What's Out There and How Do We Know? An Overview of Astrochemistry

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Assoc. Prof. of Chemistry
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III Chilean Astrochemistry School, November 28, 2022

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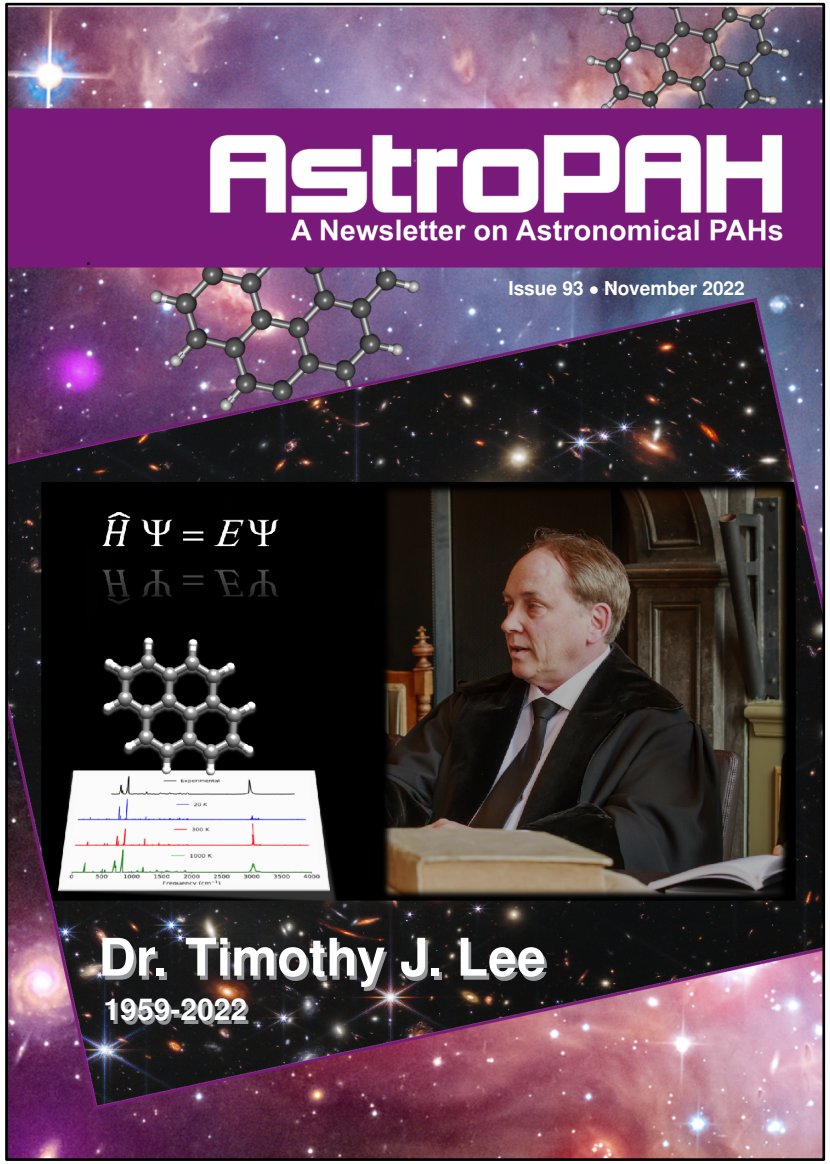

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Chapter 7

Vibrational and Rovibrational Spectroscopy Applied to Astrochemistry

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7.1. Introduction

Quantum chemistry and electronic structure theory have played a crucial role in the detection of molecules in space largely since molecules have been detected in space. In the early- and mid-1970s radioastronomical observations were increasing the census of extraterrestrial molecules nearly from zero. Observation of the protonated nitrogen cation (N_2H^+) was among the first detection studies and also among the first that utilized the self-consistent field (SCF) Hartree–Fock (HF) approach to compute an equilibrium geometry and provide corresponding rotational constants for comparison to astronomically derived spectral constants.[1,2] Similarly, detections of C_2H, C_4H, and C_3N also employed a similar approach utilizing quantum chemical *ab initio* theoretical data for corroborating evidence of detection.[3–5] During this era, the famed "X-ogen" lines were reported,[6] but these lines were conclusively linked to HCO^+ by Herbst and Klemperer[7] once more through the use of corroborating

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Chapter Six - Computational vibrational spectroscopy for the detection of molecules in space

Ryan C. Fortenberry [a], Timothy J. Lee [b]

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Electronic Structure

ACCEPTED MANUSCRIPT

Reparameterized semi-empirical methods for computing anharmonic vibrational frequencies of multiply-bonded hydrocarbons

Brent R. Westbrook[1], Joshua P. Layfield[2], Timothy Lee[3] and Ryan Fortenberry[1]

Accepted Manuscript online 18 November 2022 •

What is an Accepted Manuscript?

DOI 10.1088/2516-1075/aca458

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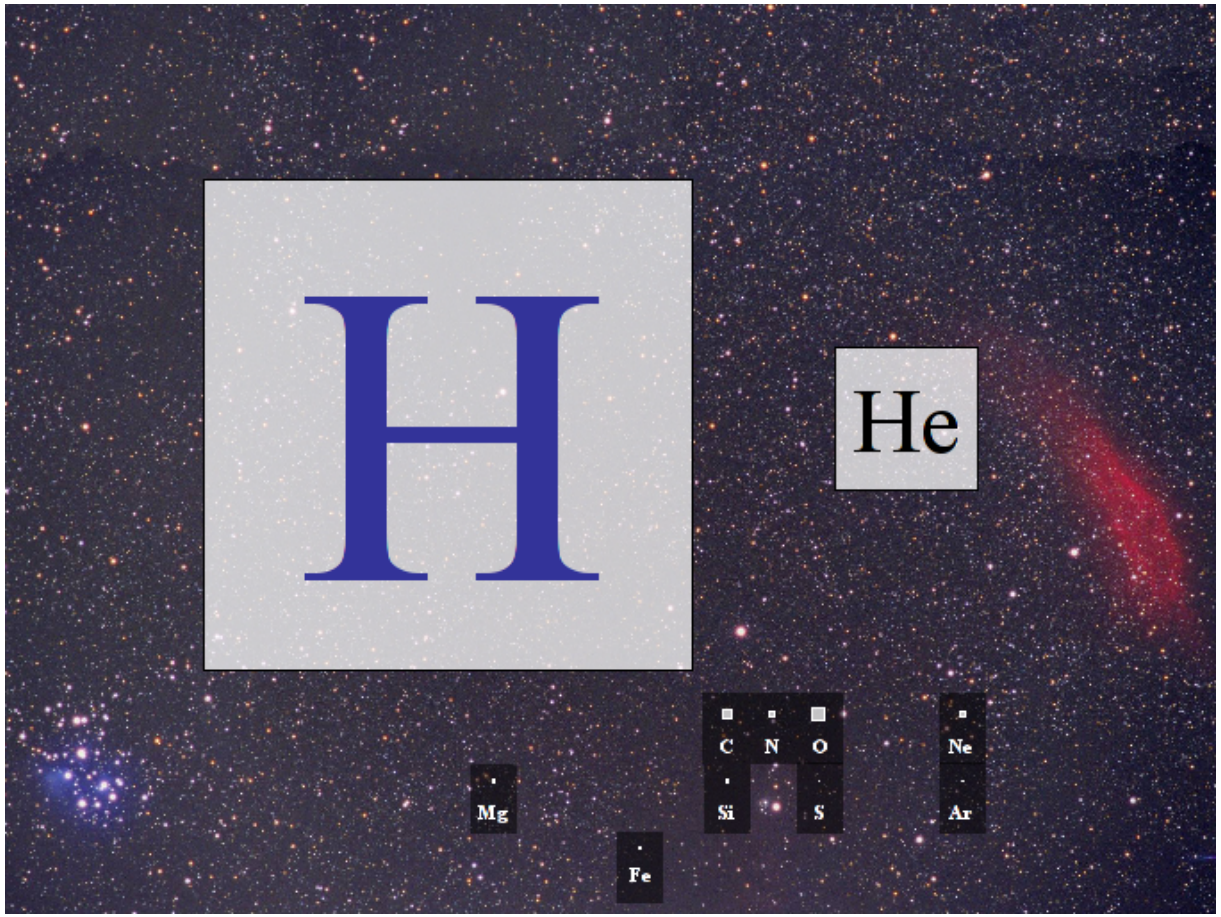
Astronomer's Periodic Table

