

Radiative Transfer & Interstellar Molecular Lines

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Photons

Particles

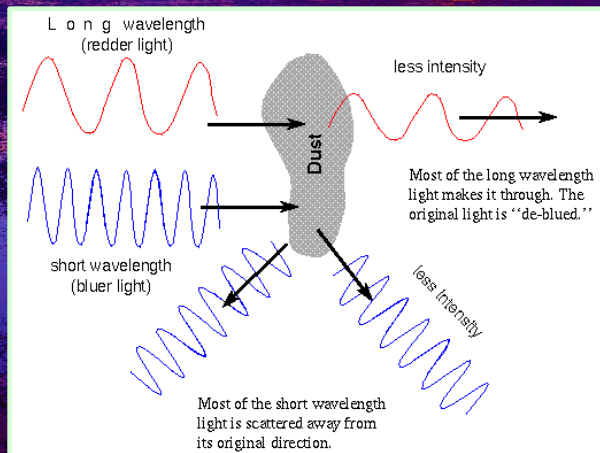
Gravitational Waves

Meteorites,... Space Missions

1. Radiative Transfer
2. Spectral Line Emission – Molecular Lines
3. Probes of Physical Conditions
4. Molecule Formation – Astrochemistry
5. Basics of Molecular Parameters
6. Examples of Molecular Line Observations
7. Summary

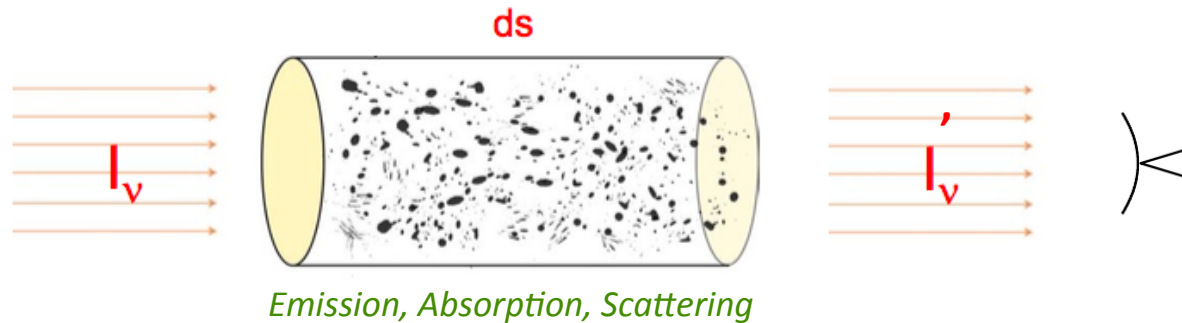


Reddening and Extinction by Dust



Radiative transfer is the physical phenomenon of energy transfer in the form of electromagnetic radiation. The propagation of radiation through a medium is affected by absorption, emission, and scattering processes. The equation of radiative transfer describes these interactions mathematically.

1. Basic Equation



loss of intensity in the beam (true absorption/scattering)

$$dI_v^{abs} = -\kappa_v I_v ds \quad \kappa_v : \text{absorption coefficient} \left[\text{cm}^{-1} \right]$$

energy added by emission processes within dV

$$dE_v^{em} = \varepsilon_v dV d\omega dv dt \quad \varepsilon_v : \text{emission coefficient} \left[\text{erg cm}^{-3} \text{sr}^{-1} \text{Hz}^{-1} \text{s}^{-1} \right]$$

$$dI_v = dI_v^{abs} + dI_v^{em} = \left(-\kappa_v I_v + \varepsilon_v \right) ds$$

$$\frac{dI_v}{ds} = -\kappa_v I_v + \varepsilon_v$$

$$\frac{dI_v}{d\tau_v} = -I_v + S_v(\tau_v)$$

$$\tau_v = \int_0^s \kappa_v ds \quad \text{Optical depth}$$

$$S_v = \frac{\varepsilon_v}{\kappa_v} \quad \text{Source Function}$$

$$I_v(0) = I_v(\tau_v) e^{-\tau_v} + \int_0^{\tau_v} S_v e^{-t} dt$$

Solution for simple cases: the normal direction, the source function (S_v) independent of location (*actual solution can be complex, since S_v can depend on I_v*),

$$I_v(0) = I_v(\tau_v) e^{-\tau_v} + S_v \int_0^{\tau_v} e^{-t} dt$$

$$I_v(0) = I_v(\tau_v) e^{-\tau_v} + S_v (1 - e^{-\tau_v})$$

Optically thick: $\tau \rightarrow \infty$

$$I_v(0) = I_v(\tau_v) e^{-\tau_v} + S_v (1 - e^{-\tau_v})$$

$$= S_v$$

Optically thin: $e^{-\tau_v} \approx 1 - \tau_v$

$$I_v(0) = I_v(\tau_v) + [S_v - I_v(\tau_v)] \tau_v$$

$$I_v(0) = S_v \tau_v$$

if $I_v(\tau_v) = 0$

$$\tau_v = \int_0^s \kappa_v ds$$

$$e^{-\tau_v}$$

$$T_B = T_{bg} e^{-\tau_v} + T_{ex} (1 - e^{-\tau_v})$$

In the $R-J$ approximation (T_B), in a homogeneous medium, for a specific line (T_{ex}), in the case of thermal EQ, with Boltzmann distribution

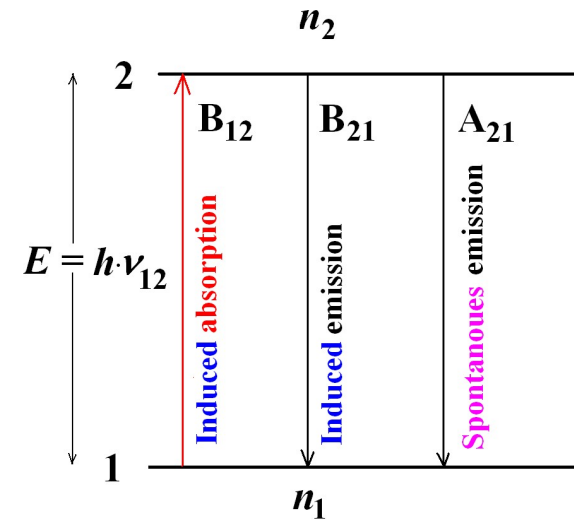
For the line transition:

$$\epsilon_v = \frac{h\nu}{4\pi} n_2 A_{21} \phi(\nu)$$

4π : assumption of isotropic emission

$\phi(\nu)$: the line shape (for simplicity, a rectangle or a gaussian profile)

$$\kappa_v = \frac{h\nu}{4\pi} (n_1 B_{12} - n_2 B_{21}) \phi(\nu)$$



The line source function for the transition $2 \rightarrow 1$:

Einstein relations:

$$g_1 B_{12} = g_2 B_{21}$$

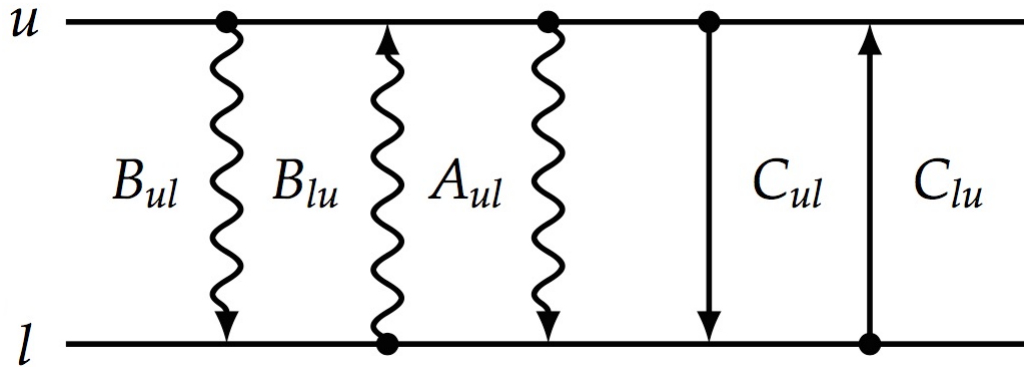
$$A_{21} = \frac{2h\nu^3}{c^2} B_{21}$$

$$S_v = \frac{\epsilon_v}{\kappa_v} = \frac{n_2 A_{21}}{n_1 B_{12} - n_2 B_{21}} = \frac{A_{21}}{B_{21}} \frac{1}{\frac{n_1 g_2}{g_1 n_2} - 1} = B_v(T_{ex})$$

$$\frac{n_2}{n_1} = \frac{g_2}{g_1} e^{-\frac{h\nu}{kT_{ex}}}$$

Radiative transfer is an exchange of energy between the radiation field and the energy levels of molecules and atoms (defined by the Boltzmann temperature). **Local Thermodynamic Equilibrium (LTE)** when the Boltzmann temperature is in equilibrium with the kinetic temperature.

$$S_v = B_v(T_{ex})$$



$$C_{ij} = n_{col} K_{ij}$$

C_{ij} : Collision rate

K_{ij} : Collision rate coefficient
(velocity integrated cross section)

For a two-level system in thermodynamic equilibrium,

$$n_1 C_{12} = n_2 C_{21} \quad C_{12} = \frac{g_2}{g_1} C_{21} e^{-\frac{\Delta E}{kT}}$$

LAMDA (Leiden Atomic and Molecular Database)
<https://home.strw.leidenuniv.nl/~moldata/>

Statistical equilibrium:

$$\frac{dn_1}{dt} = -n_1 (B_{12} \bar{J} + C_{12}) + n_2 (A_{21} + B_{21} \bar{J} + C_{21})$$

$$\frac{dn_2}{dt} = n_1 (B_{12} \bar{J} + C_{12}) - n_2 (A_{21} + B_{21} \bar{J} + C_{21})$$

The chance that a newly created photon can escape from the cloud, **Escape Probability** : β

$$\bar{J} = S(1 - \beta)$$

It is **the amount of radiation “inside” the source**, so for a completely opaque source it equals the (profile averaged) source function S . So we can solve the level populations and the radiation field separately; they are decoupled. [<https://home.strw.leidenuniv.nl>]

$$\frac{dn_2}{dt} = n_1(B_{12}\bar{J} + C_{12}) - n_2(A_{21} + B_{21}\bar{J} + C_{21})$$

$$\frac{dn_2}{dt} = n_1C_{12} - n_2C_{21} - \beta n_2A_{21}$$

$$\begin{aligned} \frac{dn_2}{dt} &= n_1(B_{12}\bar{J} + C_{12}) - n_2(A_{21} + B_{21}\bar{J} + C_{21}) \\ &= n_1C_{12} - n_2C_{21} + (n_1B_{12} - n_2B_{21})\bar{J} - n_2A_{21} \\ &= n_1C_{12} - n_2C_{21} + (n_1B_{12} - n_2B_{21})S(1 - \beta) - n_2A_{21} \\ &= n_1C_{12} - n_2C_{21} + n_2A_{21}(1 - \beta) - n_2A_{21} \\ &= n_1C_{12} - n_2C_{21} - \beta n_2A_{21} \end{aligned}$$

Simple one-dimensional case: $\beta = \langle e^{-\tau_v} \rangle = \frac{1}{\tau} \int_0^\tau e^{-\tau'} d\tau' = \frac{1 - e^{-\tau}}{\tau}$

An expanding sphere (Sobolev or LVG approximation), A homogeneous slab;
A turbulent medium; A uniform sphere; ...
Monte Carlo Method; Accelerated Λ Iteration; Gauss-Seidel Algorithm; ...

