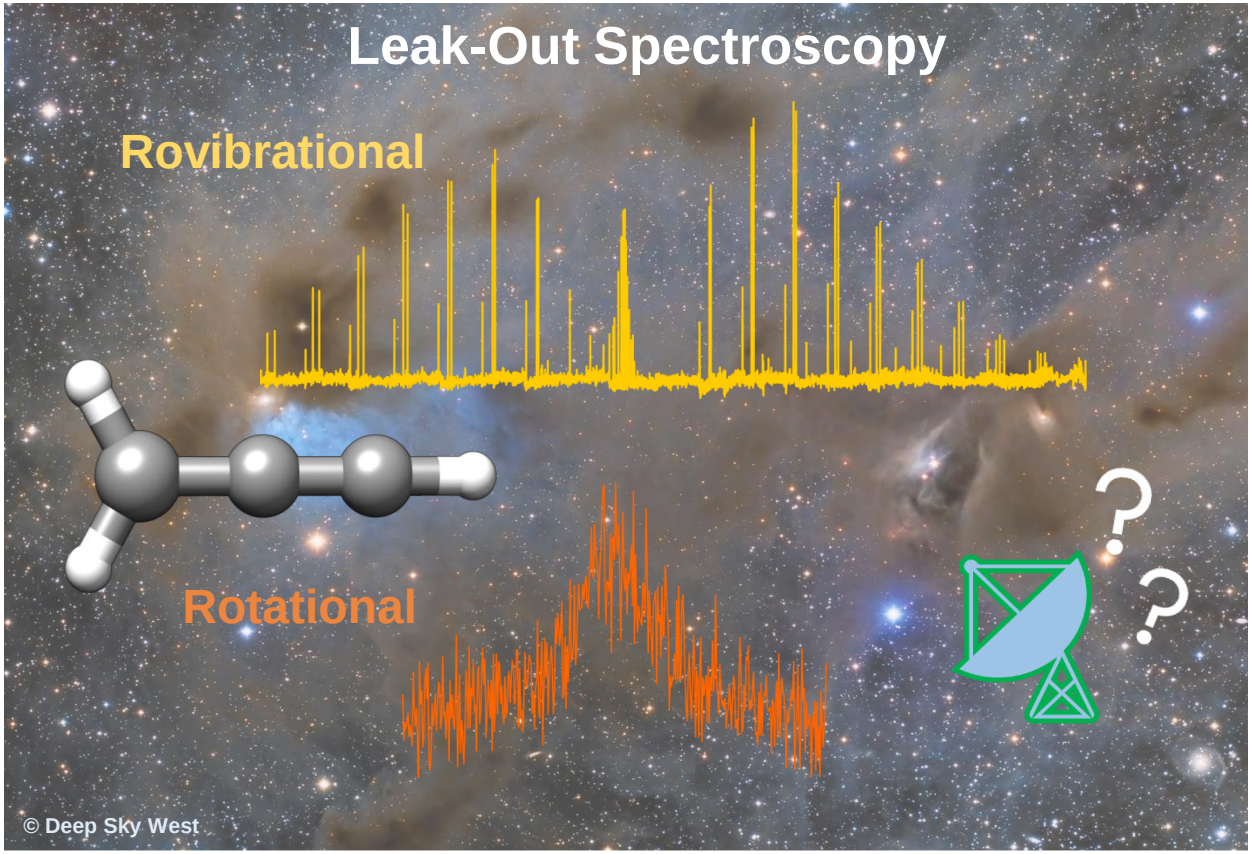
Vibrational and Rotational Action Spectroscopy of H_2CCCH^+



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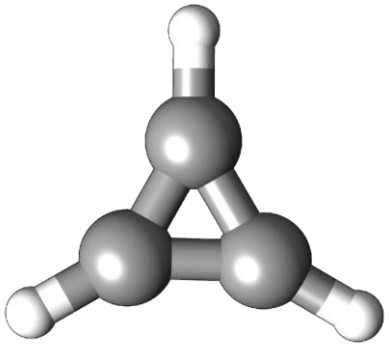
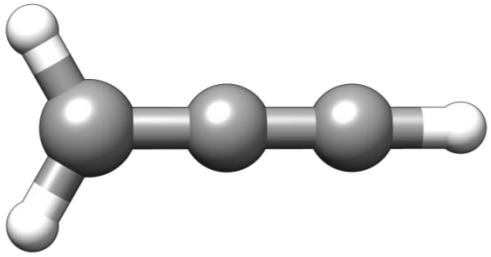
Ions in space and the $C_3H_3^+$ story