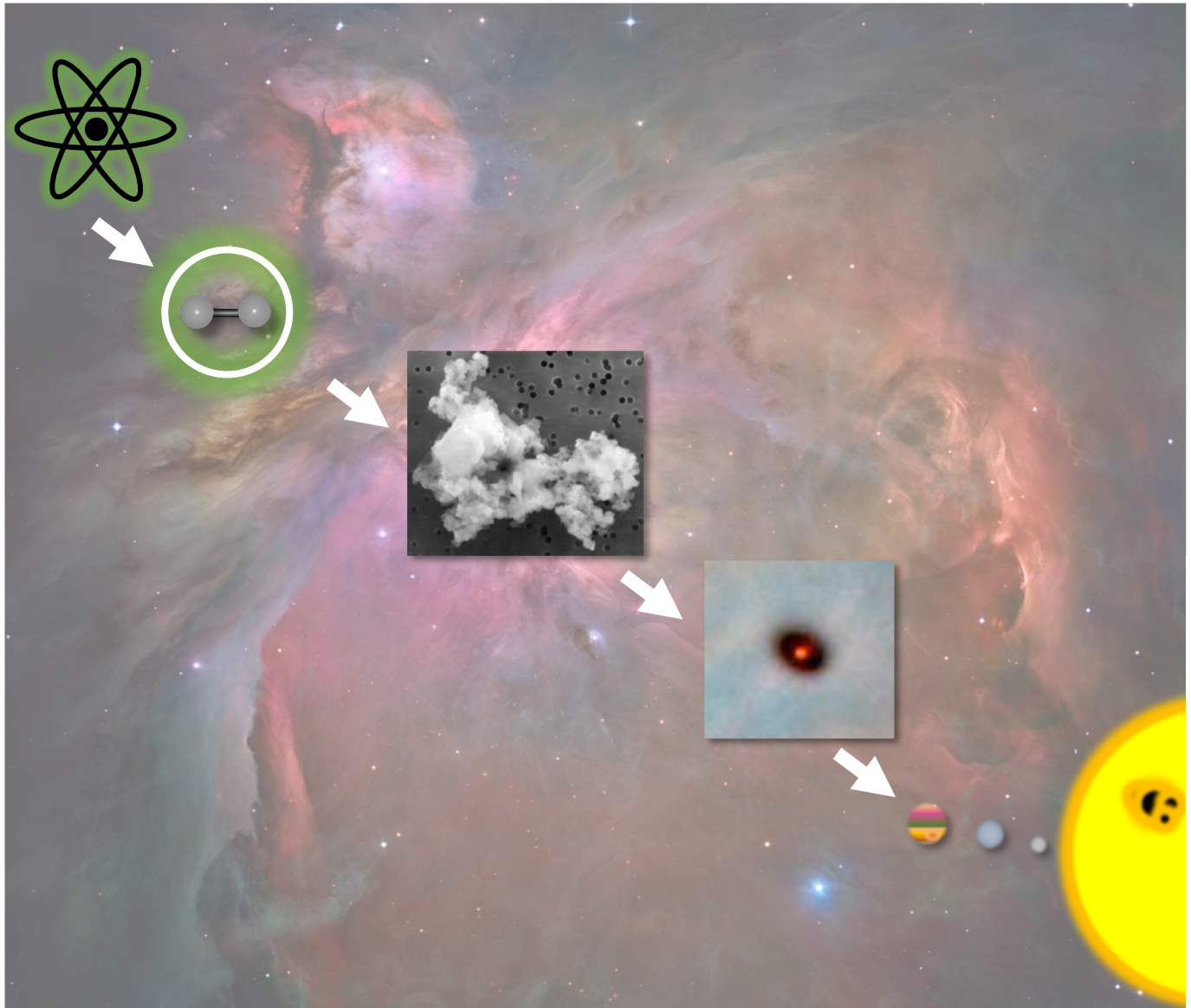
Tabla Periódica del Astrónomo

Tabla Periódica del Astróquimica

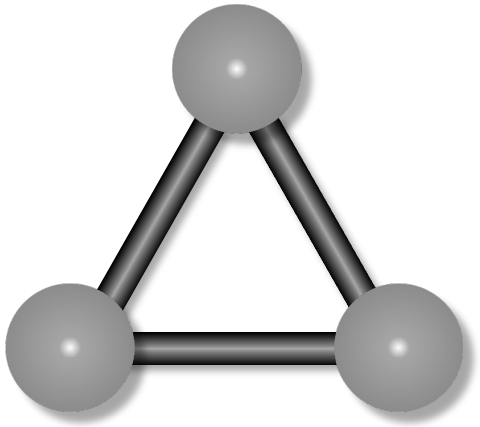


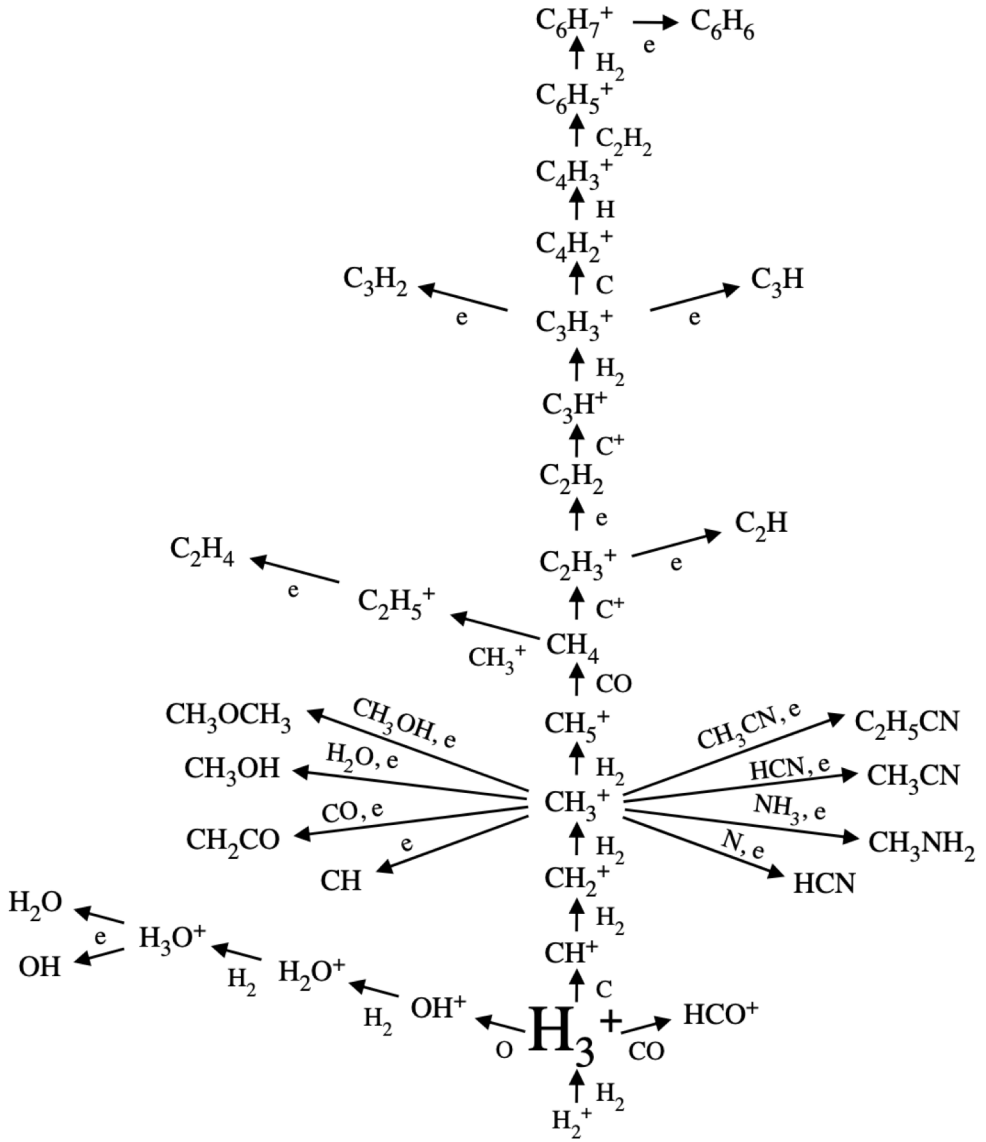