2. Electromagnetic radiation – Spectral Line Emission – Molecular Lines

Electromagnetic radiation is produced whenever charged particles are accelerated.

In general, by one of two means, either thermal or non-thermal mechanisms.

Thermal emission: which depends only on the temperature of the emitting object, includes blackbody radiation, free-free emission in an ionized gas, and spectral line emission.

Non-thermal emission: which does not depend on the temperature of the emitting object, includes synchrotron radiation, inverse Compton scattering emission, and amplified emission from masers in space.

CONTINUUM
LINE

THERMAL RADIATION

1. BLACKBODY RADIATION

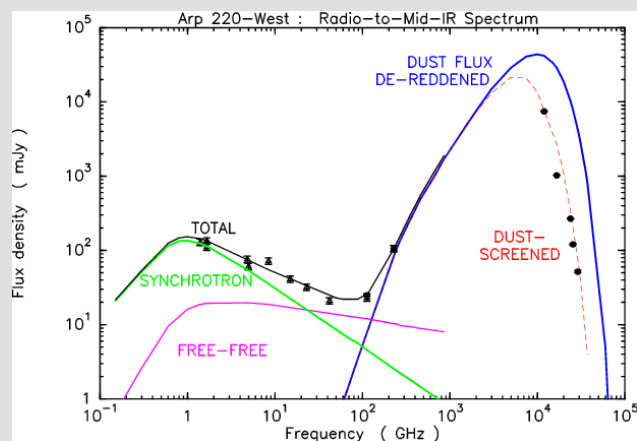
2. FREE-FREE EMISSION

4. SPECTRAL LINE EMISSION

NON-THERMAL RADIATION

3. SYNCHROTRON RADIATION

5. ASTRONOMICAL MASERS



CONTINUUM

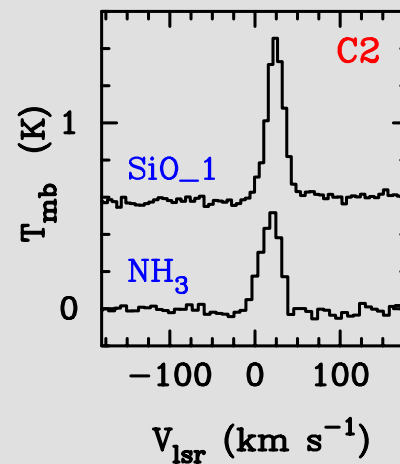
- Spectral index
- Abundance

■ Total power

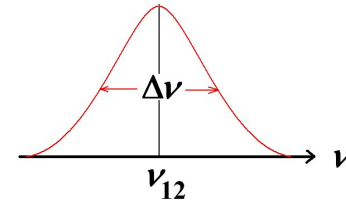
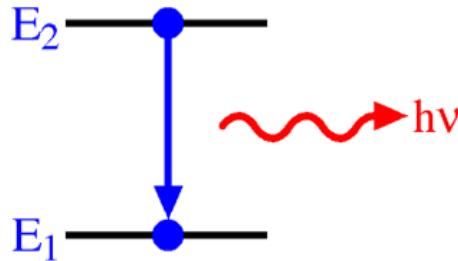
LINE

- Kinematics
- Abundance

■ Baseline



Spectral Line Emission – Molecular Lines



Spectral line emission involves the transition of electrons from a higher energy level to lower energy level, determined by the quantum properties of the atom or molecule. When this happens, a photon is emitted with the same energy as the energy difference between the two levels.

Accurate frequency: The emission of this photon at a certain discrete energy shows up as a discrete "line" or wavelength in the electromagnetic spectrum.

Astronomically Important Lines

(1) H I hyperfine line

(2) Atomic lines

(3) Molecular lines

Interstellar molecules listed by number of atoms

Diatomic	Triatomic	Four atoms	Five atoms	Six atoms	Seven atoms	Eight atoms	
H ₂	C ₃	<i>c</i> -C ₃ H	C ₅	C ₅ H	C ₆ H	CH ₃ C ₃ N	
AlF	C ₂ H	<i>l</i> -C ₃ H	C ₄ H	<i>l</i> -H ₂ C ₄	CH ₂ CHCN	HCOOCH ₃	
AlCl	C ₂ O	C ₃ N	C ₄ Si	C ₂ H ₄	CH ₃ C ₂ H	CH ₃ COOH(?)	
C ₂	C ₂ S	C ₃ O	<i>l</i> -C ₃ H ₂	CH ₃ CN	HC ₅ N	C ₇ H	
CH	CH ₂	C ₃ S	<i>c</i> -C ₃ H ₂	CH ₃ NC	HCOCH ₃	H ₂ C ₆	
CH ⁺	HCN	C ₂ H ₂	CH ₂ CN	CH ₃ OH	NH ₂ CH ₃	CH ₂ OHCHO	
CN	HCO	CH ₂ D ⁺ (?)	CH ₄	CH ₃ SH	<i>c</i> -C ₂ H ₄ O	CH ₂ CHCHO	
CO	HCO ⁺	HCCN	HC ₃ N	HC ₃ NH ⁺	CH ₂ CHOH		
CO ⁺	HCS ⁺	HCNH ⁺	HC ₂ NC	HC ₂ CHO			
CP	HOC ⁺	HNCO	HCOOH	NH ₂ CHO			
CSi	H ₂ O	HNCS	H ₂ CHN	C ₅ N			
HCl	H ₂ S	HOCO ⁺	H ₂ C ₂ O	HC ₄ N			
KCl	HNC	H ₂ CO	H ₂ NCN				
NH	HNO	H ₂ CN	HNC ₃				
NO	MgCN	H ₂ CS	SiH ₄				
NS	MgNC	H ₃ O ⁺	H ₂ COH ⁺				
NaCl	N ₂ H ⁺	NH ₃					
OH	N ₂ O	SiC ₃					
PN	NaCN	C ₄	Nine atoms	Ten atoms	Eleven atoms	Twelve atoms	Thirteen atoms
SO	OCS		CH ₃ C ₄ H	CH ₃ C ₅ N(?)	HC ₉ N	CH ₃ OC ₂ H ₅	HC ₁₁ N
SO ⁺	SO ₂		CH ₃ CH ₂ CN	(CH ₃) ₂ CO			
SiN	<i>c</i> -SiC ₂		(CH ₃) ₂ O	NH ₂ CH ₂ COOH			
SiO	CO ₂		CH ₃ CH ₂ OH	CH ₃ CH ₂ CHO			
SiS	NH ₂		HC ₇ N				
CS	H ₃ ⁺		C ₈ H				
HF	SiCN						
SH	AlNC						
FeO(?)	SiNC						

Table from A. Wootten (www.cv.nrao.edu/~awootten/allmols.html).

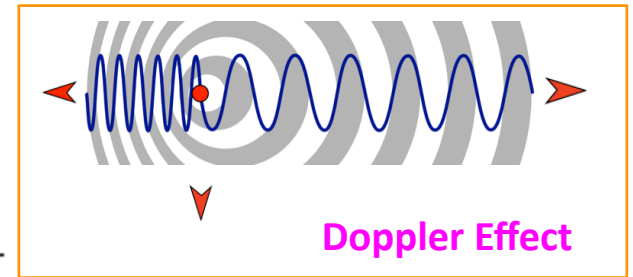
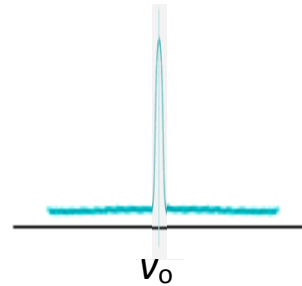
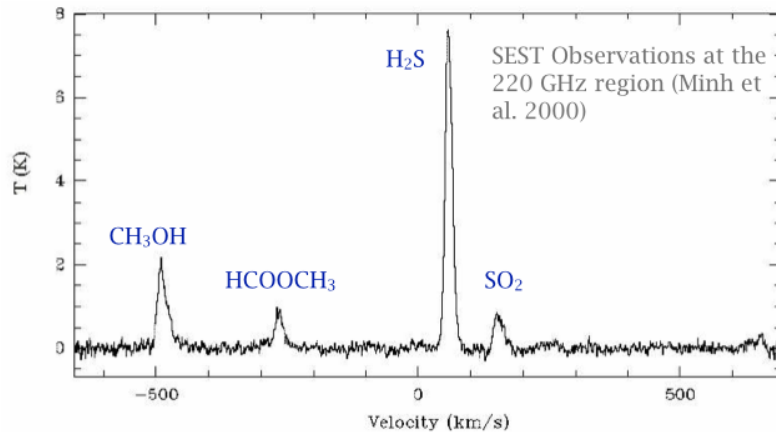
Identified Interstellar Molecules

Many of the molecules have carbon in them → called organic molecules

The organic molecules and the water and ammonia molecules are used in biochemical reactions to create the building blocks of life: amino acids and nucleotides.

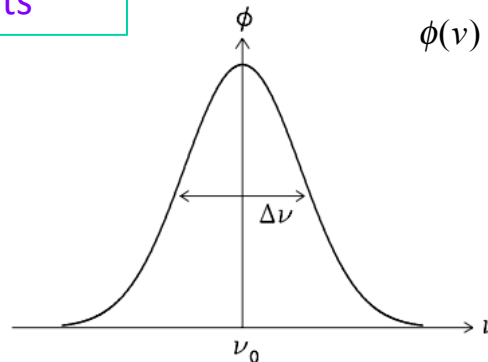
Some carbonaceous meteorites reaching the Earth have amino acids in them.

