Interstellar chemistry

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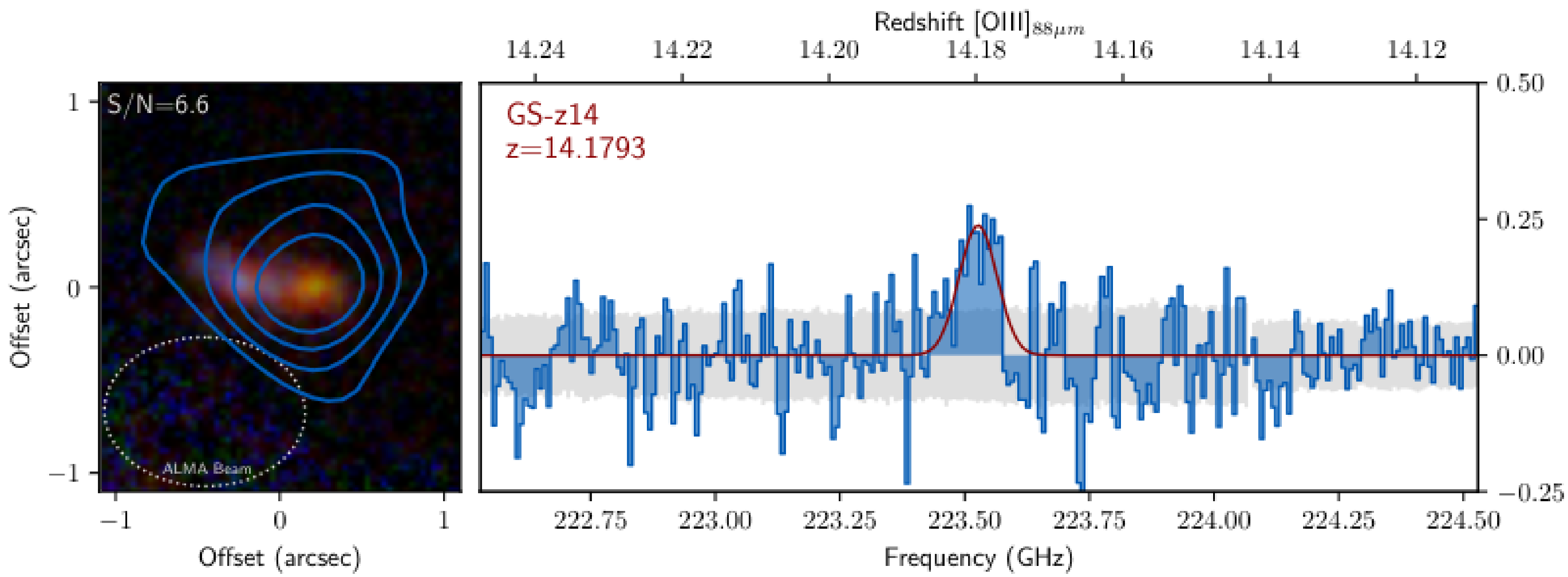
1 The chemical history of the universe

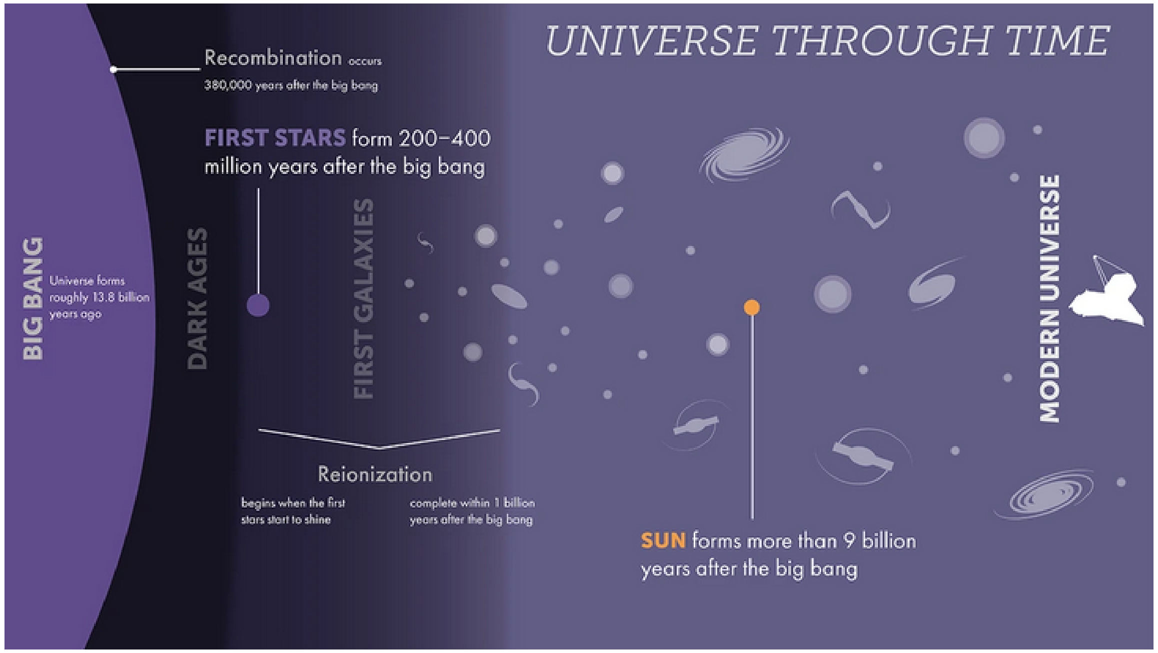


Schouws+25, Carniani+24, Helton+2025

▷ Universe was 300 Myr; metallicity ~ 0.05-0.2 solar
  - challenging our understanding of the formation of first stars