McCall et al., *PTRSA*, **364**, 2953, (2006).

Astro “chemistry”



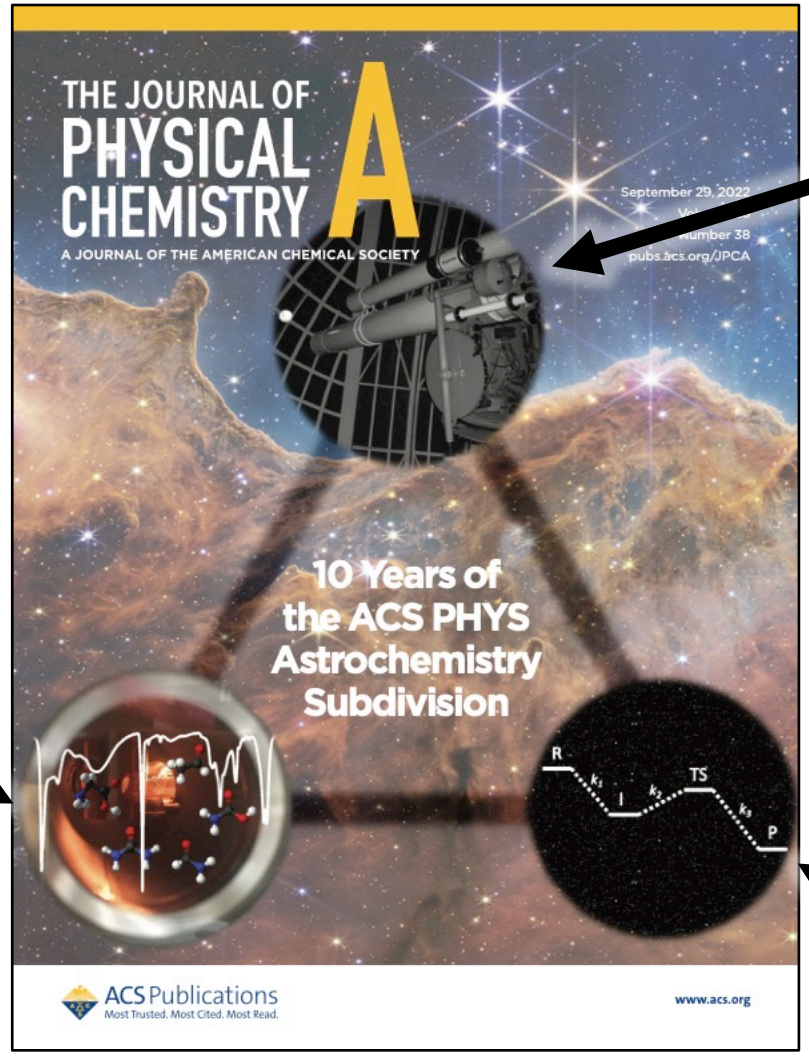
Astro “chemistry”





McCall et al., *PTRSA*, **364**, 2953, (2006).