- Key intermediates for chemical evolution
- Ions ~15% of molecules detected in ISM
- Lack of experimental data on bare ions



Cyclopropenyl cation
c-$C_3H_3^+$



Propargyl cation
H_2CCCH^+

Formation of neutrals via $C_3H_3^+$

$$c\text{-}C_3H_3^+ + e^- \longrightarrow \boxed{c\text{-}C_3H} + H_2$$
$$c\text{-}C_3H_3^+ + e^- \longrightarrow \boxed{c\text{-}C_3H_2} + H$$

$$l\text{-}C_3H_3^+ + e^- \longrightarrow \boxed{l\text{-}C_3H} + H_2$$
$$l\text{-}C_3H_3^+ + e^- \longrightarrow \boxed{l\text{-}C_3H_2} + H$$

Sipilä *et al.*, A&A, 591, L1 (2016)

Produced from C_3H^+

$$\boxed{C_3H^+} + \boxed{H_2} \longrightarrow c/l\text{-}C_3H_3^+ + h\nu$$

Savic, I., Gerlich, D., PCCP, 7, 1026 (2005)

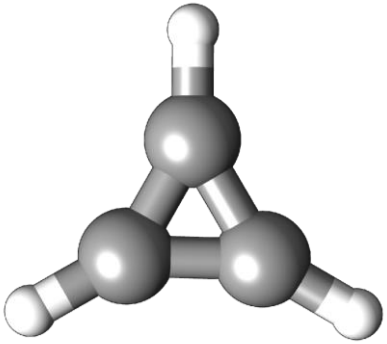
CDMS: https://cdms.astro.uni-koeln.de

Census 2021: McGuire B.A., ApJS, 59, 30 (2022)

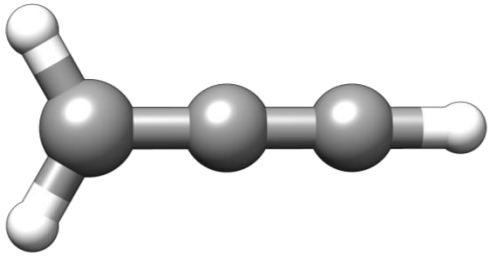
Previous knowledge on $C_3H_3^+$

2002 - 2020: IRPD– both isomers seen

- Ne, Ar, H_2, O_2, N_2, CO_2 - Messenger Tags (band origins)



D_{3h} symmetry
Non-permanent dipole moment



C_{2v} symmetry
μ_a = 0.52D (Calculated)

a) High-resolution IR - ν_4 (C-H anti-symmetric stretch)

Zhao *et al*., ApJL, 791:L28, 2014

b) *c*-$C_3H_2D^+$ (C_{2v}): Vibrational and rotational spectroscopy

- μ_a= 0.23D
- Low column density in TMC-1

Gupta *et al*., Faraday Discuss, 2023, Advanced Article

No high-resolution vibrational and rotational spectroscopy reported yet

IRPD studies: 1. Roth, D., Dopfer, O., *PCCP*, 4, 4855 (2002); **2.** Dopfer, O., Roth, D., & Maier, J. P. *JACS*, 124, 494 (2002); **3.** Ricks, A. et al., *JCP*,132, 051101; **4.** Botschwina, P., et al., *PCCP*, 13, 14163 (2011); **5.** Botschwina, P., et al., *PCCP*, 13, 7921 (2011); **6.** Marimuthu, A. N., et al., *JMS*, 374, 111377 (2020)