3. Spectral Lines as Probes of Physical Conditions



- Kinematics (velocity, linewidth, profile,...)
- Density (up to 10^{10} cm^{-3})
- Temperature ($10 \sim 10^3 \text{ K}$)
- Abundances – mass, ...
- **Astrochemistry** – Physical Environments

We actually receive the accumulated radiation from large numbers of atoms or molecules moving with different speeds, so emission lines have a finite width.



$$\phi(\nu) = \frac{c}{\nu_0} \left(\frac{M}{2\pi kT} \right)^{1/2} \exp \left[-\frac{Mc^2 (\nu - \nu_0)^2}{2kT \nu_0^2} \right]$$

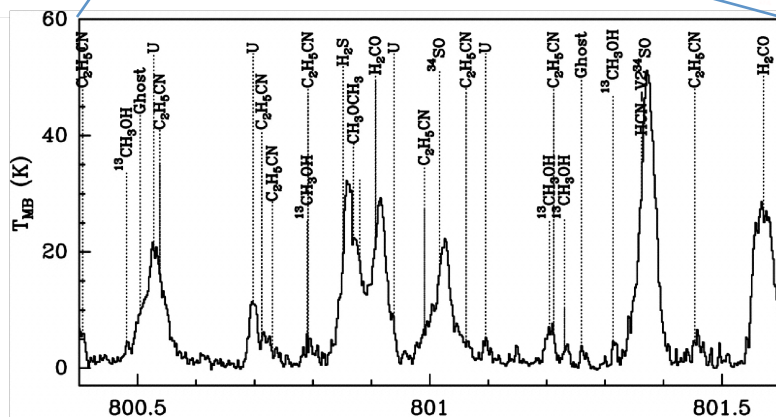
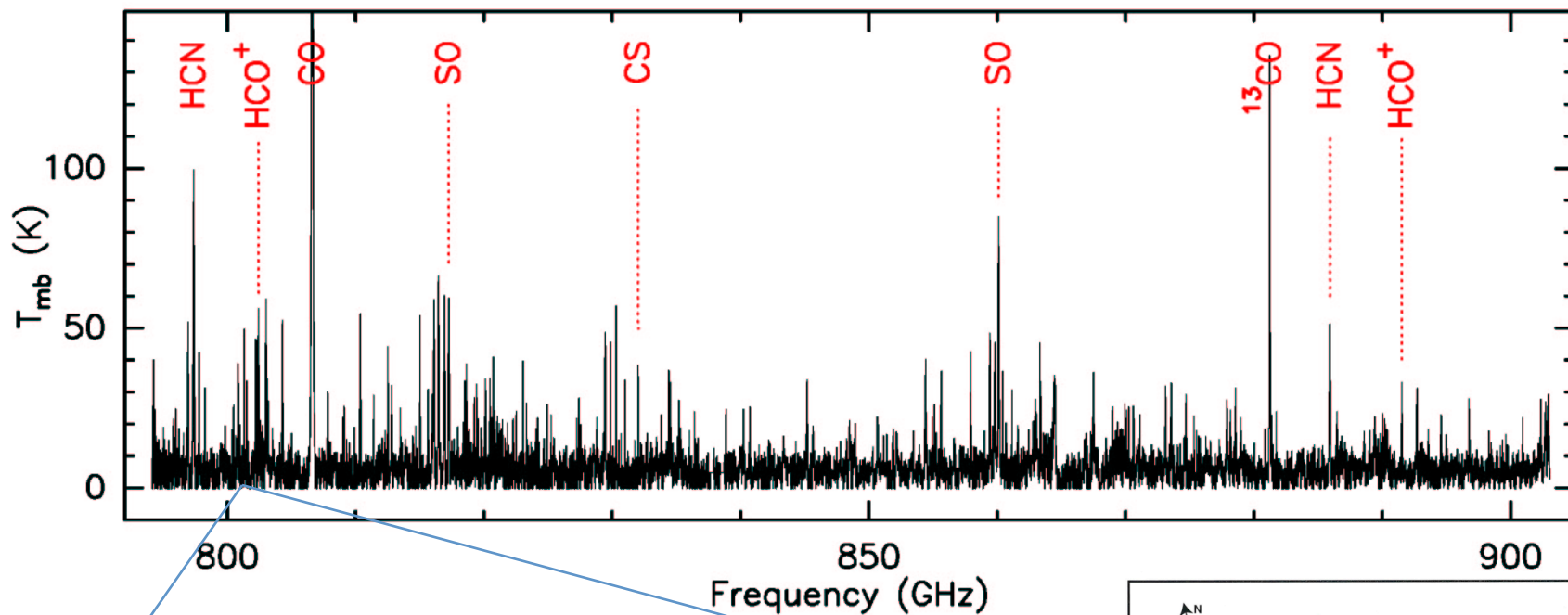
$$\Delta \nu = \left(\frac{8 \ln 2 k}{c^2} \right)^{1/2} \left(\frac{T}{M} \right)^{1/2} \nu_0$$

Molecular Lines: *Important, powerful, (sometimes only) available probes of physical conditions of astronomical sources, ...*

B335: color composite – H α (red), [SII] (green), and R band (blue). The bipolar Herbig-Haro flow HH119 are labeled. Red contours: a bipolar reflection nebular imaged at 8 μ m with Spitzer. The field of view is 5x4 min. [Gaalfalk & Olofsson 2007]



CSO 350 μ m Molecular Line Survey of Orion KL (Comito et al. 2005)



Orion Molecule Cloud-1

NICMOS NARROWBAND IMAGES OF OMC-1

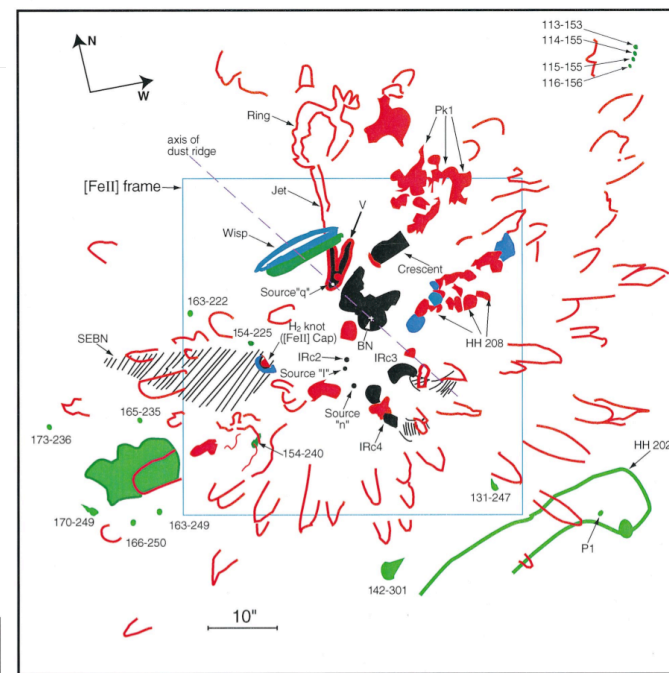
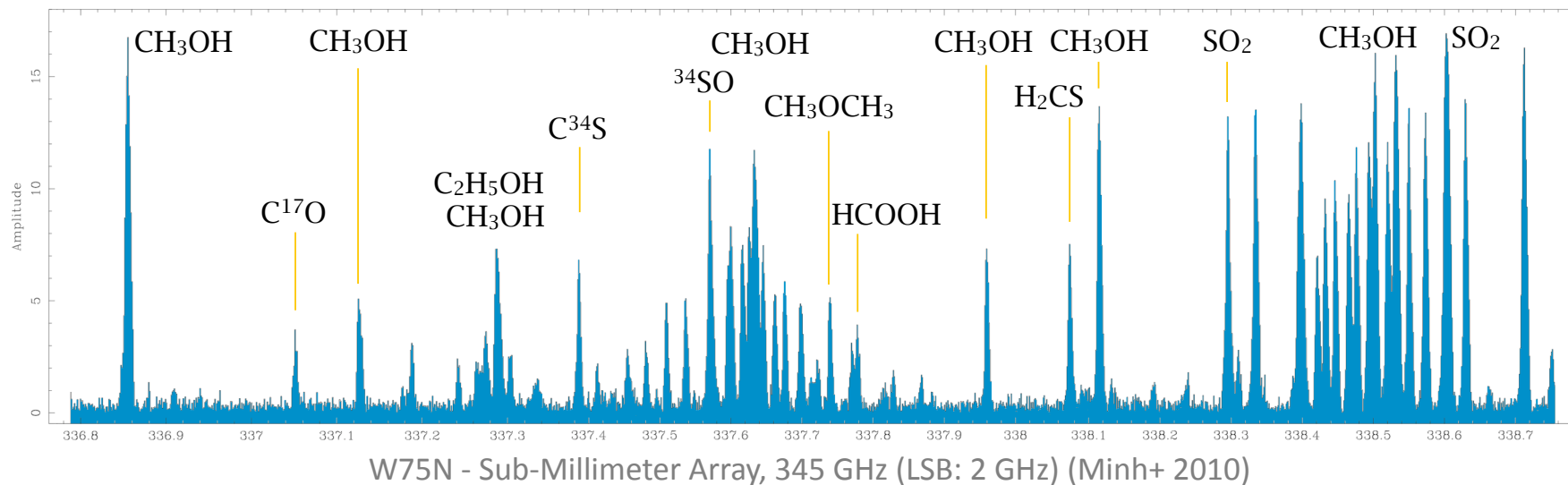


FIG. 1.—Schematic of the near-IR morphology of the OMC-1 region. Colors are as indicated. Dust disk is from Wright et al. (1992).

Each molecular line provides a unique tool for understanding the associated processes.