“Pyramid” of Astrochemistry

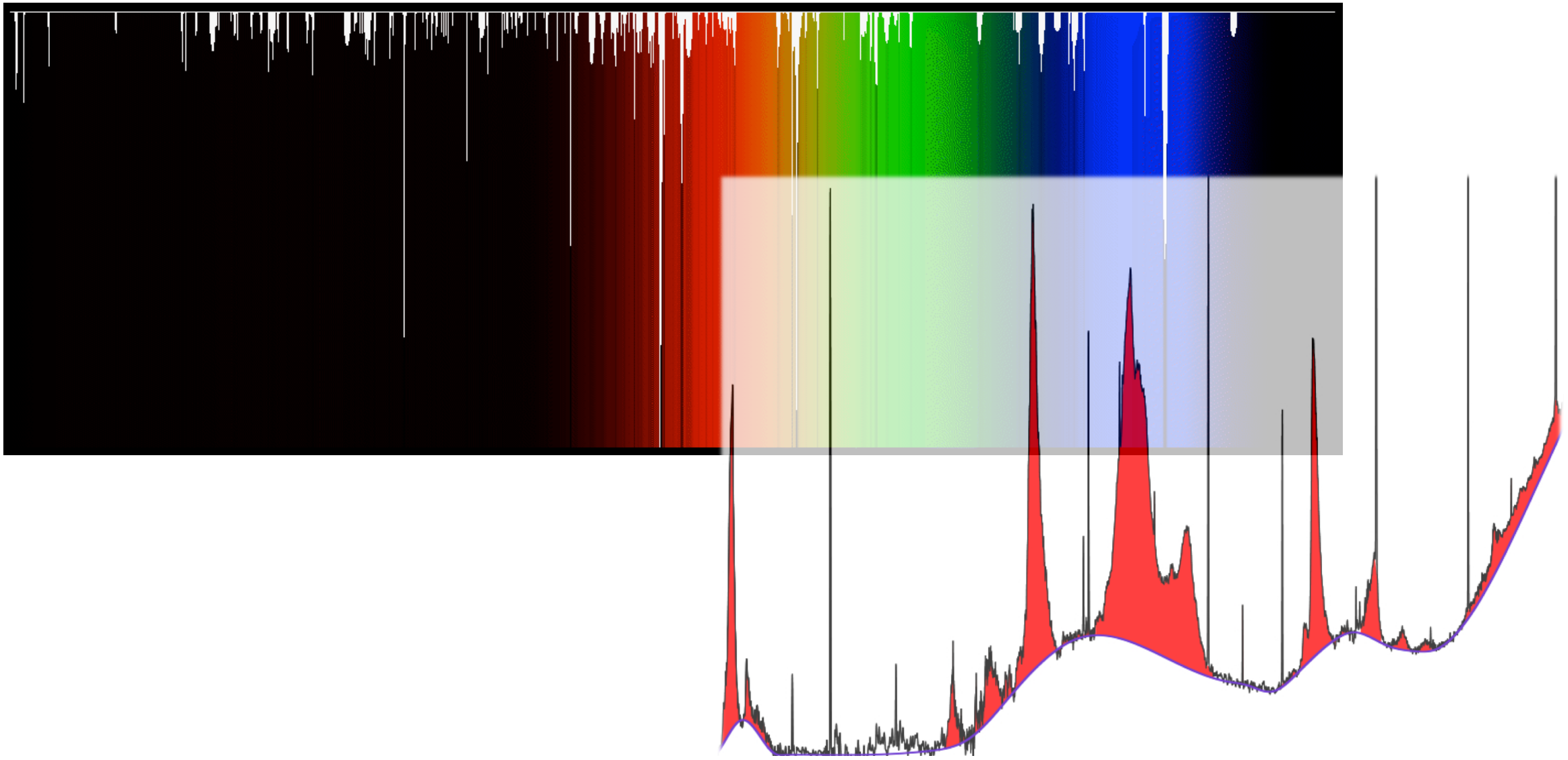


Observation

“Lab” Astro

Modeling

Observation



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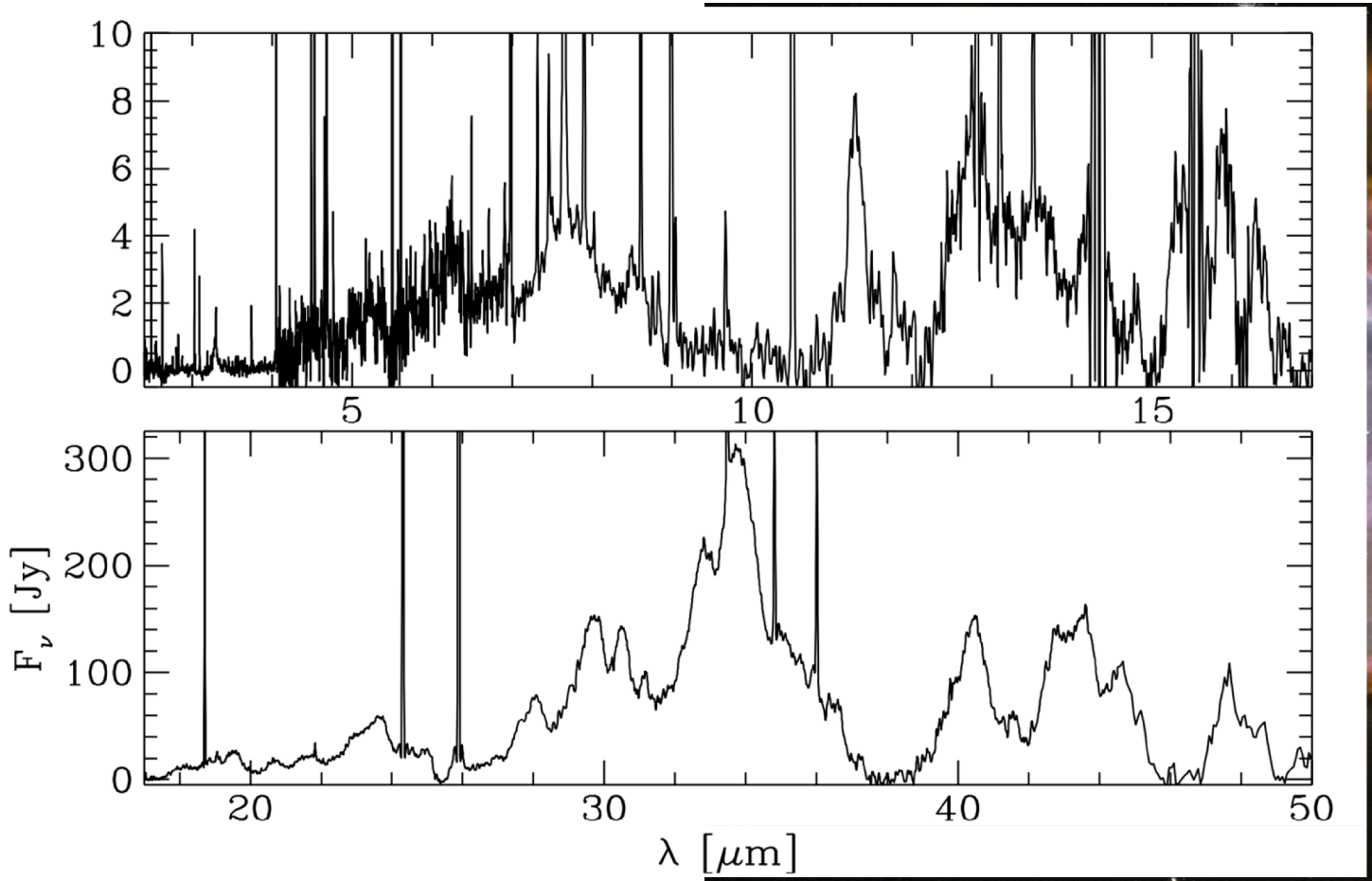

