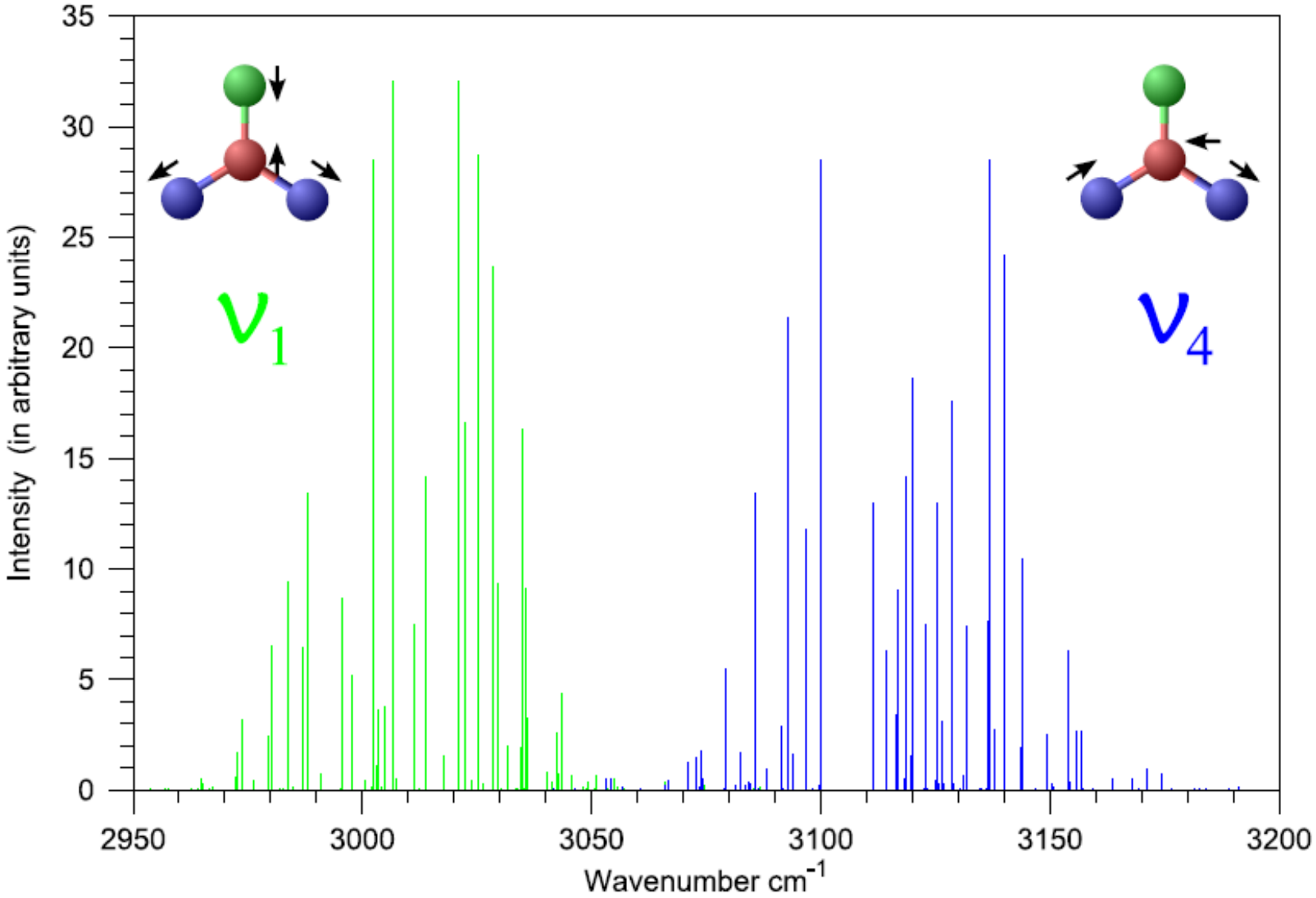
CH_2D^+ LIR Spectra



Gärtner et al., A&A 516 (2019)