4. Molecule Formation - Astrochemistry

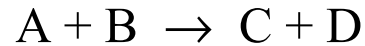
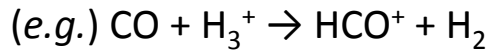
Gas phase processes

- (1) Ion-molecule reactions (2) Neutral-neutral reactions (3) PDR

Solid phase processes

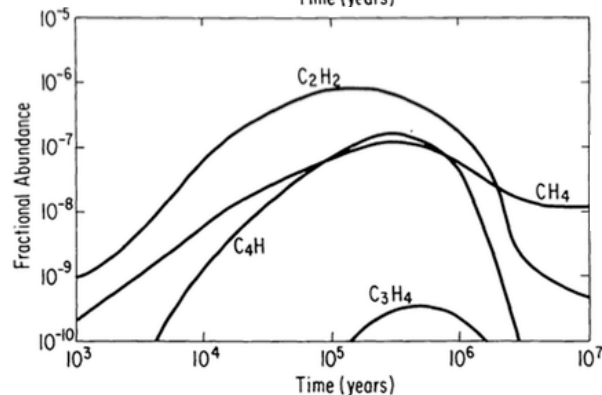
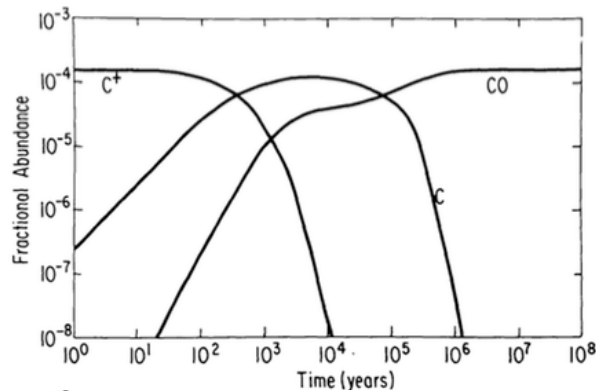
- Grain surface reactions and evaporation

Gas phase processes – (1) Ion-molecule reactions



$$\frac{d[\text{C}]}{dt} = -\frac{d[\text{A}]}{dt} = k[\text{A}][\text{B}]$$

k : rate coefficient



Basic carbon chemistry
and its coupling with
oxygen chemistry
[Prasad+ 1986]

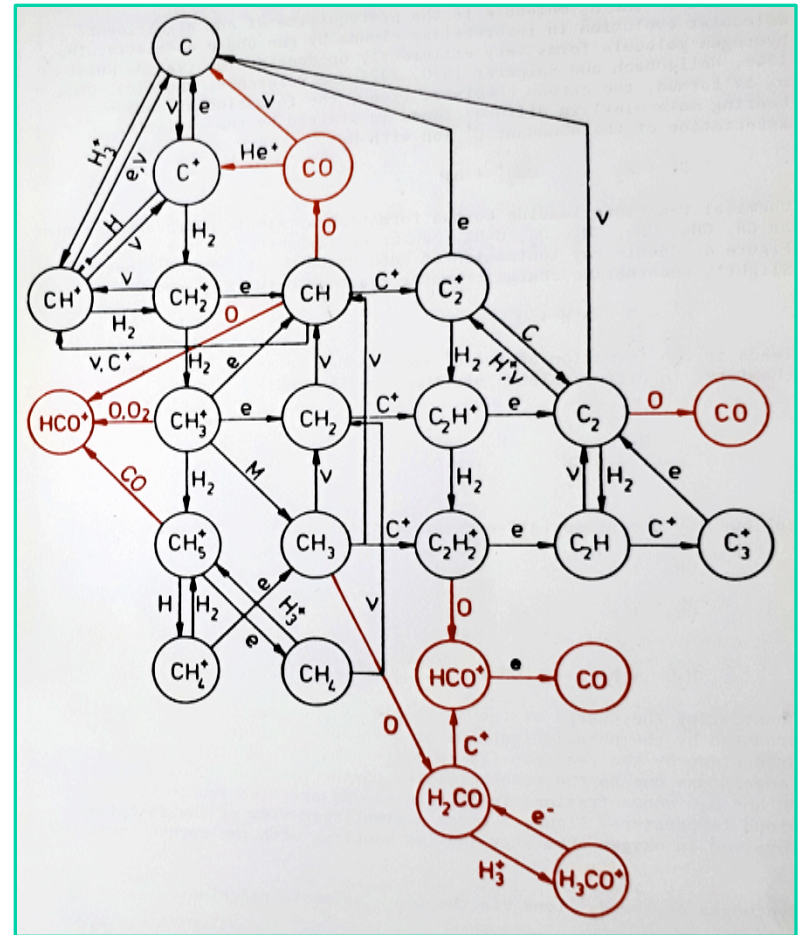


FIG. 1.—Abundances relative to H₂ of C⁺, C, and CO are plotted as function of time for a cloud of total gas density of $2 \times 10^4 \text{ cm}^{-3}$ and low-metal abundances.

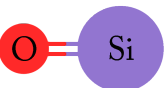
FIG. 2.—Abundances relative to H₂ of CH₄, C₂H₂, C₃H₄, and C₄H are plotted as a function of time for a cloud of total gas density of $2 \times 10^4 \text{ cm}^{-3}$ and low-metal abundances.

[Leung+ 1984]

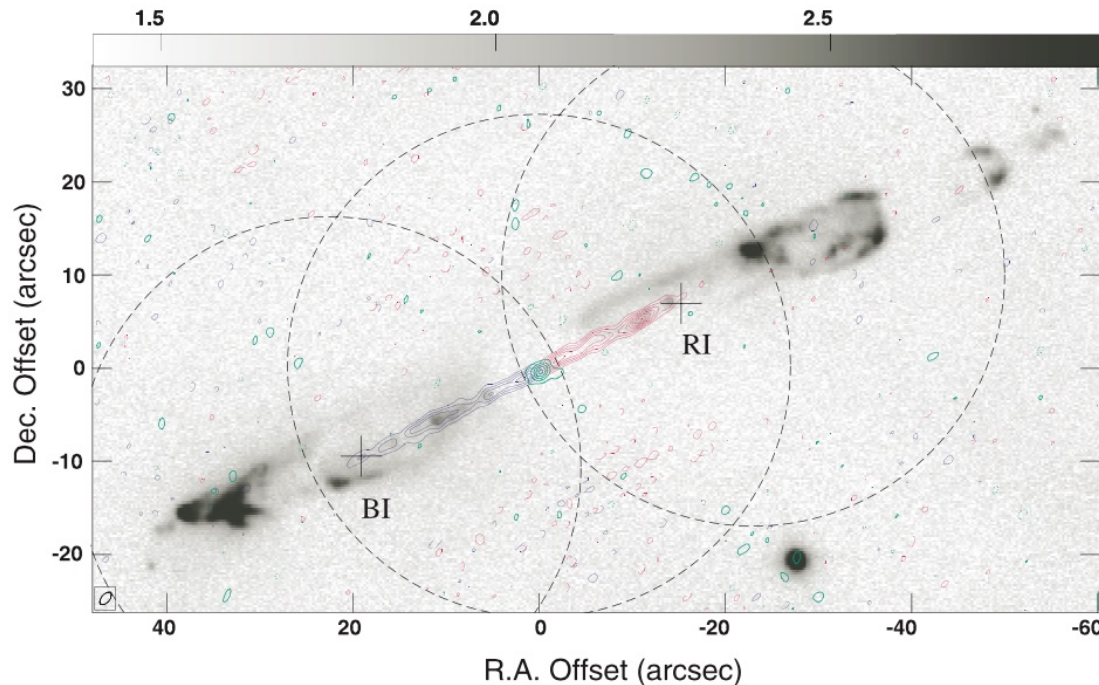
Gas phase processes – (2) Neutral-neutral reactions

- Shocked Gas (C-, J-shock): H_2O , OH, SiO, S-mols, ...

(e.g.) $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$

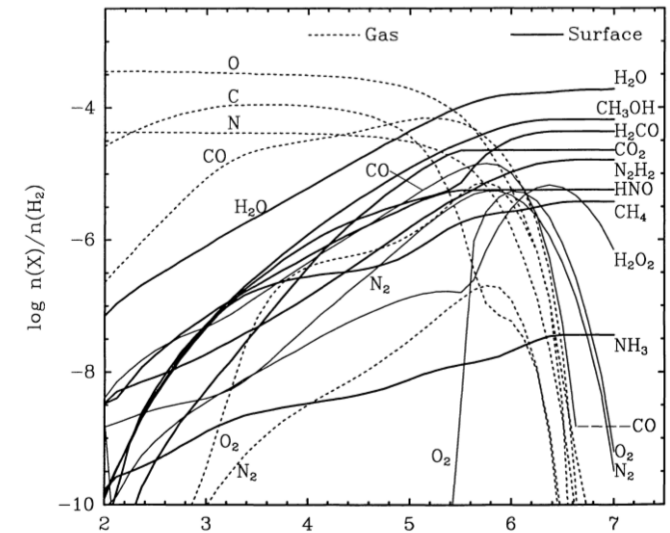
(e.g.)  *Si-containing species*
 $\rightarrow$ grain destruction, sputtering, ...

SiO chemistry: shocks



A J-shock occurs in case for $v_s > 30 \text{ km s}^{-1}$
 Pre-shock gas, shock front, post-shock gas
 (relaxation time scale is short)

The main coolants are rotational and vibrational lines from CO, H_2O , and OH.



(Hasegawa et al. 1992)

[Hirano+ 2006] The protostellar jet driven by H211 (~315 pc) observed with SMA for the SiO $J = 5-4$ (red and blue) and 220 GHz continuum (green) maps superposed on the $\text{H}_2 v = 1-0 \text{ S}(1)$ emission (gray scale).

Gas phase processes – (3) PDR

PDR (scale~0.01 pc) is mainly controlled by Far-UV photons (6-13.6 eV), heating by photo-electrons and cooling by FIR emission.

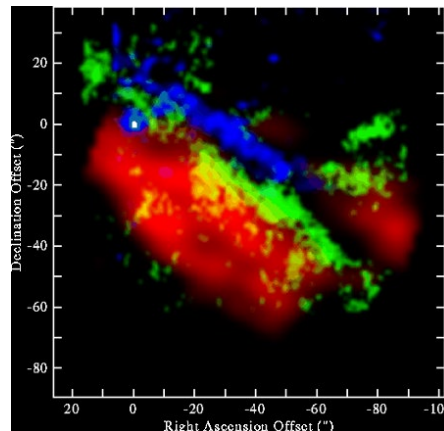
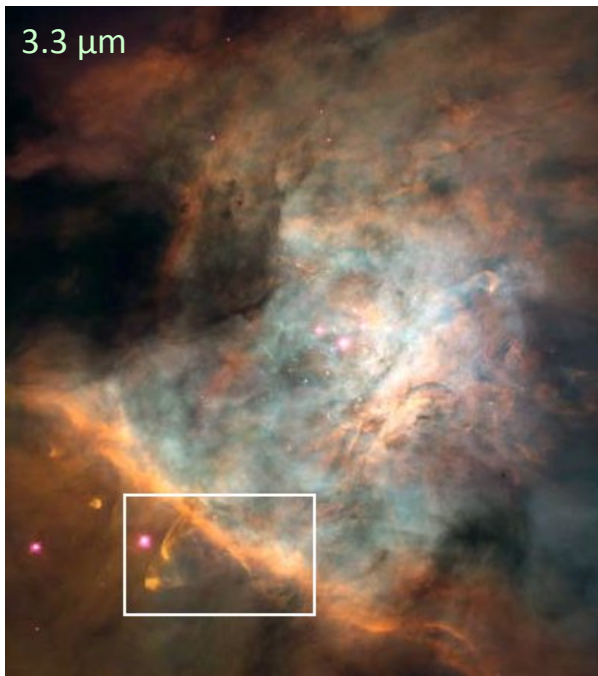
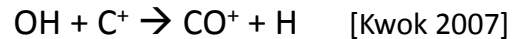
Gas phase reactions, grain surface chemistry, photo-desorption, etc., associated with CO, [CI], [CII], [OI], H₂O, OH, CH, CH⁺, NH,...