F. J. Molster, et al., *Astron. Astrophys.*, **372**, 165 (2001).


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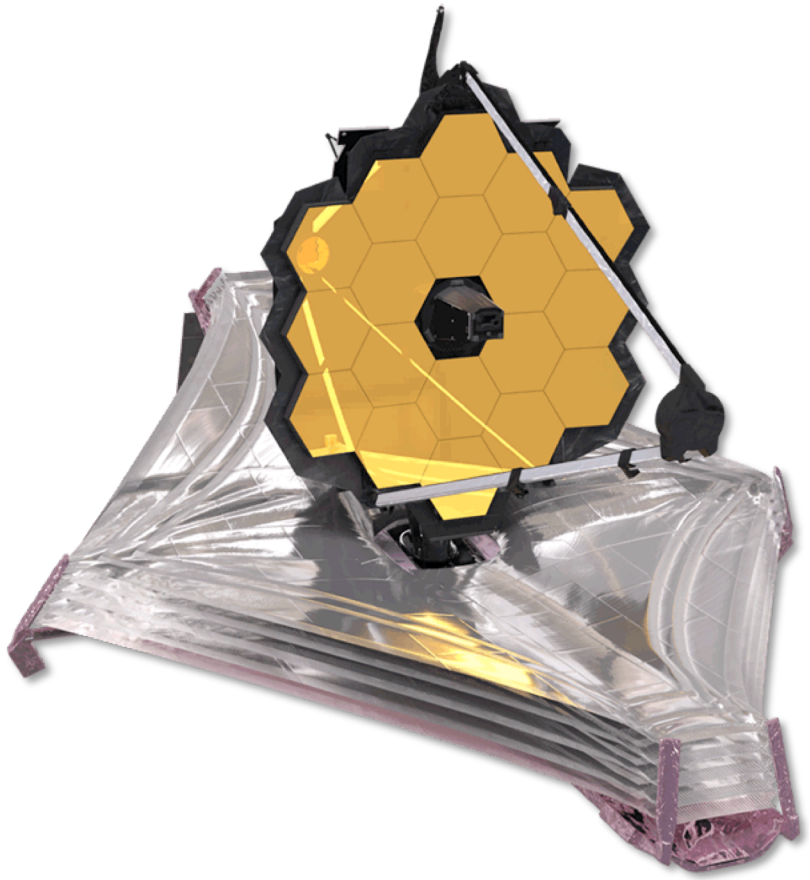
Observation



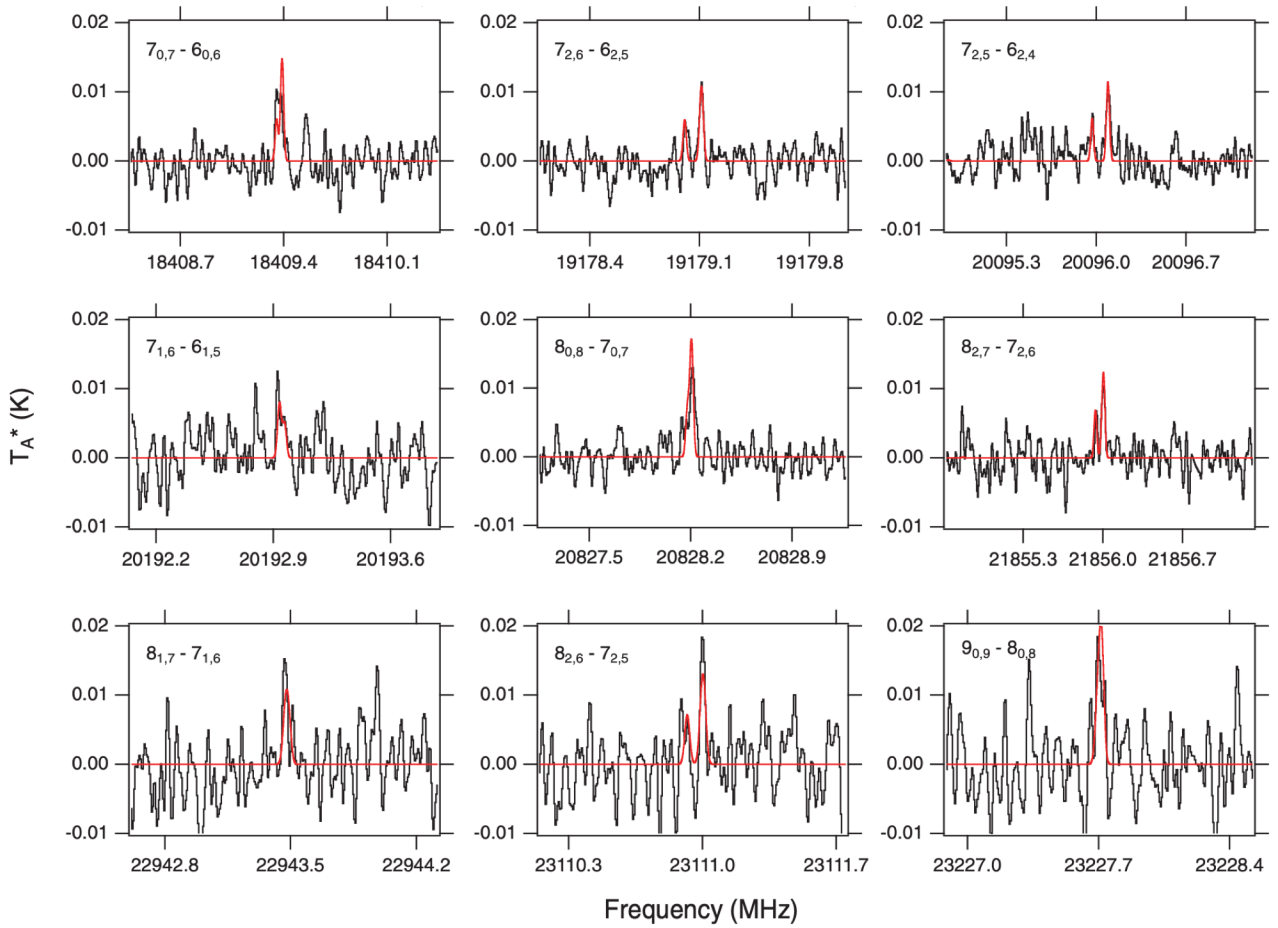
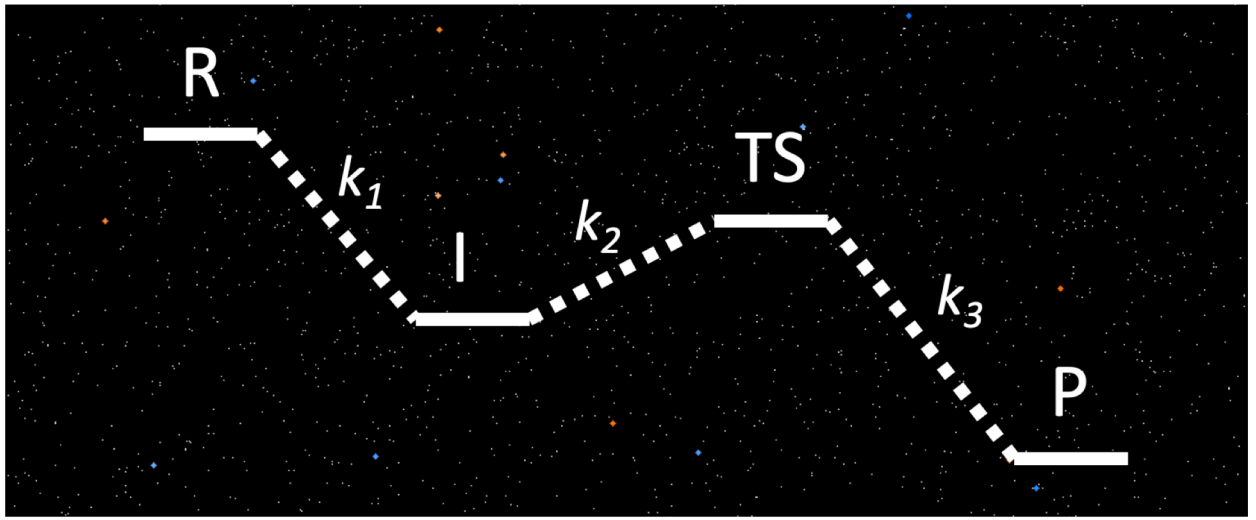