▷ ALMA-JWST synergy

The astrochemical ladder



- ▷ Infer chemical properties of primordial objects
- ▷ From local to distant astrochemistry
  - Solar system objects (Sun, planets, meteorites, pre-solar grains, etc)
  - Solar neighborhood (stars, star and planet forming regions, molecular clouds)
  - Milky Way
  - MW Satellites
  - Local Group
  - Lyman-break galaxies

2 From observations to physics and chemistry

- ▷ Dual aspects of interstellar chemistry
  - Thermodynamics remote sensing
  - Understanding the chemical evolution of the universe
- ▷ From lines to physics and chemistry
  - spectral lines: direct output
  - spectral lines = non-linear mixing of physics and chemistry
  - astrochemical and radiative transfer models
- ▷ Instrumental breakthroughs
  - ~300 interstellar species have been identified; ~90 in the last 4 years
  - **instantaneous bandwidth and high sensitivity**
    - large instantaneous bandwidth mitigates cross-calibration issues
    - make line ratios highly accurate (~5%)
- ▷ Observationally demanding
  - Heterodyne provides highest precision and accuracy for frequency
  - **Amplitude calibration**
    - critical, ~5% at IRAM-30m (20% commonly adopted)
    - standard observing procedures

Thermodynamics remote sensing

- ▷ equation of state: density, temperature
- ▷ magnetic fields intensity (Zeeman splitting, linewidth)
- ▷ ionization: ion-neutral drift, instabilities (e.g. MRI)
- ▷ fluid kinematics and dynamics: high-precision/accuracy Doppler shift velocities
- ▷ heating and cooling (endo- and exo-thermicity of reactions)

chemistry is needed to

- ▷ infer which tracer is best appropriate to some physical target
  - e.g. CF^+ tracing C^+ tracing ionization; CH^+, SH^+ tracing turbulence dissipation
- ▷ know which region is actually traced by a given species (e.g. CN in dense cores)
- ▷ ensure that different tracers are actually cospatial
- ▷ compute energy balance

References: Genzel (1992); Falgarone et al. (1994, 1998); Neufeld et al. (2006); Crutcher (2012); Godard et al. (2014); Hily-Blant et al. (2010)

Astrochemical models

- An array of processes
  - Gas phase processes (driven by ion-neutral reactions)
  - Gas-grain processes
    - Dust interplay (formation of H_2, Complex Organic Molecules)
  - Spectral lines and continuum observations work in tandem
- Chemistry is not in equilibrium
  - Kinetic chemistry is needed not just thermochemistry
- Chemical networks: from 10 to 100s of species, and ~10x more reactions
  - the art of astrochemical modelling: 50 years of work since first models
  - ISM chemistry is driven by ionization
  - kinetic rate coefficients often brought into an Arrhenius type

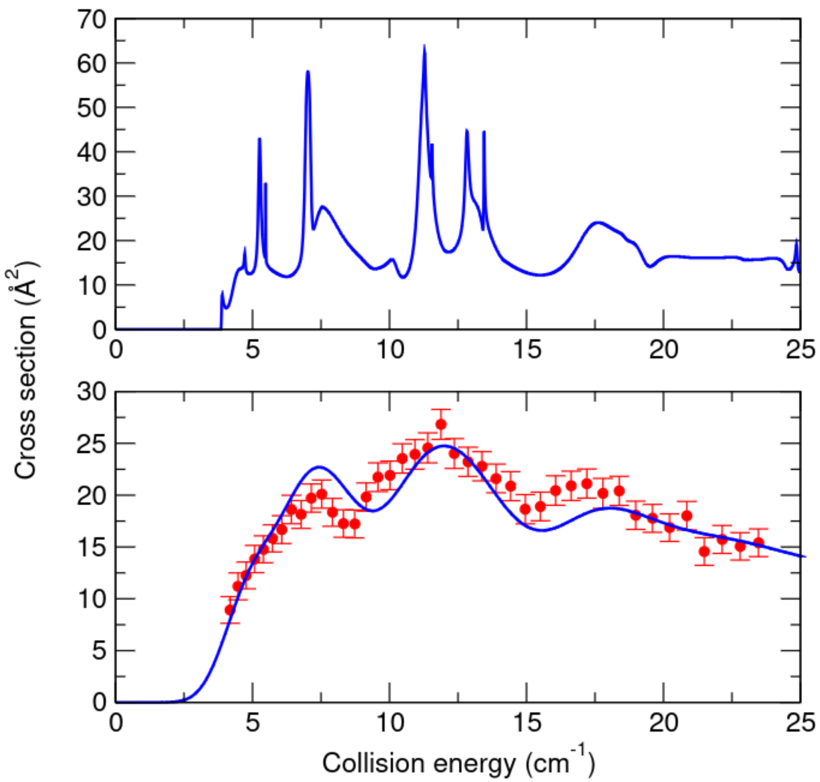
$$\frac{dn_X}{dt} = \sum_f k_f n(S_1) n(S_2) - \sum_d k_d n(S_3) n(S_4)$$