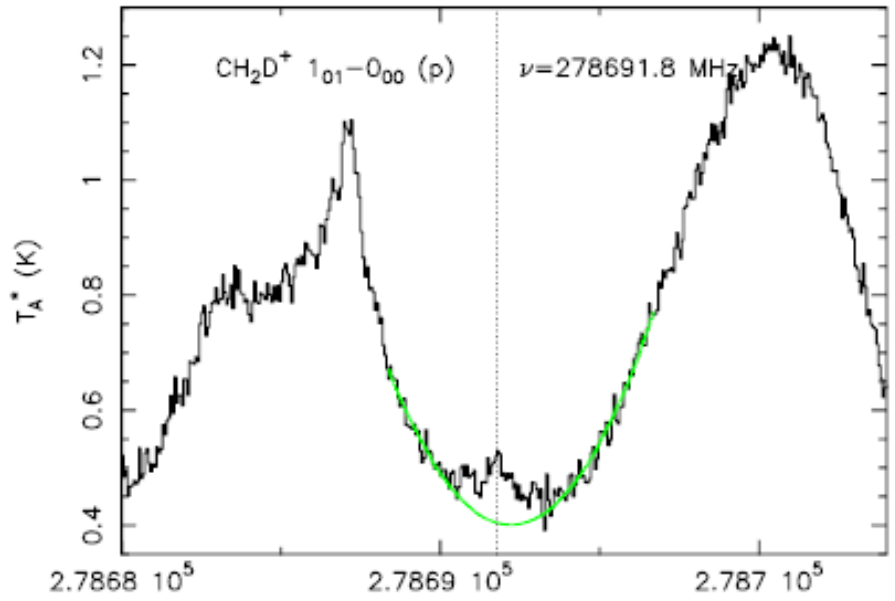
CH_2D^+ Ro-vibrational Spectra

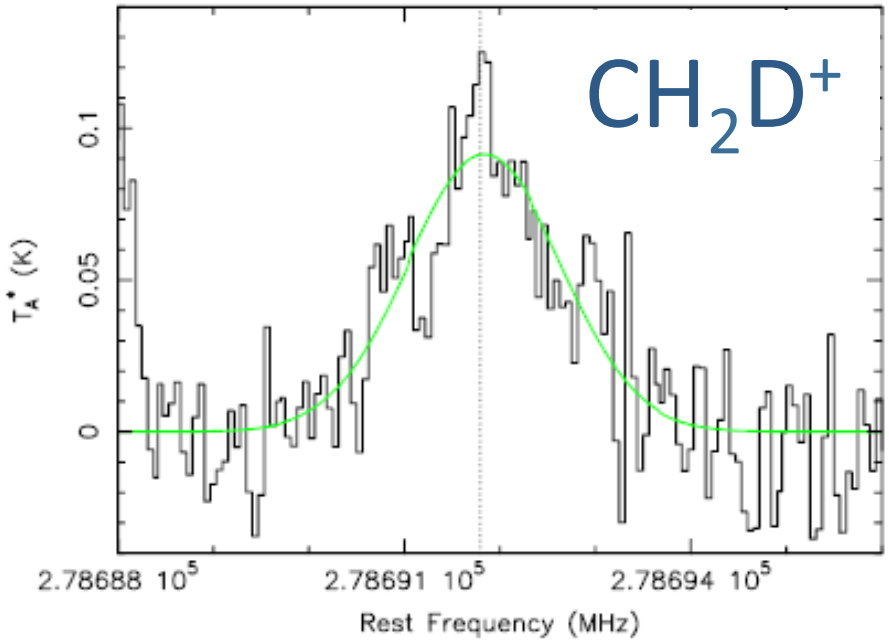
Analysis of high-resolution IR spectra yields accurate rotational transitions!
MHz accuracies or better