Fig. 2. Detected emission lines of benzonitrile in TMC-1. Observational spectra are shown in black smoothed to a resolution of 5.7 kHz (0.08 km s^{-1}) and shifted to a v_{lsr} value of 5.83 km s^{-1}. A simulated spectrum of benzonitrile (linewidth = 0.4 km s^{-1}, N_T = 4 × 10^{11} cm^{-2}, T_{ex} = 7 K) is overlaid in red (*25*). Rotational quantum numbers are displayed at the upper left of each panel. The four transitions with well-resolved hyperfine structure are shown on an expanded frequency axis in (*25*).

Observation

Observation + Modeling

$$A = \varepsilon b c$$



Lab Astro: Primero Parte

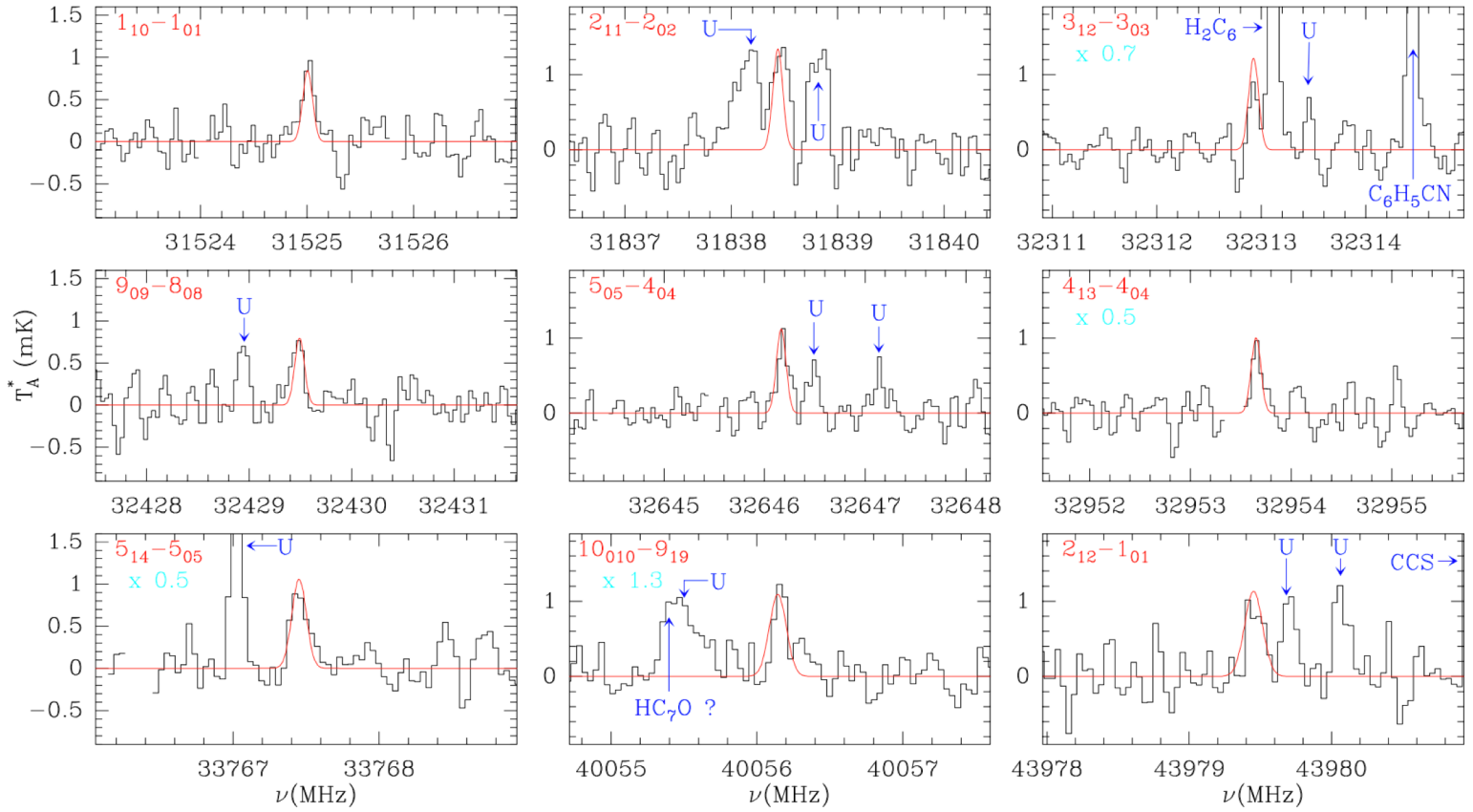
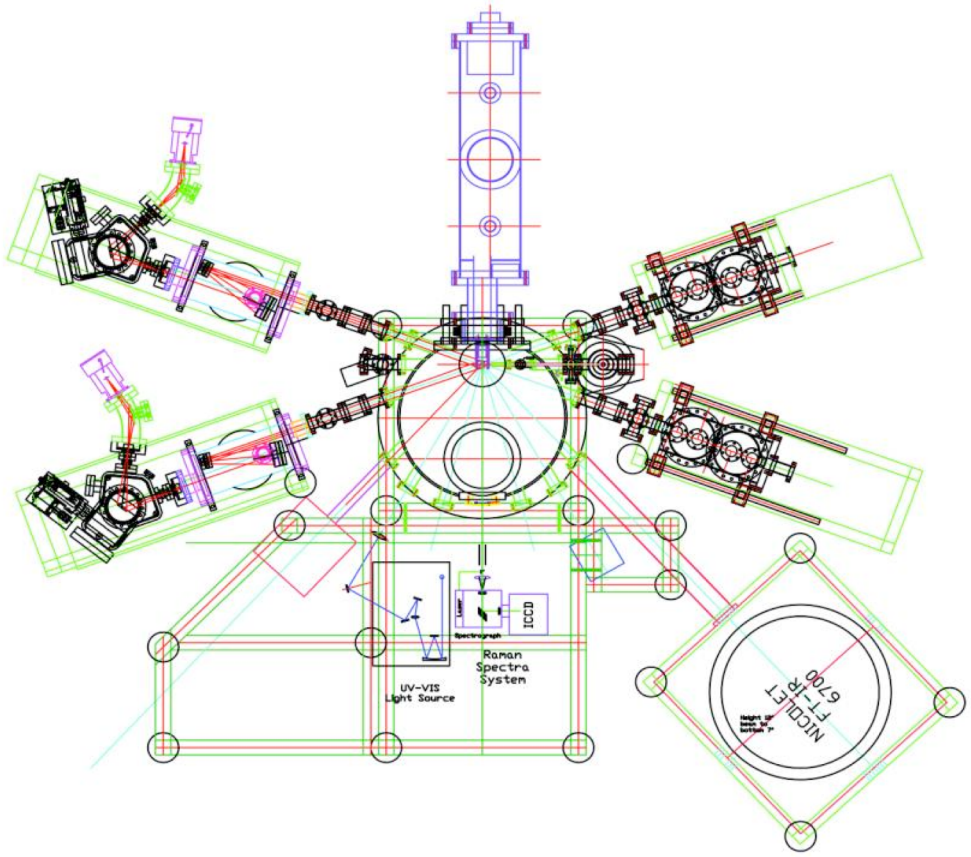
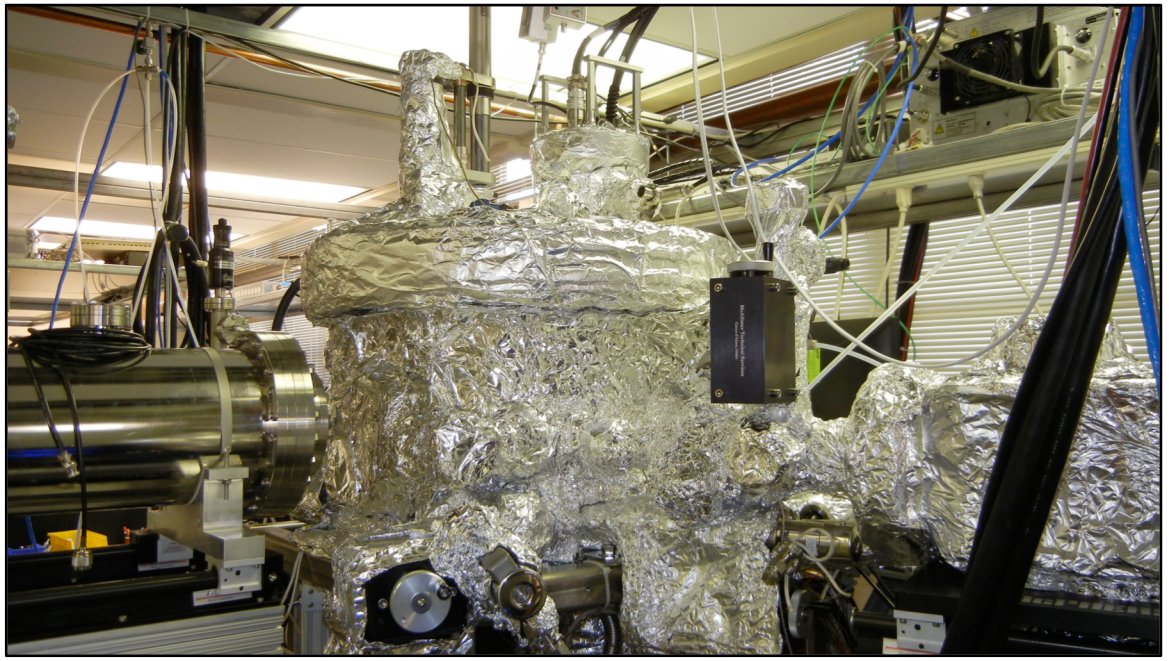