$$k(T) = \alpha (T/300)^\beta exp^{-\gamma/T}$$

  - KIDA, UMIST general databases

References: Lique & Faure (2019); Herbst (2014); Watson (1976)

Molecular astrophysics



Faure et al. (2016); Chefdeville et al. (2015)

▷ PCMI community: unique strengths and skills
- Laboratory (kinetic rates, spectroscopy), theory
- EMAA database for collision rate coefficients

New trends

- State-to-state astrochemistry: take into account quantum state of colliding species
  - quantum state resolved laboratory and theory: challenging
  - ortho-para chemistry (UGAN chemical network)
- Isotopic chemistry
- 3D modeling of molecular clouds
  - full coupling of physics and chemistry in a time-dependent fashion
  - 3D radiative transfer in molecular clouds

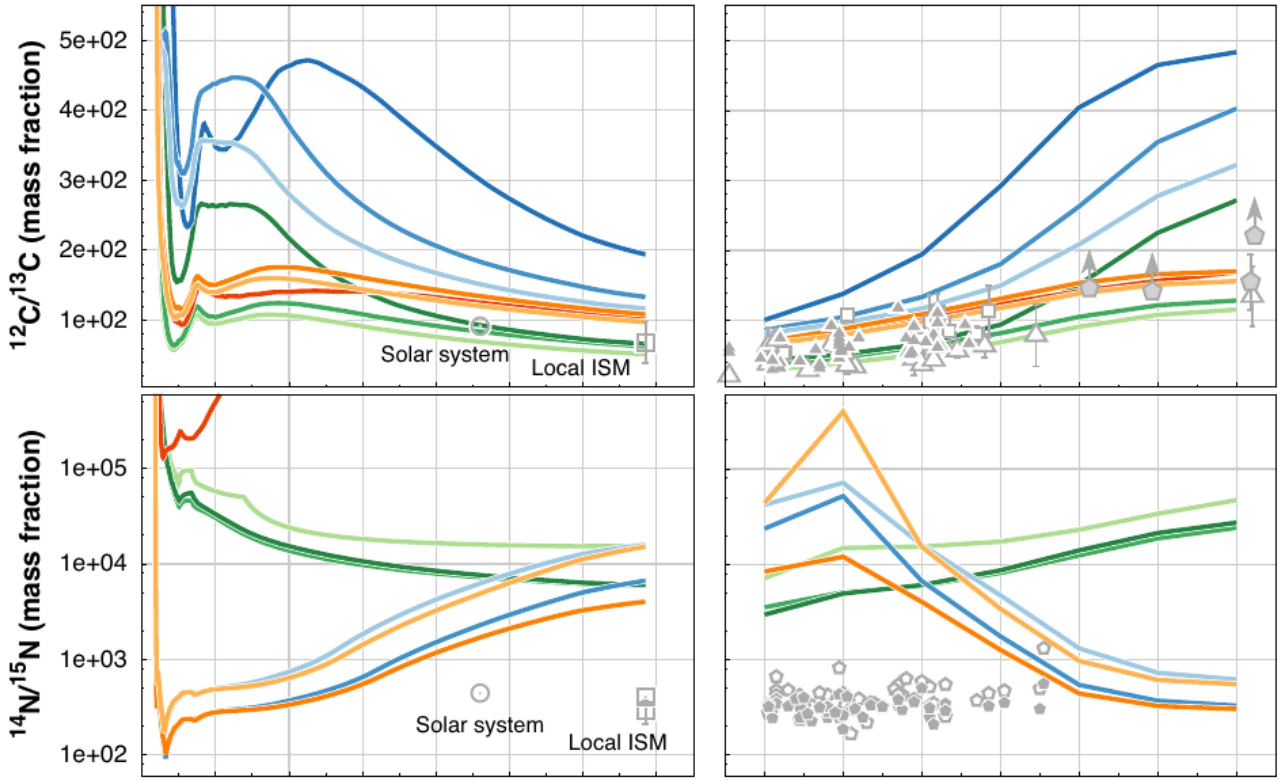
References: Roueff et al. (2015); Gong et al. (2017); Seifried et al. (2017); Pety et al. (2017); Hily-Blant et al. (2018); Borchert et al. (2022); Jensen et al. (2023)