CH_2D^+ in Space and Laboratory

Ori IRc2



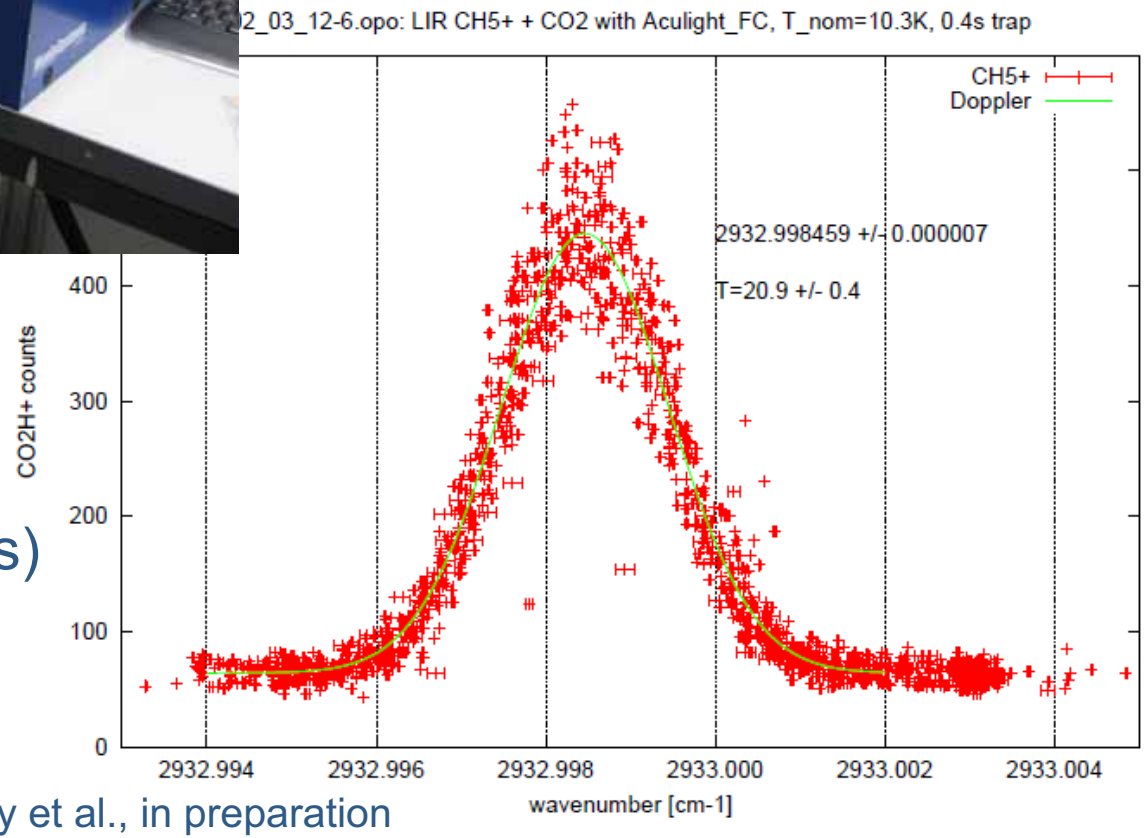


Laboratory & Model MHz	Observation MHz	Δ MHz
201751.537(1339)	201754.2	2.66
278691.849(868)	278691.8	-0.05