Fig. 2. Selected transitions of *c*-C_3HCCH in TMC-1. The abscissa corresponds to the rest frequency of the lines, assuming a local standard of rest velocity of the source of 5.83 km s^{-1}. Frequencies and intensities for the observed lines are given in Table A.1. The ordinate is the antenna temperature, corrected for atmospheric and telescope losses, in millikelvins. The quantum numbers for each transition are indicated in the upper left corner of the corresponding panel. The red lines show the computed synthetic spectrum for this species for $T_r = 10$ K and a column density of 3.1×10^{11} cm^{-2}. Cyan labels indicate the multiplicative factor applied to the model to match the intensity of the observed lines.

Lab Astro: Segundo Parte





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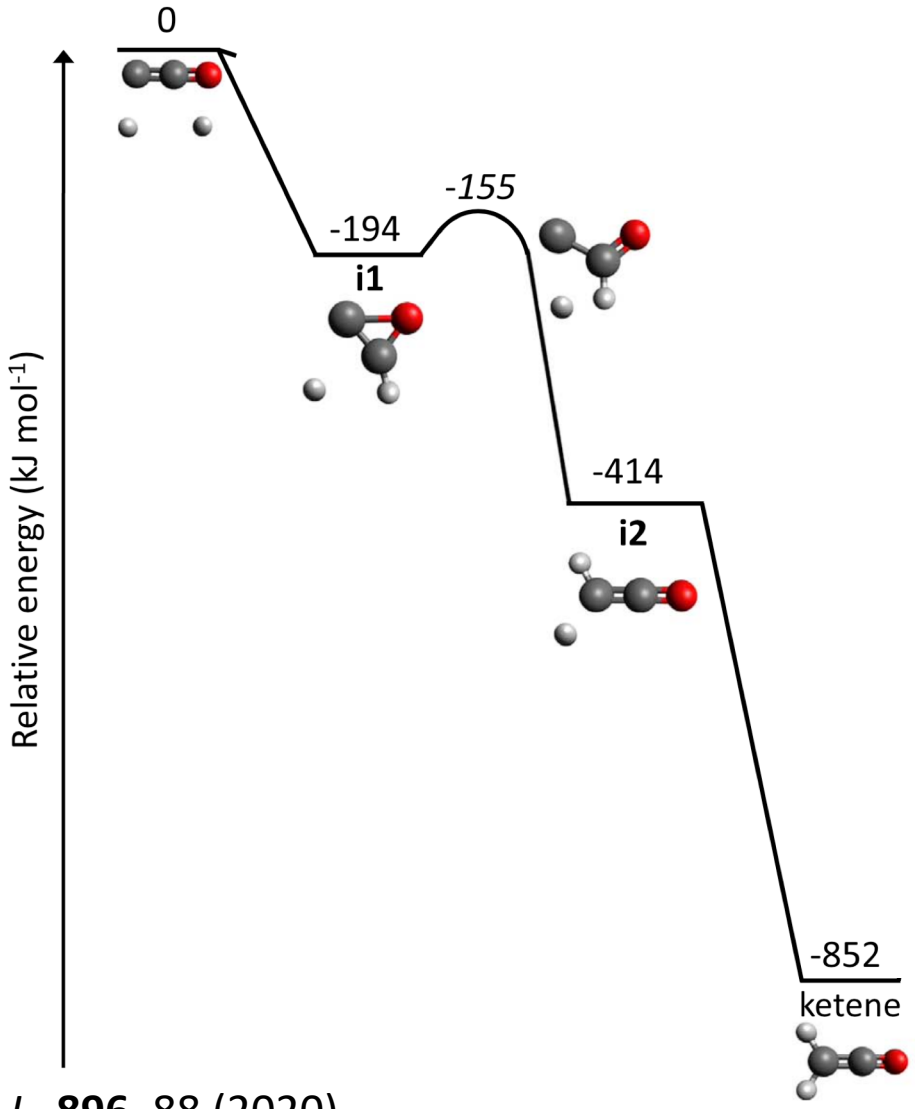
Lab Astro: Theory



Turner, A. M. et al., *Astrophys. J.*, **896**, 88 (2020).