3 Galactic chemical evolution

- ▷ GCE models and Galactic archeology
  - predict the space-time chemical evolution of galaxies
  - Main uncertainties: stellar nucleosynthesis yields
  - Milky Way as a calibrator to understand primordial galaxies
- ▷ Solar system history
  - comparison of isotopic ratios in SS with presolar grains; was the environment of the forming Sun normal or atypical?
- ▷ Isotopic ratios as tools to go back through chemical history
  - Depend on stellar nucleosynthesis
  - Coupling of Galactic star formation history (stellar IMF) and Galactic dynamics

References: Kobayashi et al. (2011); Kobayashi & Nakasato (2011); Prantzos (2016); Romano et al. (2019); Wilson (1999)

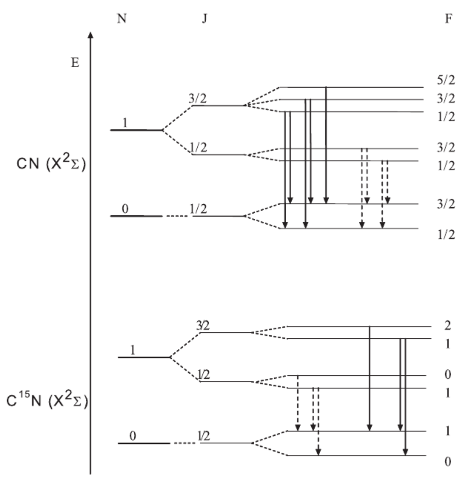
Chemical history: Galactic gradients of isotopic ratios

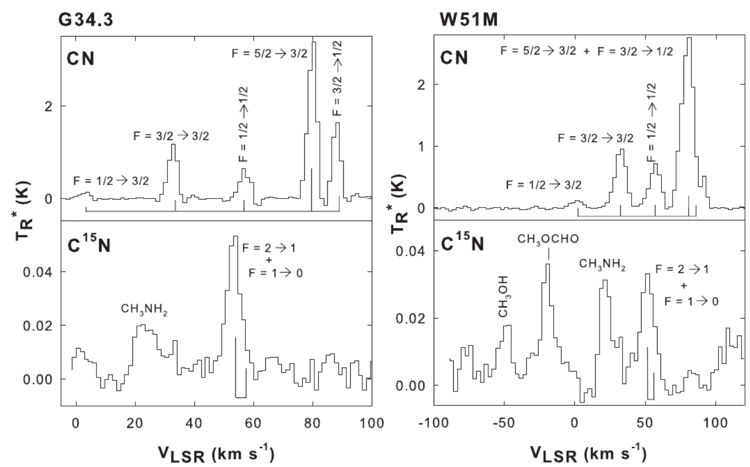


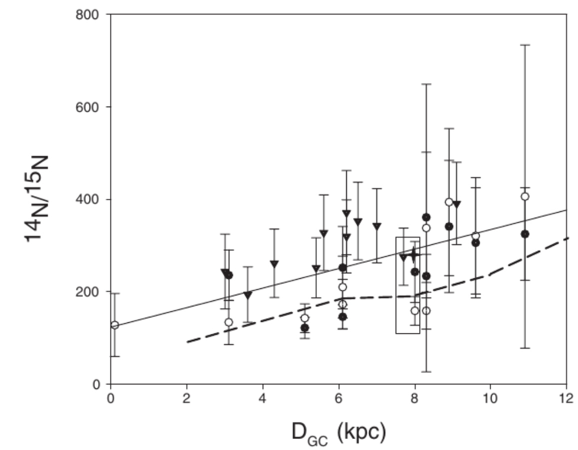
Romano et al. (2019)

- ▷ Isotopic ratios are probes of chemical history
  - Probes of metallicity
  - Time and location are related due to radial migration
- ▷ Constraining GCE models: surveys of isotopic ratios

Observations







- ▷ Measuring the 14N/15N ratio over the galactic disk taking advantage of hyperfine splitting

Challenging requirements

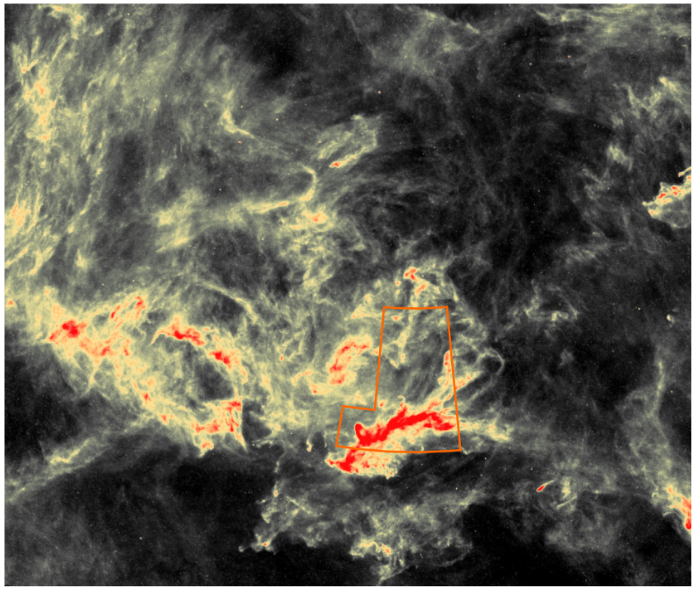
- ▷ Isotopic ratios often involve weak lines: 16O/18O ~ 500, 14N/15N ~ 330
- ▷ Line ratios for simultaneous observations (cross-calibration): bandwidths
- ▷ Cold star forming regions: high spectral resolution (40 kHz at 3mm)