Lis et al., ASPCS 417 (2009); E. Roueff

Towards higher (microwave!) accuracy in the IR

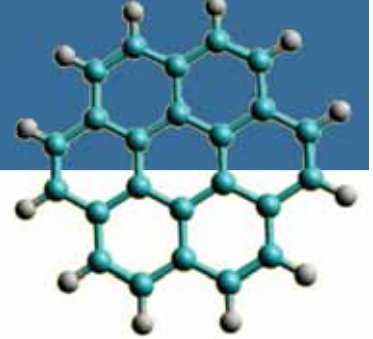
Accuracy: 2.3×10^{-9}

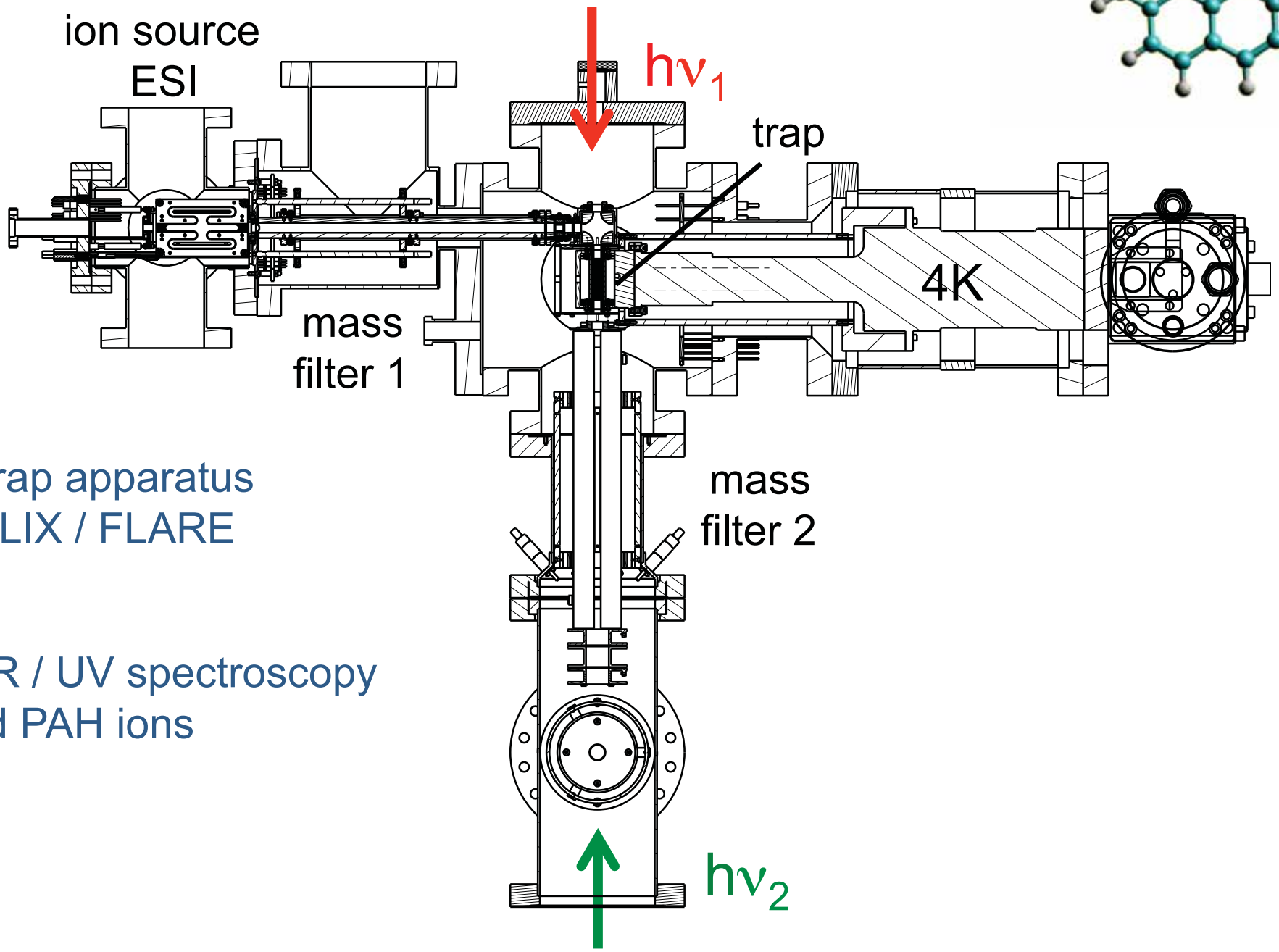


Calibration: Wavemeter & Frequency Comb (Menlo Systems)