(e.g.) $\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H}$ (endo by 900 K plus the activation $E=2000$ K)

$\text{C}^+ + \text{H}_2 \rightarrow \text{OH} + \text{H}$ (endo by 4640 K)

CO⁺ : an important indicator (signature molecule) of a PDR

CO ionization energy = 14 eV (larger than 13.6 eV for H),
so CO⁺ cannot be produced by photoionization of CO, instead:



(Tielens+ 1993, Sloan+ 1997): the PAH emission layer in blue, the H₂ emission in green, and the CO emission in red. The yellow area results from an overlap of green and red.

The Orion Bar is called a photo-dissociation region (PDR), because of the ionization from the Trapezium, photo-dissociating molecules into atoms and then ionizing them.

Problems: interplay between chemistry, dynamics, and radiative transfer; various models predict different results

Solid phase processes – Grain surface reactions

Interstellar H₂O ice at 3 μm in 1973 (Gillet & Forrest); Solid CO detections in the 1980s (Lacy+ 1984: Palomar 5m).

More than 40 H₂O ice bands: mostly in the cold outer envelopes of high-mass protostars, low-mass objects (*ISO*), ... *(in the crystalline form rather than the amorphous phase)*

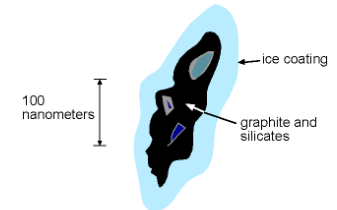
Ice mantle: H₂O, CH₃OH (1-30%), NH₃ (a few – 30%), CO, CO₂, OCS,...

*At densities below 10⁴ cm⁻³, H is more abundant than O, and **hydrogenation** will be expected.*

*At higher densities, O is more abundant than H and **oxygenation** is expected.*

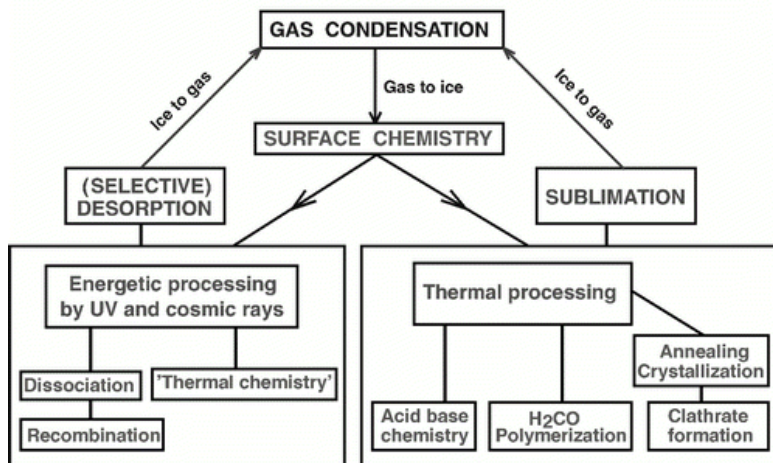
Daughter molecules: CH₃CN, HCOOCH₃, HCN, CH₃CH₂CN, CH₃CH₂OH,...

Accretion and Desorption: Heating by CRs or UV followed by thermal evaporation of the surface molecules (~ binding E); UV photodesorption: direct interaction with surface molecules

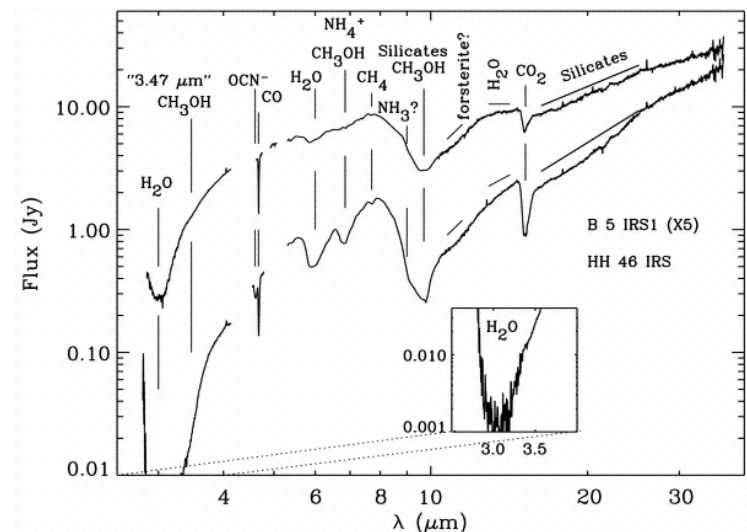


A typical dust grain (note the tiny scale!).

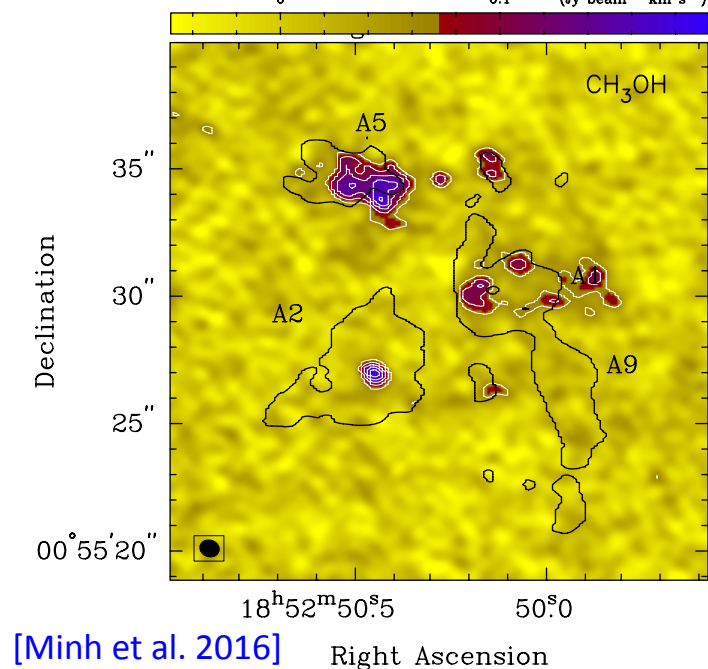
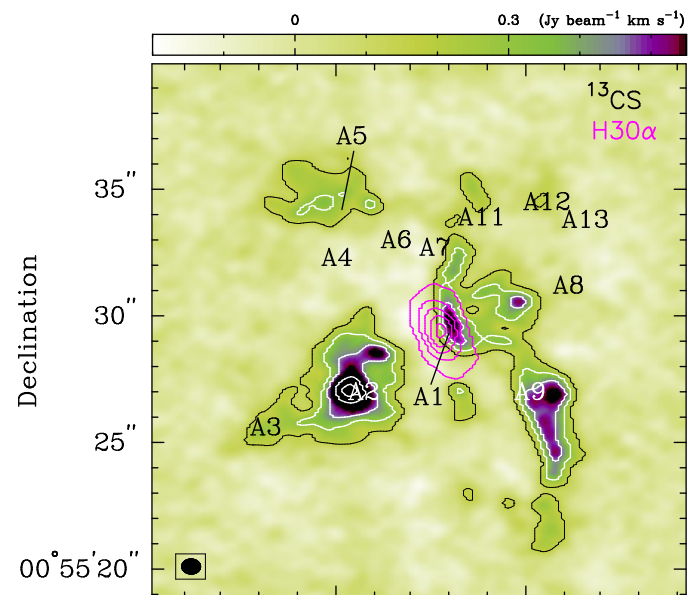
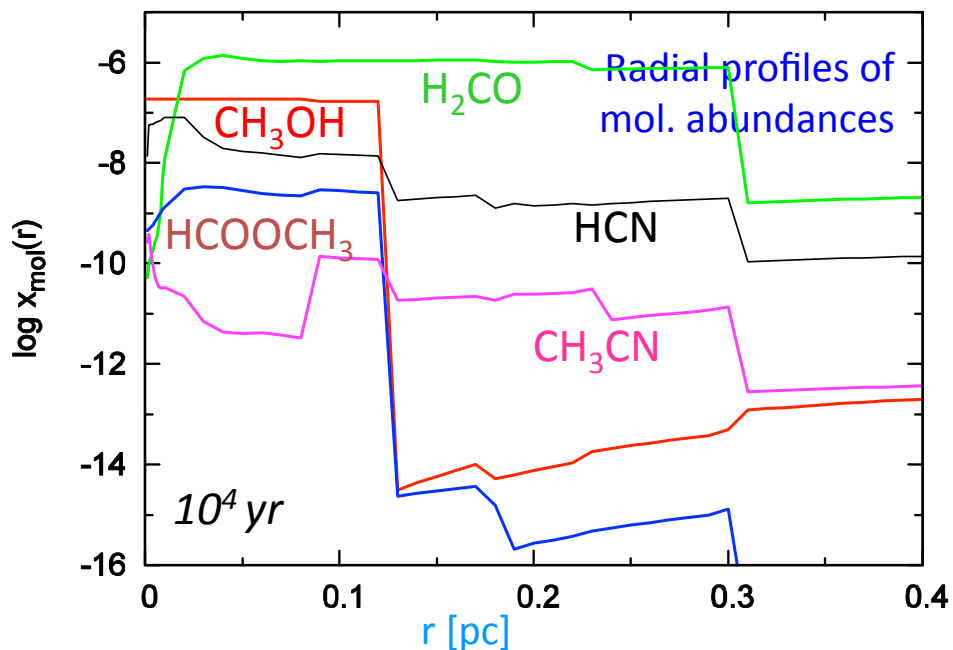
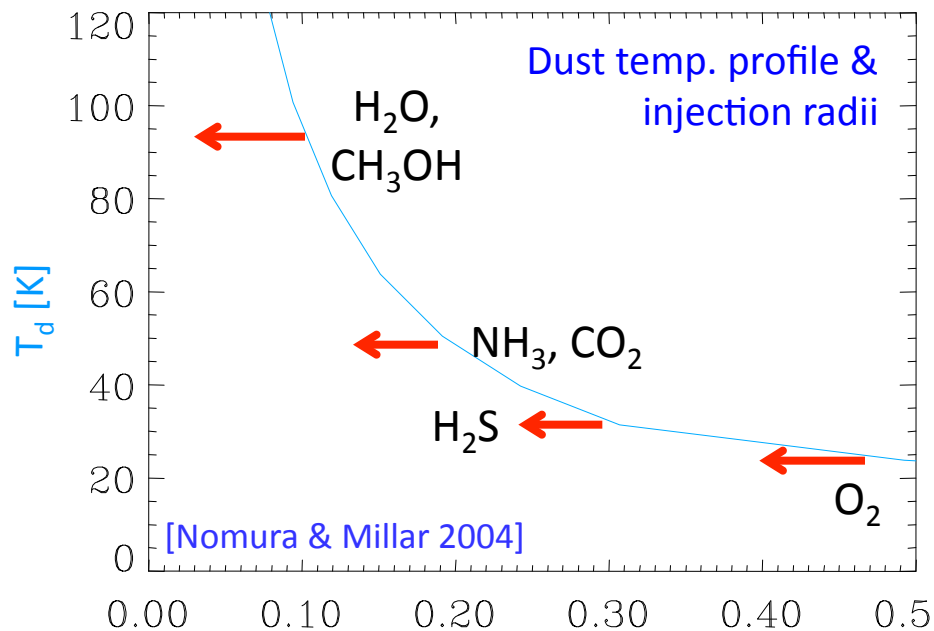
THE CYCLE OF ICE AND GAS IN DENSE CLOUDS