Cryogenic Ion Trap and Leak-Out Spectroscopy

COLTRAP T= 4K

light source
IR, mm-wave

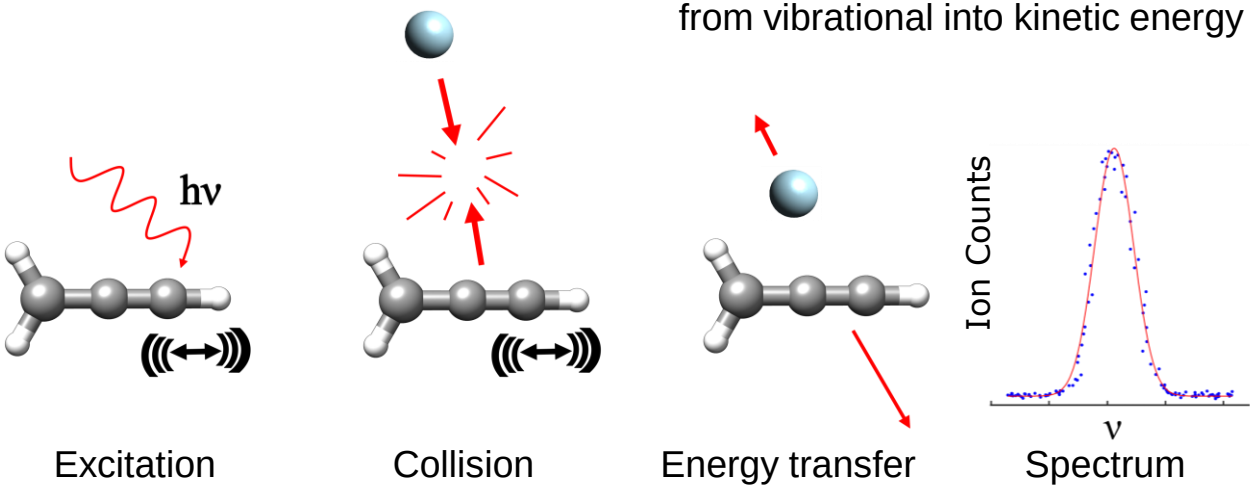
source → mass filter → trap → mass filter → detector

allene (C_3H_4) | 39 u | $C_3H_3^+$ ions | 39 u

1:3 Ne:He mixture

LOS scheme

Escape of trapped ions after collision-induced transfer from vibrational into kinetic energy