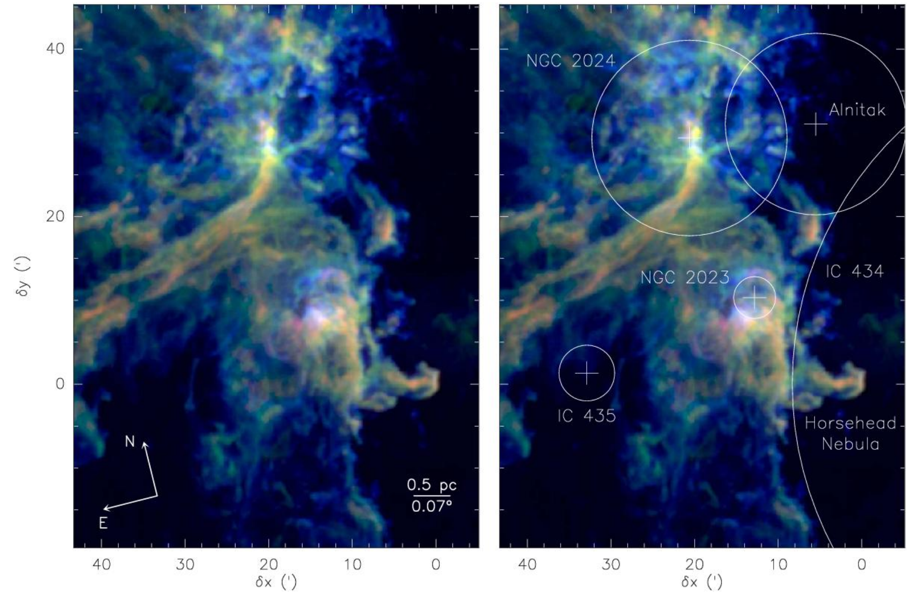
References: Adande & Ziurys (2012); Colzi et al. (2018); Zhang et al. (2019)

4 Star formation

- ▷ A corner stone of our understanding of the universe
- ▷ Fundamental issue: universality of the Stellar Initial Mass Function
- ▷ Interplay between gravity and turbulence
  - Formation of star forming regions
  - Interplay between clouds, filaments, and cores: from 30pc to 0.03 pc
- ▷ Role of turbulence: tracing gas turbulent dynamics
  - huge spatial dynamics: Large/small scales ~ (Reynolds number)$^{3/4}$
  - Re ~ 10^6 or more: spatial dynamics ~ 10^5
- ▷ Explore parameter space
  - Large-scale environment 30-100 pc scale
  - Energy injection (solenoidal, compressive)

Large-scale observations

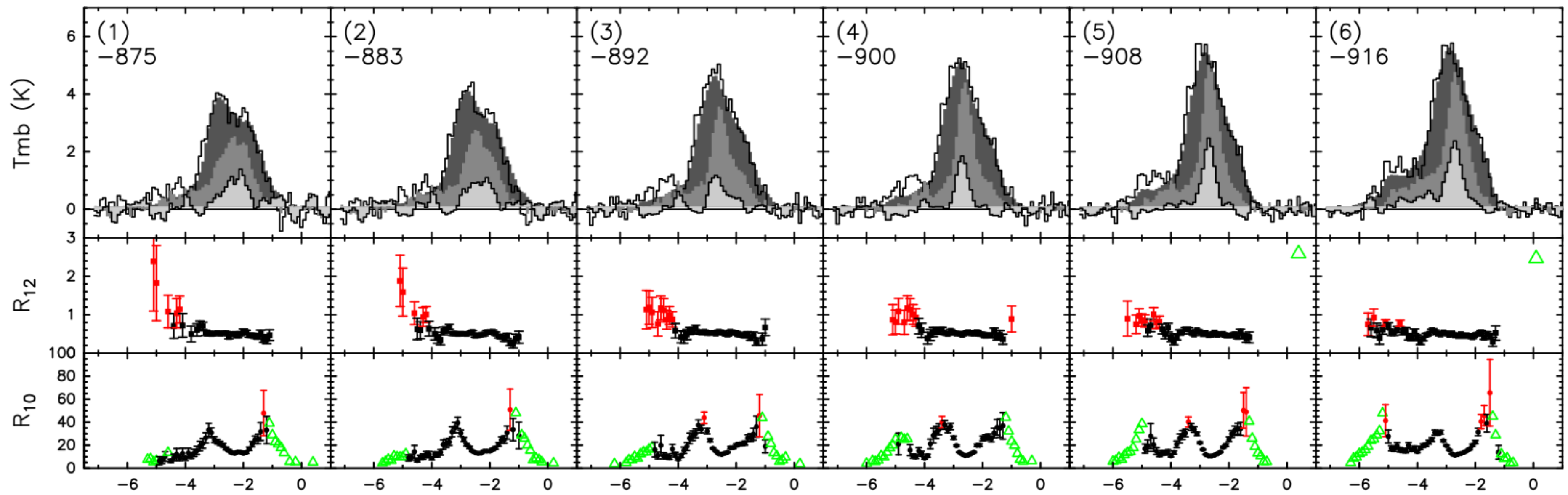




- ▷ Diffuse molecular clouds (left: Polaris Molecular Cloud): $A_V \sim$ 1-3
  - Birth place of filaments and embedded cores: best places to study interplay between gravity and turbulence prior to star formation
  - Best tracers: CO (blue), ^{13}CO(green), $C^{18}O$(red) (1-0) peak intensity
  - Right: ORION-B
- ▷ Observation needs: Hyperspectral data covering large areas over large parameter space