Boogert et al. 2004 (Spitzer)



Hot core molecules exist concentrated in compact region



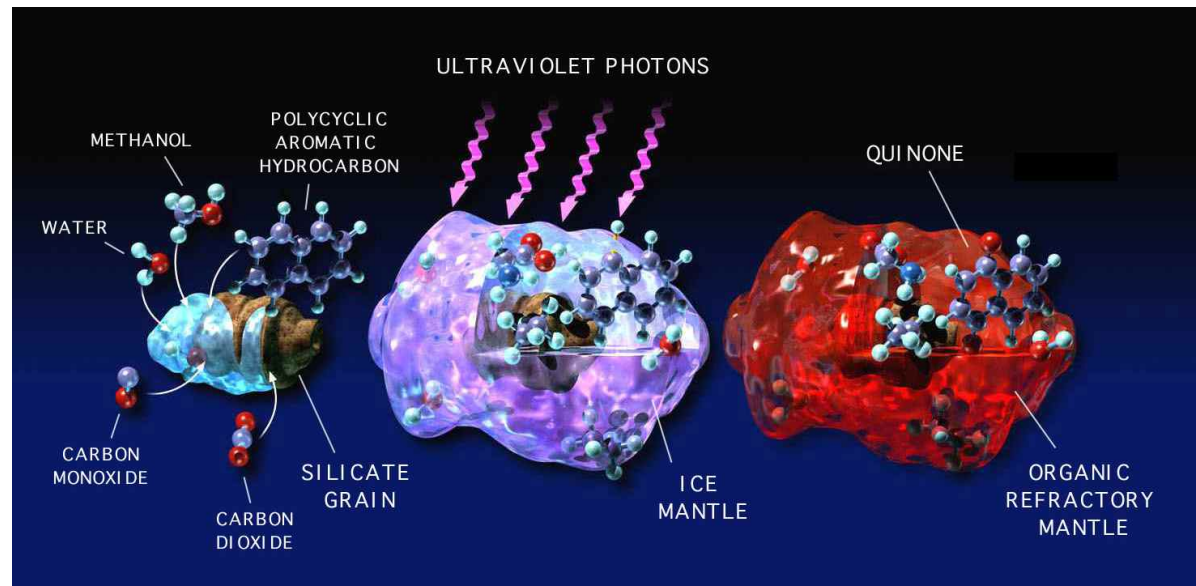
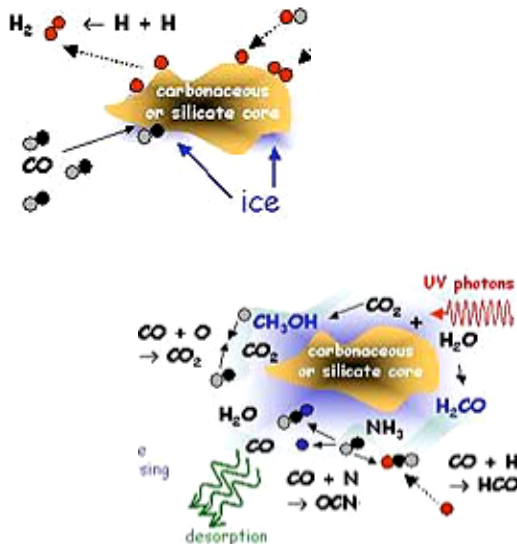
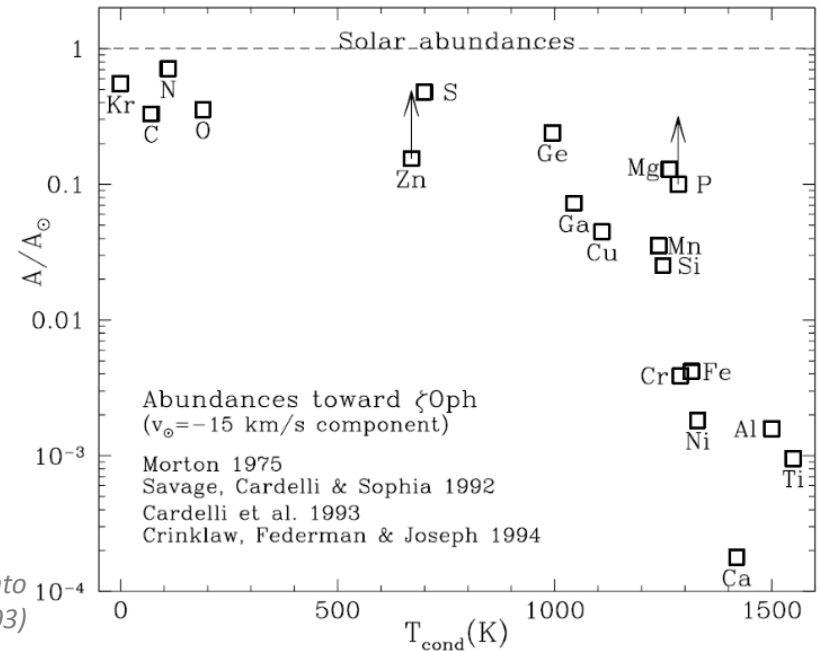
[Minh et al. 2016]

Right Ascension

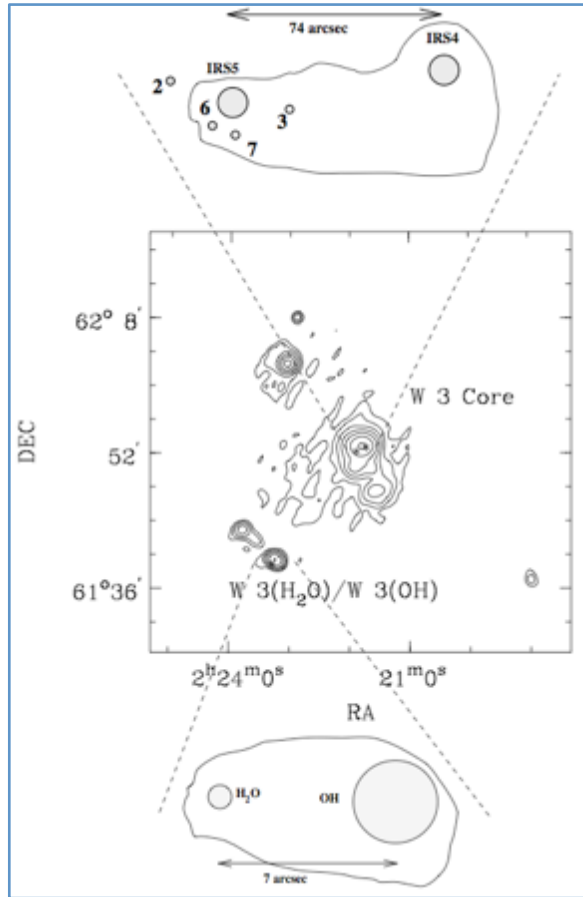
Dust is Crucial in ISM Chemistry

- ◆ 50% of C and 20% of O : locked up in dust grains in dense gas (Interstellar chemistry is carbon-dominated)
- ◆ Most Si and Fe locked up in dense dust grain cores
- ◆ Dust grain surfaces: shield molecules from UV radiation field, produce H_2 through catalysis: $H + H + \text{grain} \rightarrow H_2 + \text{grain}$
- ◆ Drives much of gas-phase chemistry
- ◆ UV photolysis on the surface to form complex molecules in dense gas