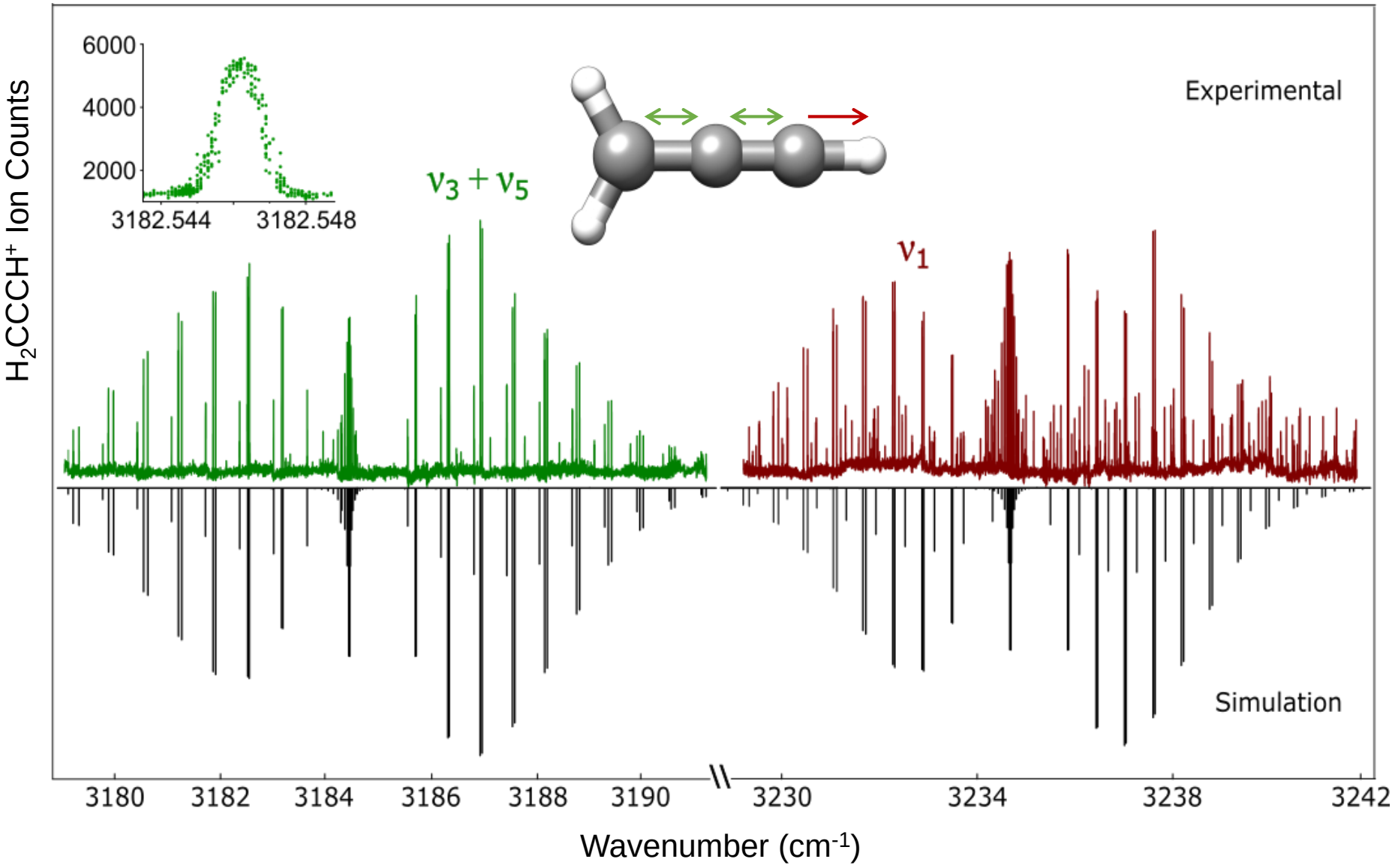


Excitation | Collision | Energy transfer | Spectrum

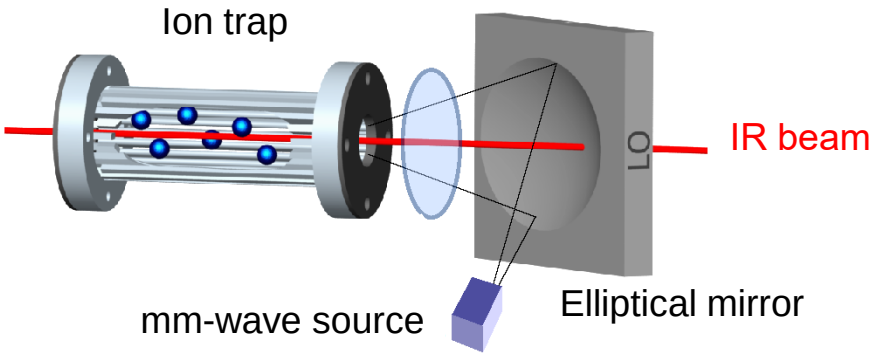
COLTRAP: Asvany, O., Brünken, S., Kluge, L., Schlemmer, S., *Appl. Phys. B*, 124, 203 (2014)

LOS: Schmid, P. C., Asvany, O., Salomon, T., Thorwirth, S., Schlemmer, S. JPCA, 126, 43 (2022)

Rovibrational Spectroscopy

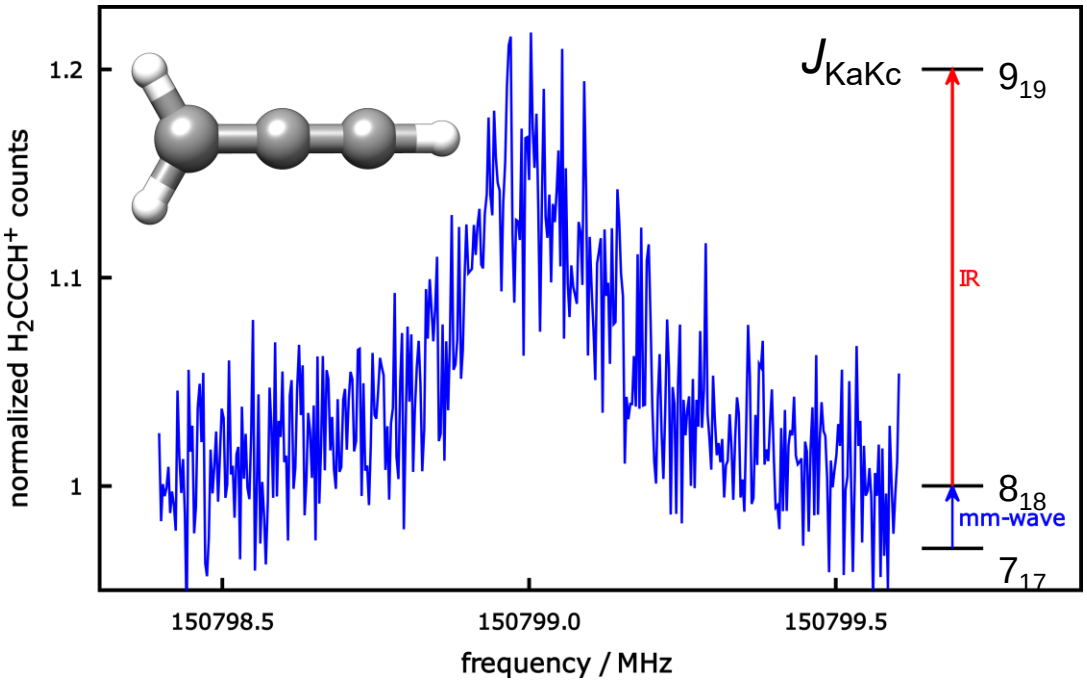


Double-Resonance Vibrational-Rotational Spectroscopy



Double-resonance: Asvany, O., Schlemmer, S. *PCCP*, 23, 26602 (2021)