References: Goldsmith et al. (2008); Hily-Blant et al. (2008); Hily-Blant & Falgarone (2009); Pety et al. (2017); Orkisz et al. (2017), Hily-Blant & Falgarone 2025 (in prep)

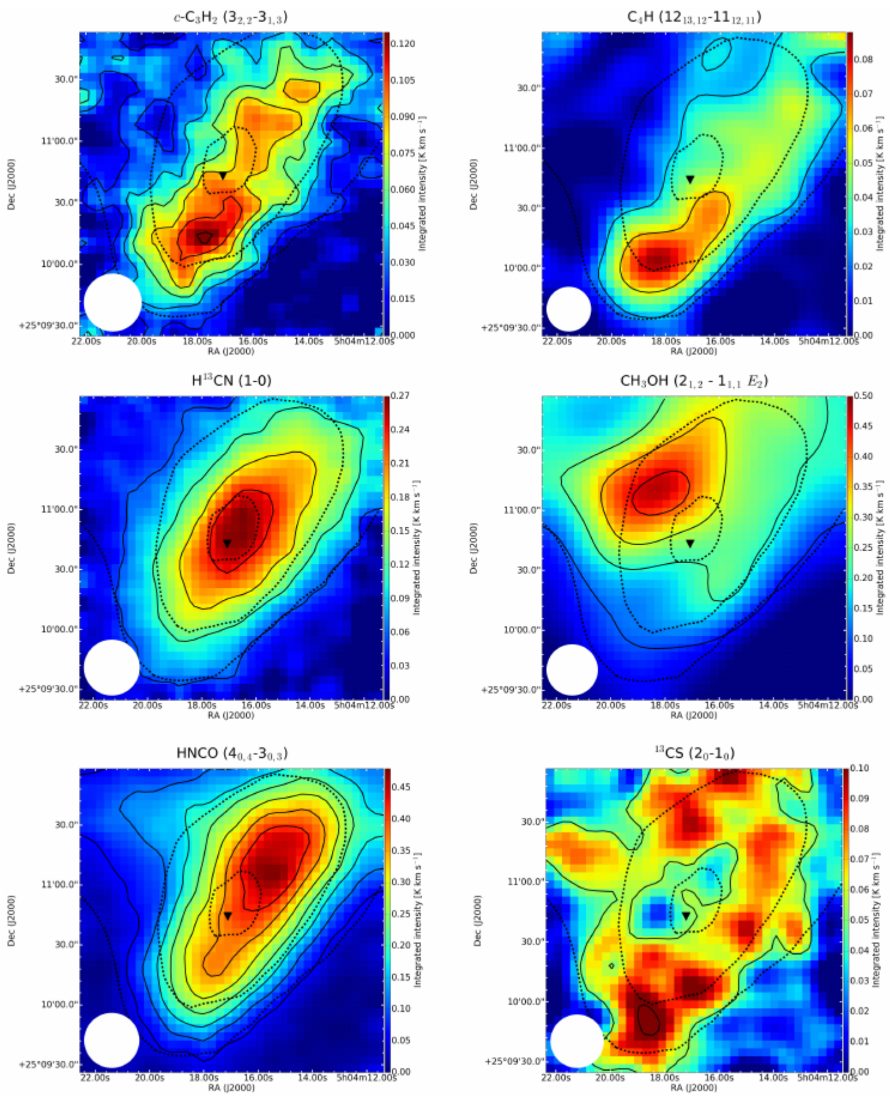
■ Multi-line, pointed observations



- ▷ Pinpoint critical regions based on velocity field analysis
- ▷ Multi line: line ratios to trace density/temperature (turbulence dissipation)
- ▷ Challenge: sensitivity, calibration

References: Goldsmith et al. (2008); Hily-Blant et al. (2008); Hily-Blant & Falgarone (2009); Pety et al. (2017); Orkisz et al. (2017), Hily-Blant & Falgarone 2025 (in prep)

Small-scale observations



▷ Typical star forming region: dense core
- Chemical factories: spectral signatures are very rich (≠ diffuse molecular clouds)
- 0.1 pc in size; better than 10" resolution at 150pc
- T=10K, narrow lines: <40kHz spectral resolution at 3mm