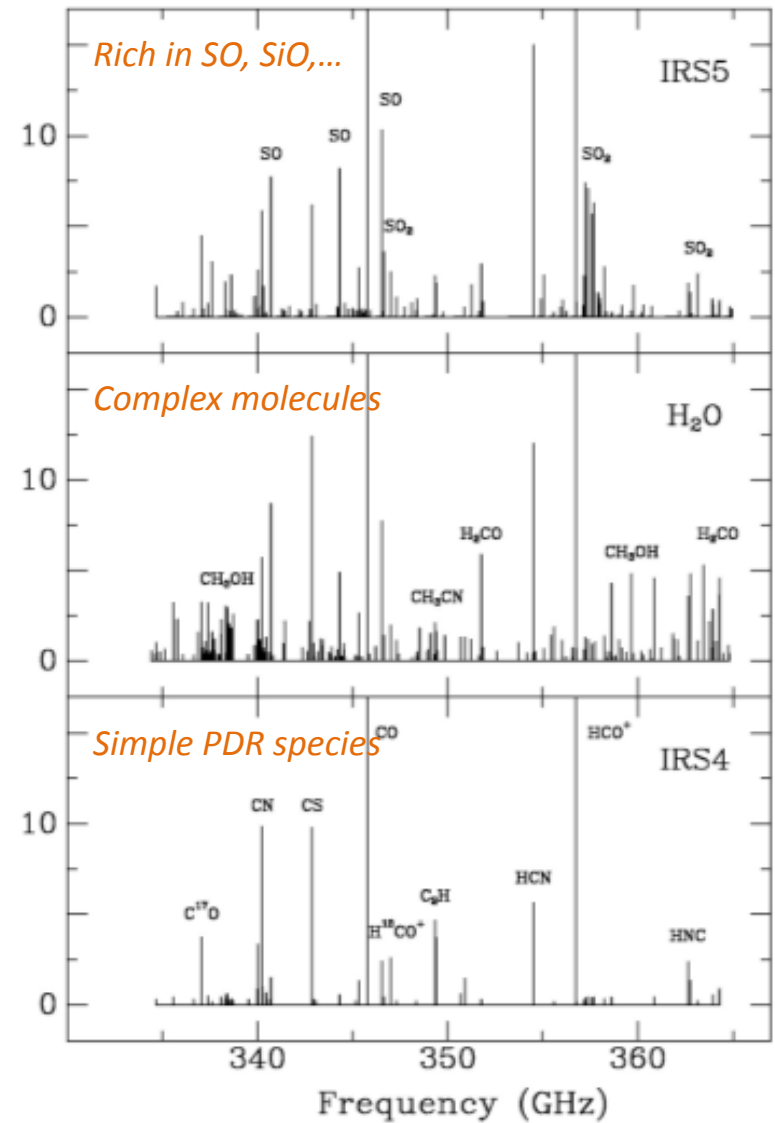
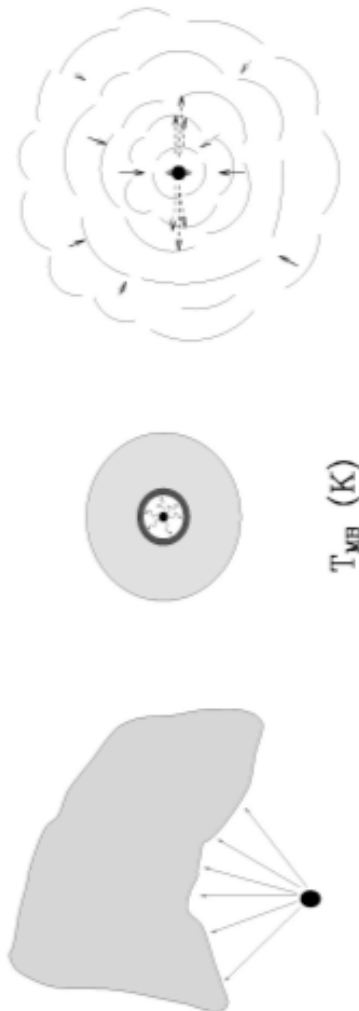
Pattern of the depletion of gas-phase elements onto dust grains measured toward ζ Oph (Drain 2003)



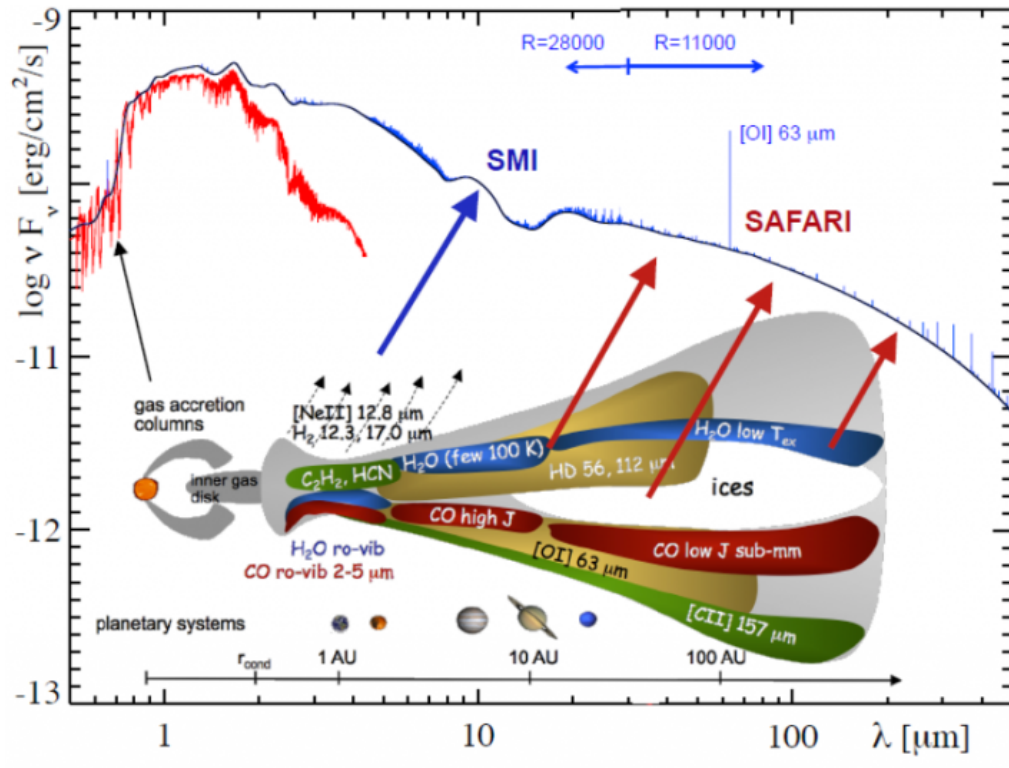
Observational Example of Chemical Evolution: W3



[Helmich & van Dishoeck 1997]



Protoplanetary Disk



Hot Topics:

- Exoplanets
- Formation of Planetesimals
- Transient Disks
- Observation of Disk Gas

[SPICA: <https://spica-mission.org>]

Detected species toward disks (e.g.):

UV: H₂

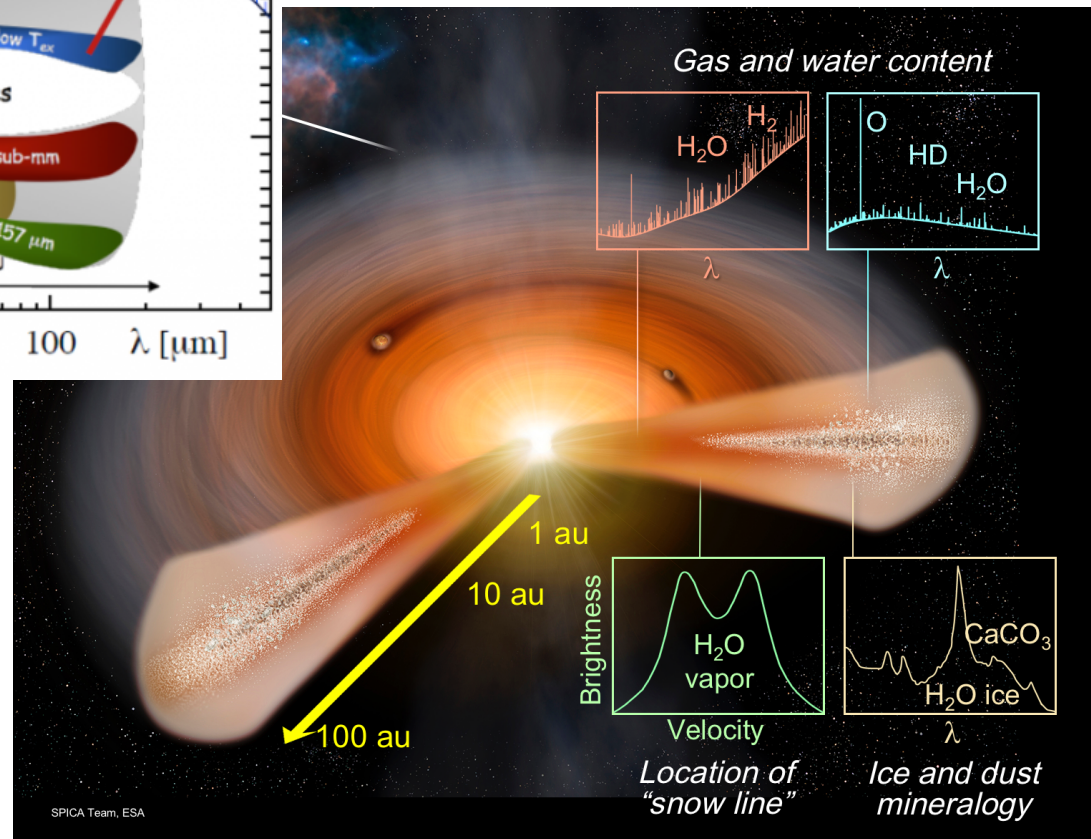
Optical: OI

NIR: H₂, CO, H₂O, OH

mid-IR: H₂, Ne⁺, C₂H₂, HCN, CO₂

Radio: CO, CN, HCN, CS, H₂CO, C₂H, CH₃OH, HCO⁺, DCO⁺, N₂H⁺, ...

Solid: amorphous & crystalline silicates, PAH, ice (H₂O, CO, CO₂, NH₄⁺ ...)



5. Basics of Molecular Parameters: (1) Classification depending on the shapes

- **Linear Molecules** : CO, CS, HCN, HC₃N, ...
- **Asymmetric Tops** : HNCO, SO₂, H₂CO, ...
- **Symmetric Tops** : NH₃, CH₃CN, CH₃CCH, ...

Molecular axis: a, b, c

Moment of Inertia: I

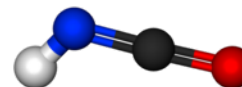
$$I_b = m_b r_b^2$$
$$= \frac{h}{8 \pi^2 B}$$

Molecular constant: A, B, C



Carbon monoxide
(CO)

$B=57.636$ GHz

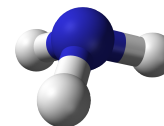


Isocyanic acid
(HNCO)

$A=912.712$ GHz

$B=11.071$ GHz

$C=10.910$ GHz



Ammonia
(NH₃)

$A=B$

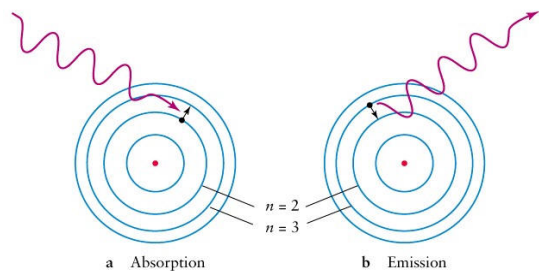
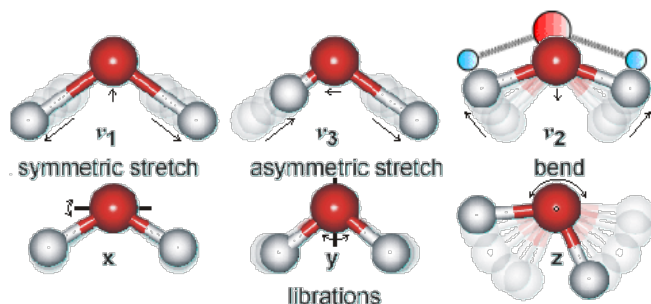
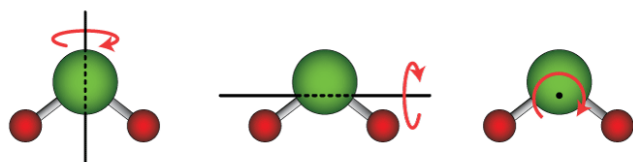
$B=29.819$ GHz