Double-resonance + LOS: Asvany, O., et al., *PCCP*, Submitted (2023)

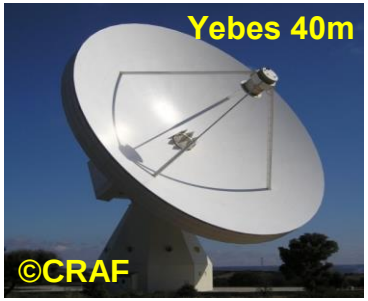


- 14 pure rotational lines
  - 94–192 GHz

Radio Astronomical Searches in TMC-1

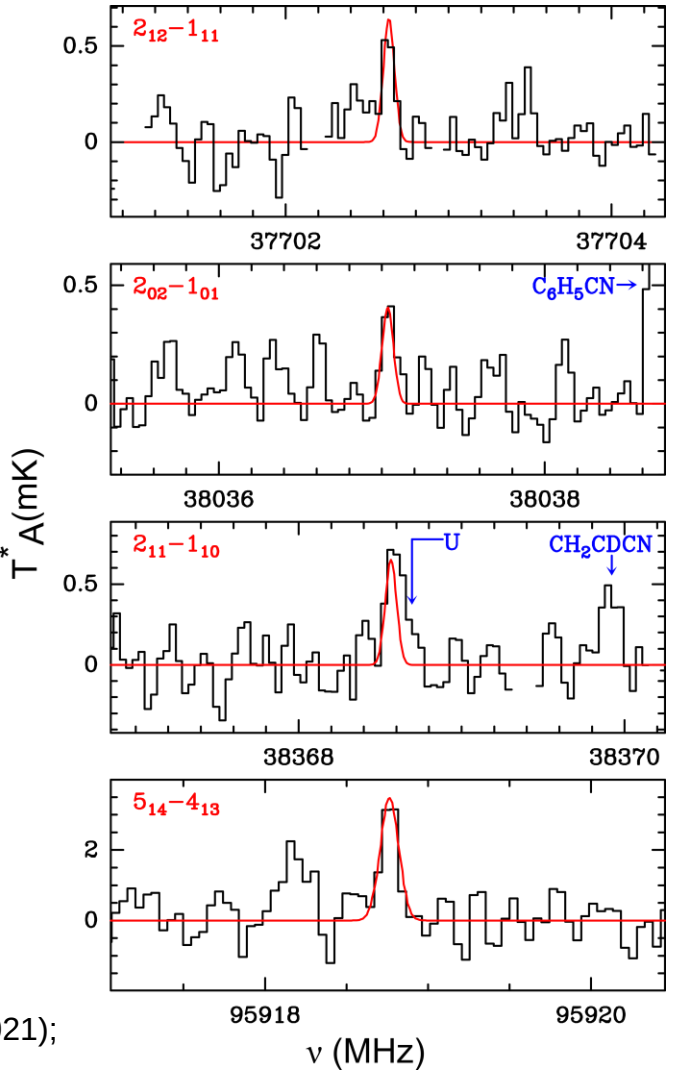
Q-band **U**ltrasensitive **I**nspection **J**ourney to the **O**bscure **T**MC-1 **E**nvironment (**QUIJOTE**)

José Cernicharo's Group (Spain)



Sensitivity= 0.17-0.25 mK
Frequency= 31.0–50.3 GHz (Q-band)
Resolution= 38.15 kHz