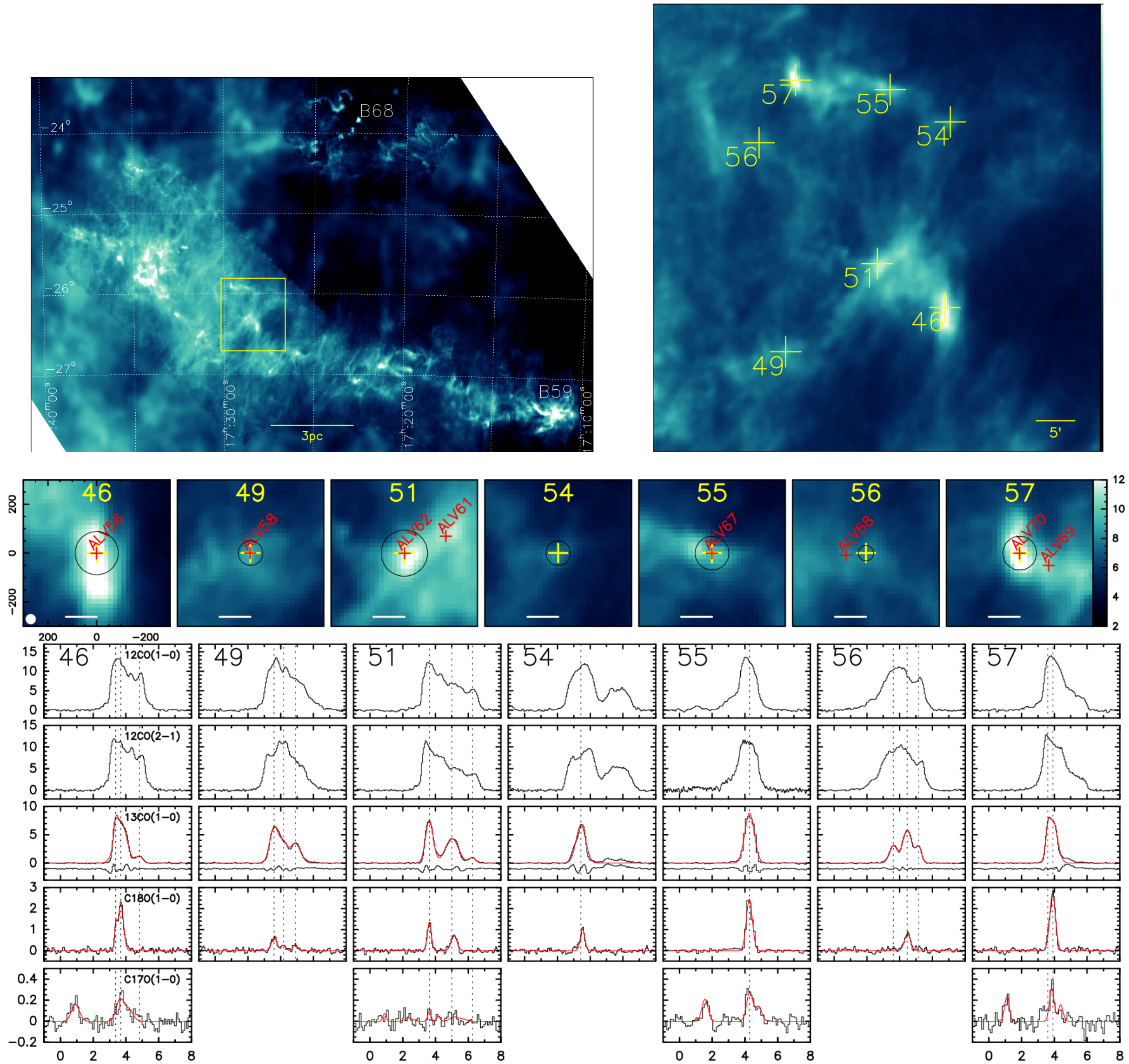
▷ Hyperspectral data: surveys needed covering physical parameter space (environments, location in MW)

▷ Towards machine learning analysis
- Building template spectral signatures from observations and models
- Unbiased measurements of the dense core mass function (DCMF)

▷ Line identification tools (e.g CLASS/WEEDS) and databases (e.g. CDMS, JPL)

References: Spezzano et al. (2017); Maret et al. (2011)