Asvany et al., in preparation

Spectroscopy of PAH ions – FELION

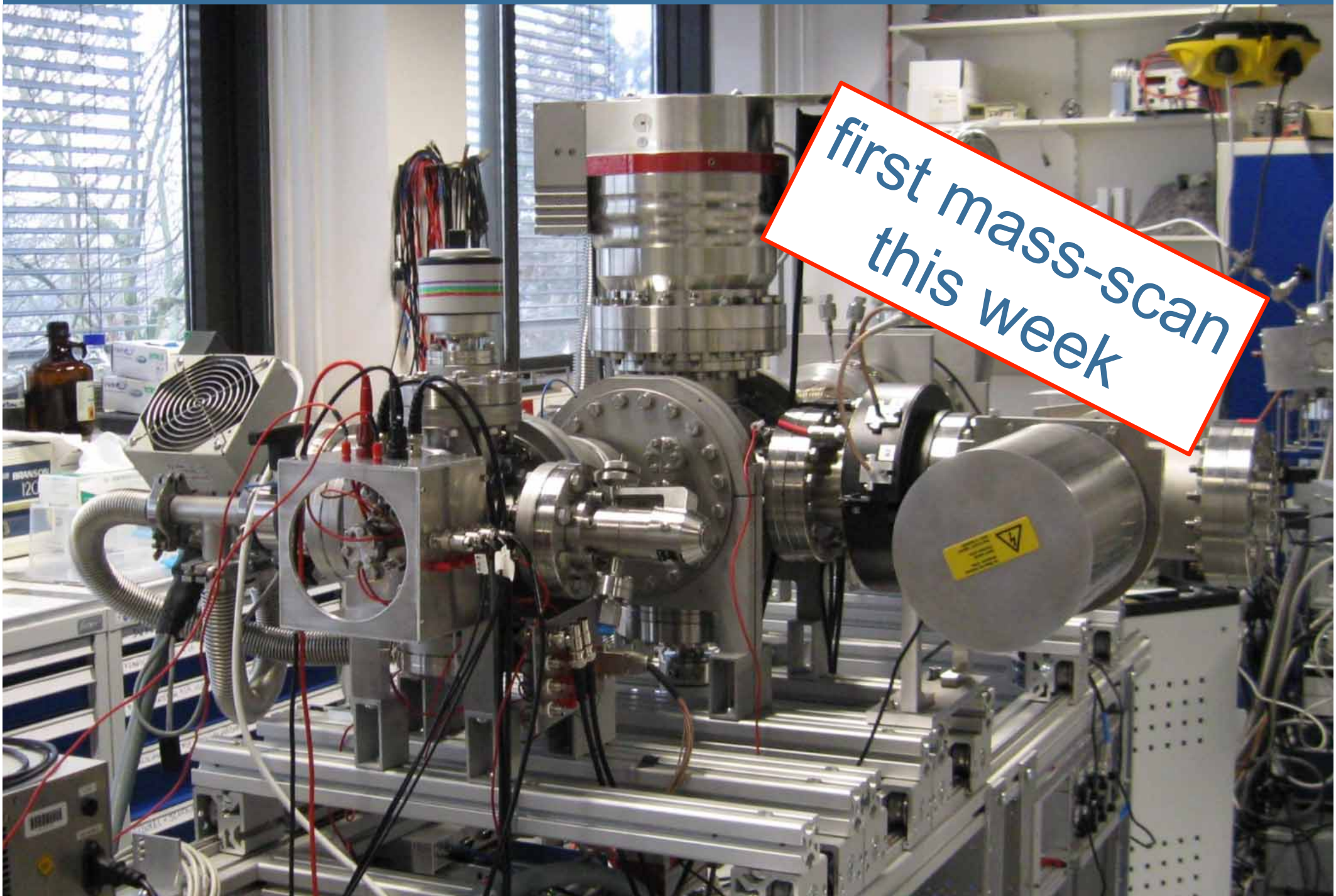




New trap apparatus
for FELIX / FLARE

IR & IR / UV spectroscopy
of cold PAH ions

Spectroscopy of PAH ions - FELION



Cologne Laboratory Astrophysics Group 2011

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