Sensitivity= 2-10 mK
Frequency: ~71-119 GHz (3 mm region)
Resolution= 40-49 kHz



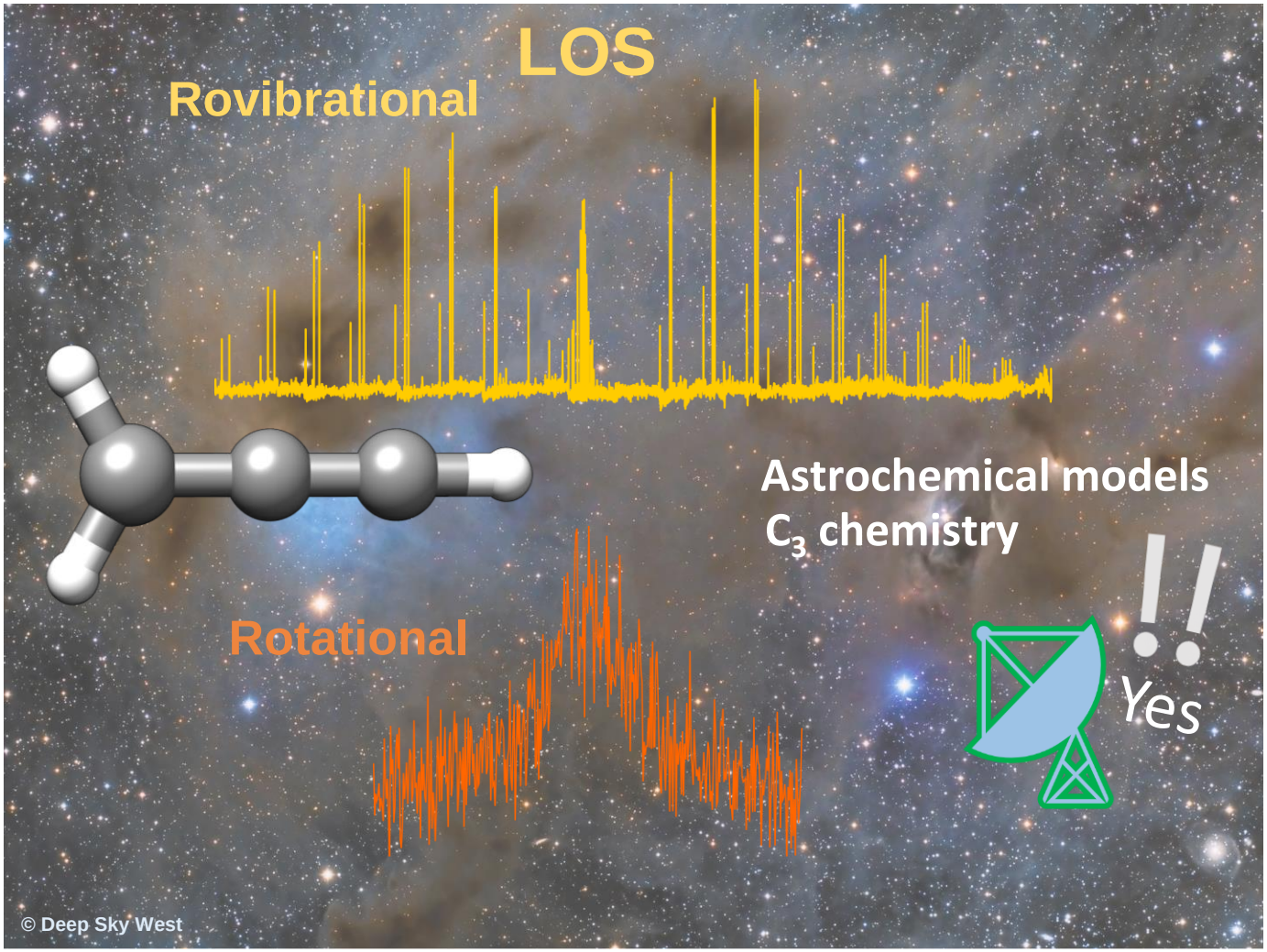
Column density (H_2CCCH^+)= 7.8(1.5)x10^{11} cm^{-2}

n(H_2CCC)/n(H_2CCCH^+) = 2.5(0.7)

Detection of H_2CCCH^+ in TMC-1, *Submitted to A&A*, (2023)

QUIJOTE: **1.** Cernicharo, J., Agúndez, M. Kaiser, R., *et al.*, *A&A*, 652, L9 (2021);
2. Cernicharo, J., Pardo, J., Cabezas, C. *et al.*, *A&A*, 670, L19 (2023)

Take-Home Summary



Acknowledgements

Thank you for listening!!

Cologne group (Laboratory Astrophysics)
https://astro.uni-koeln.de/schlemmer/research

Laboratory Team (Uni. Cologne)

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Divita Gupta
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P. de Vicente (OAN, IGN, Spain)
J.-C. Loison (CNRS, France)
V. Wakelam (CNRS, France)
W. Kim (University of Cologne, Germany)

Funding Agencies

Alexander von HUMBOLDT STIFTUNG
University of Cologne
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