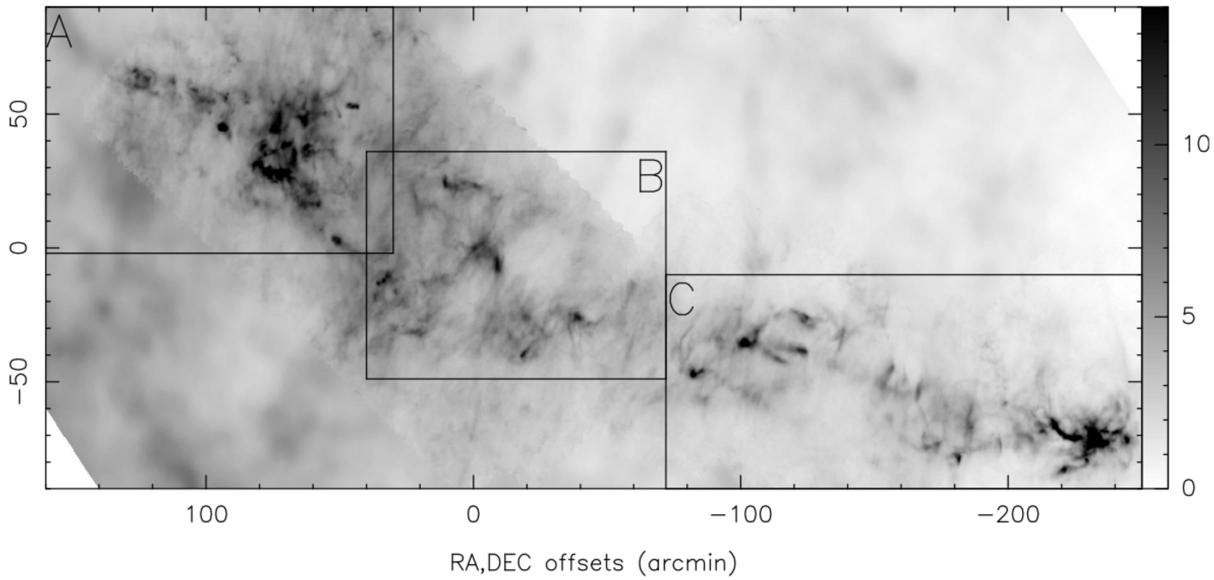
■ The origin of the stellar IMF

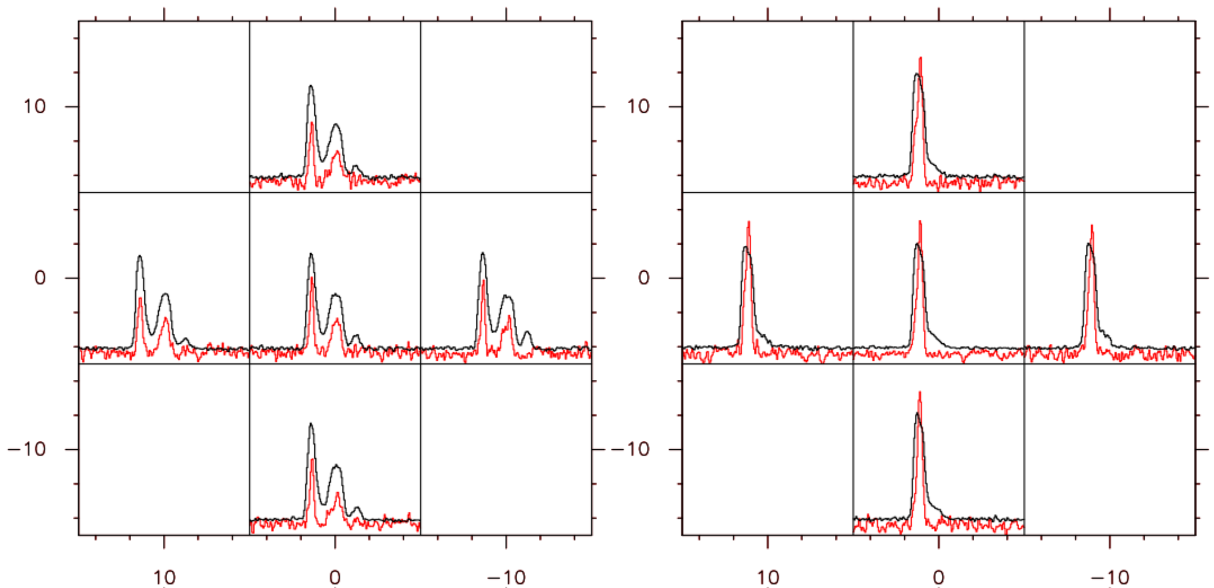


- ▷ Dense Core Mass Function (DCMF)
- ▷ High-sensitivity spectral lines of CO and isotopologues
- ▷ SED: Multi-band continuum observations
  - dust temperature, total column density

References: Delcamp and HB in prep

■ Increase data samples





References: HB et al prep

- ▷ Dense Core Mass Function (DCMF)
- ▷ High-sensitivity spectral lines of CO and isotopologues
- ▷ SED: Multi-band continuum observations
  - dust temperature, total column density
- ▷ Spatial variations carry a wealth of information

5 Openings

- ▷ Chemical history of the universe and the astrochemical ladder
  - Ratios (isotopic, ortho/para): highest accuracy for simultaneous observations
  - Chemistry-oriented tools to optimize instrumental settings
- ▷ Gravo-turbulence theory
  - covering large spatial dynamics (10^4 or more)
  - multi-line CO and isotopologues to trace the low-column density environment
- ▷ Origin of the stellar IMF
  - Dense core mass function
  - Consistent continuum and spectral line hyperspectral cubes
  - Large sample
- ▷ Machine learning to go from ppv to 3D structure
  - Training requires hyperspectral maps
  - Observations and models
  - Building models: astrochemical models and radiative transfer: constraints from observations
- ▷ Warning to models: challenge the 5% accuracy of cutting-edge facilities

6 Bibliography

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