Lab Astro: Theory

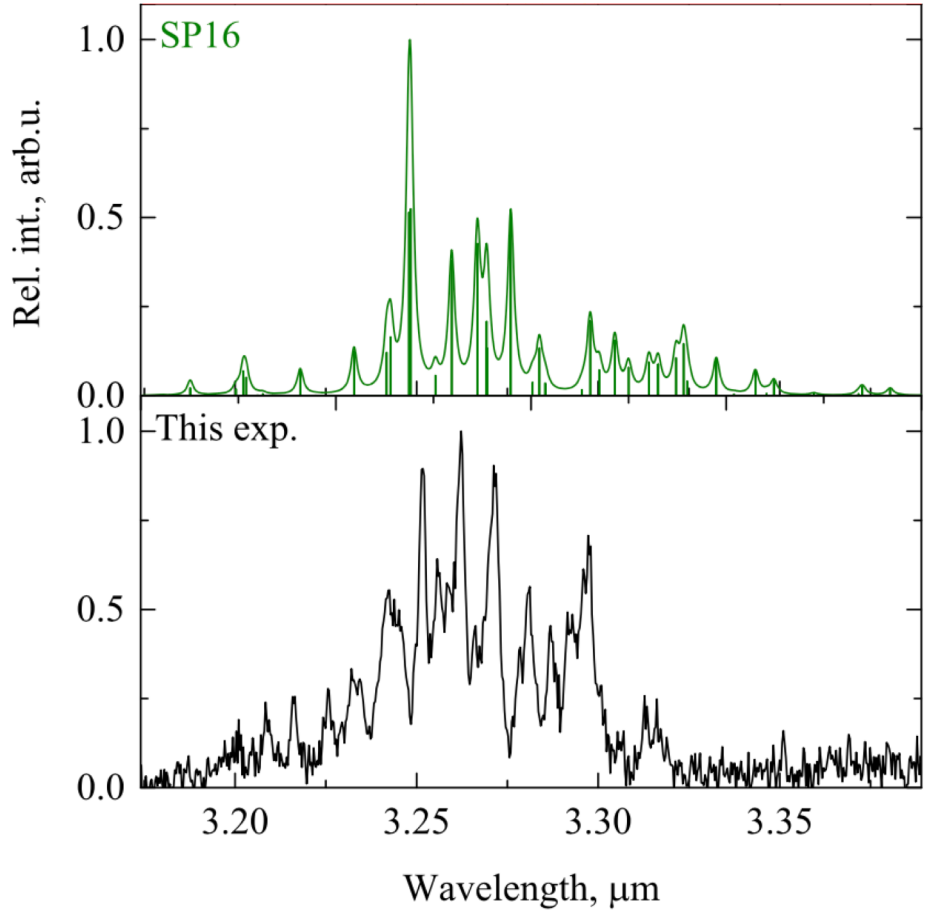
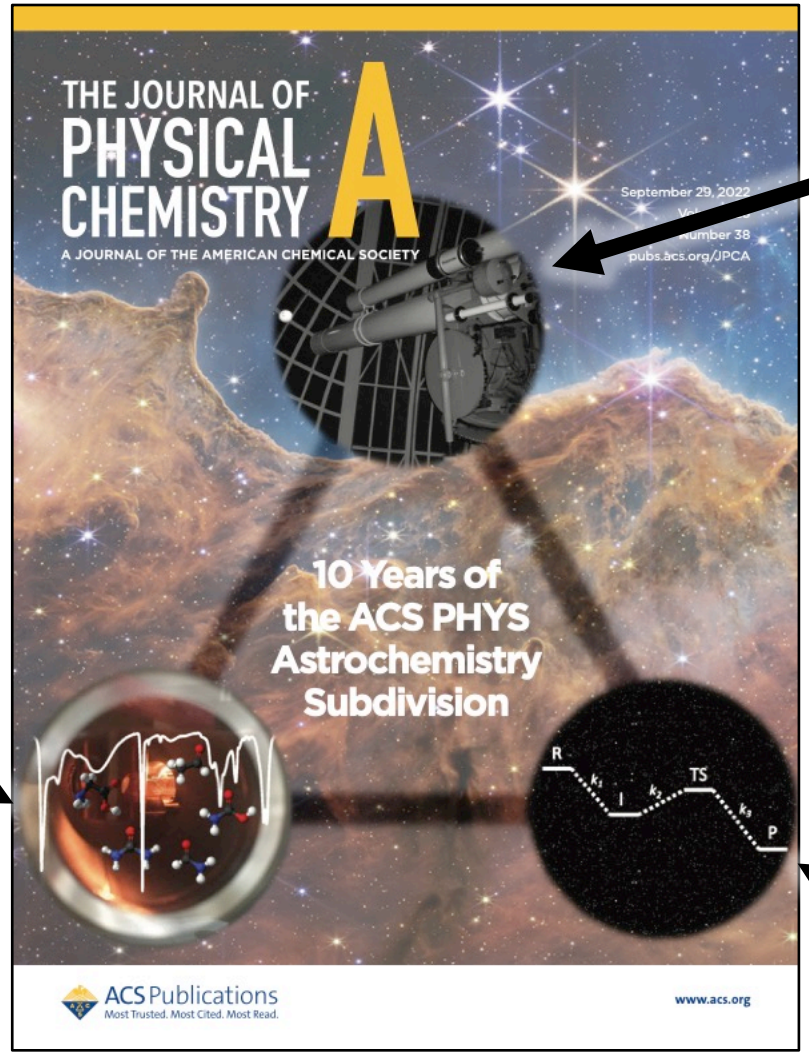


Figure 1. IR absorption spectrum of phenanthrene as predicted by G09-h (scaling factor sf = 0.961) and SP16 calculations (not scaled) together with the molecular beam gas-phase spectrum as measured in the present experiments. The number of hydrogens is mentioned in the following order: solo/duo/trio/ quartet/bay H's. See Figure 8 for more details.

Maltseva, E. et al., *Astrophys. J.*, **831**, 58 (2016).

“Pyramid” of Astrochemistry



Observation

“Lab” Astro

Modeling

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Ryan C. Fortenberry

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