$C=18.670$ GHz

(2) Molecular Transition Modes

Rotational Transitions, Vibrational Transitions, and Electronic Transitions

(e.g.) H_2O



Rotational transitions:

- *Rotational state*: radio and millimeter-wave ($E/k \sim 0.1\text{-}1000\text{K}$)

Vibrational transitions:

- *Vibrational state*: infrared

Electronic transitions:

- *Electronic state*: visible, UV

(3) Rotational Energy Levels: *Quantum Mechanical Solution*

For a linear molecule:

Energy at level J :

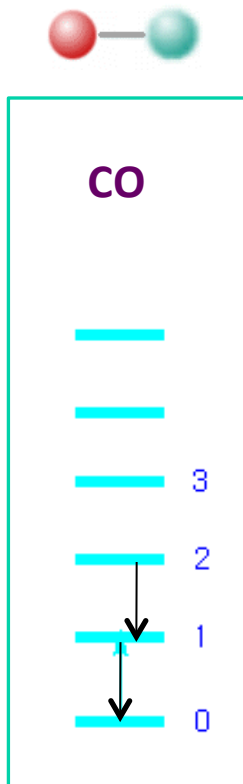
$$E_J = \frac{h^2}{8\pi^2 I} J(J+1)$$

$$= hBJ(J+1)$$

Line frequency between level J and $J-1$:

$$\nu_{J,J-1} = E_J - E_{J-1}$$

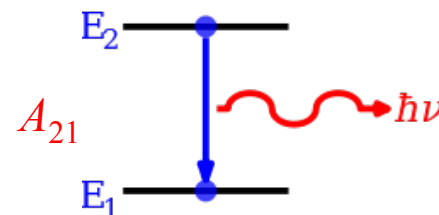
$$= 2B(J+1)$$



$J=2-1$ 230 GHz

$J=1-0$ 115 GHz

Einstein A Coefficient



$$A_{J,J-1} = \frac{64}{3} \frac{\pi^4}{h} \frac{\nu^3}{c^3} \mu^2 \frac{J}{2J+1}$$

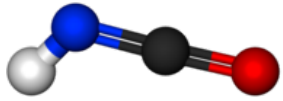
$$= 9.3 \times 10^{-11} B^3 \mu^2 \frac{J^4}{2J+1}$$

Electric dipole moment: μ

CO: $\mu_b = 0.11$ D

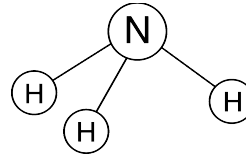
a measure of the separation of positive and negative electrical charges within a system, that is, a measure of the system's overall polarity. The electric-field strength of the dipole is proportional to the magnitude of dipole moment. The SI units for electric dipole moment are coulomb-meter (C·m); however, the most common unit is the debye (D). (Wikipedia)

HNCO



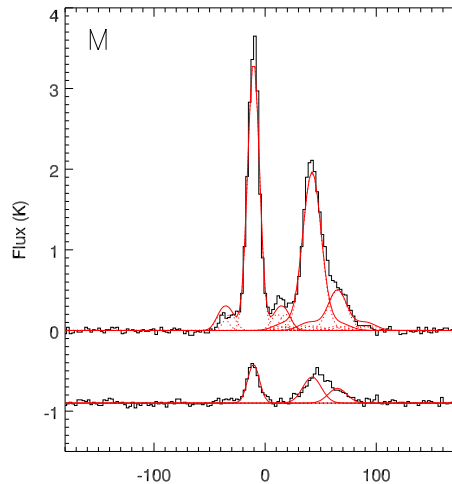
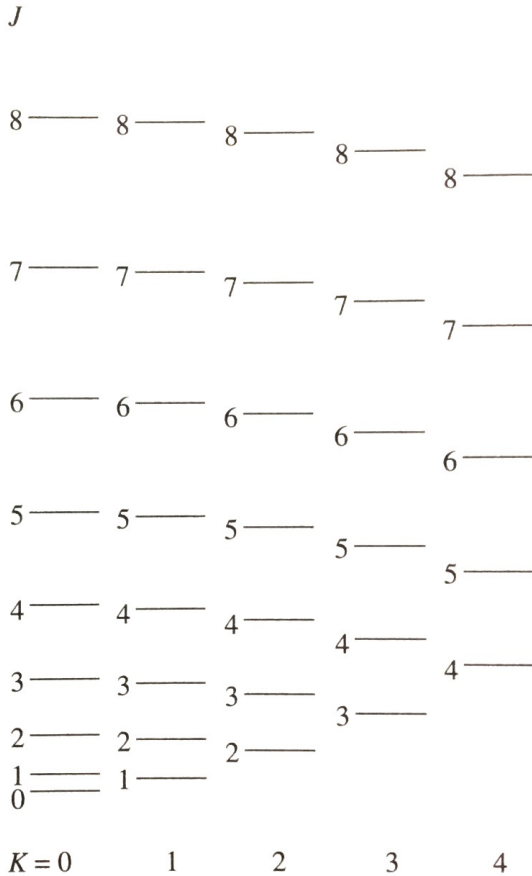
- Prolate (oblate)
- $\mu_a = 1.60$ D
- $\mu_b = 1.35$ D

Ammonia



$$\mu_c = 1.47 \text{ D}$$

A symmetric top with inversion, ortho- and para-, and hyperfine structure



NH_3 (3, 3) & (6, 6) taken
at our Galactic Center
[GBT, Minh et al. 2013]

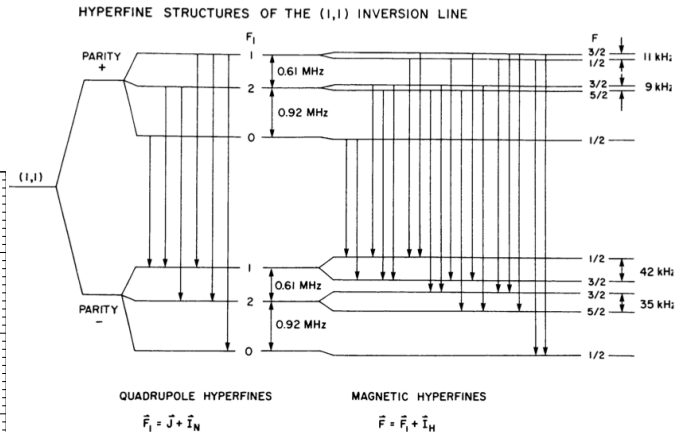
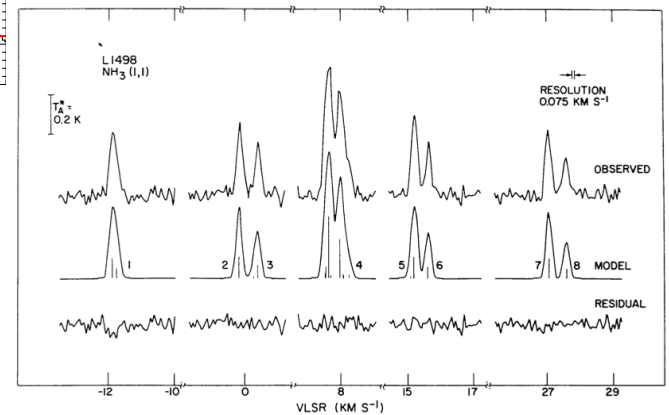


Figure 2 Hyperfine splitting of the $(J, K) = (1, 1)$ transition. The allowed transitions are indicated.



(4) Abundance: Total Column Density

Radiative Transfer - *Optically thin case*:

$$I_\nu(0) = I_\nu(\tau_\nu) + [S_\nu - I_\nu(\tau_\nu)] \tau_\nu$$

$$N_u [\text{cm}^{-2}] = 1.94 \times 10^3 \frac{\nu^2 [\text{GHz}]}{A_{ul} [\text{s}^{-1}]} f_{bc} \int T_B d\nu [\text{K km s}^{-1}]$$

Fractional abundance in the energy level u :

$$f_u = \frac{N_u}{N_{\text{total}}} = \frac{g_u}{Q(T)} e^{-E_u/kT}$$

Partition function: $Q = \sum_{i=1}^M e^{-E_i/kT}$

$$f(E) = \frac{1}{A e^{E/kT}}$$

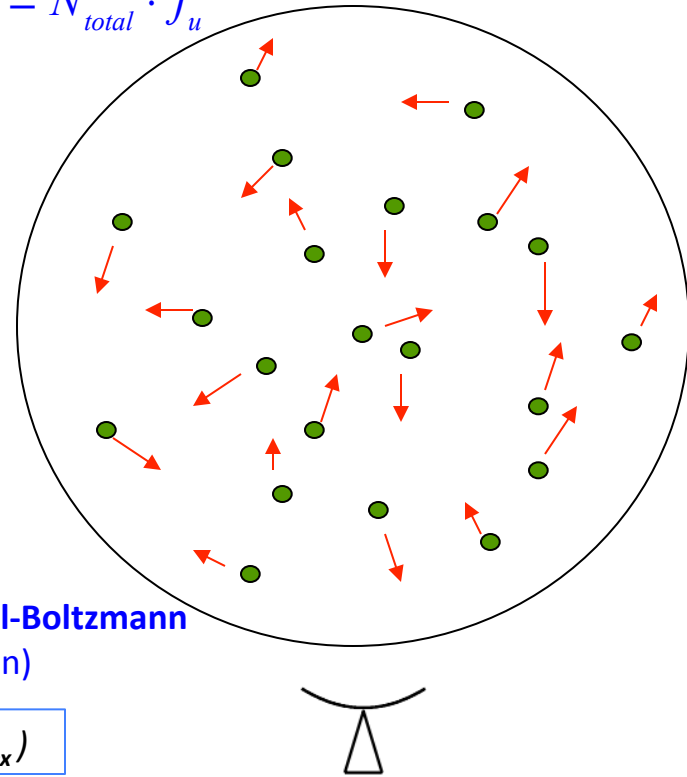
Probability distribution function: Maxwell-Boltzmann Distribution (also called Gibbs distribution)

$T \rightarrow$ Excitation Temperature (T_{ex})

cf: Minh 1994

$$\tau = \frac{c^2}{8 \pi \nu^2} \phi(\nu) A_{ul} N_u \left(e^{\frac{h\nu}{kT_{\text{ex}}}} - 1 \right)$$

$$N_u = N_{\text{total}} \cdot f_u$$



T_B

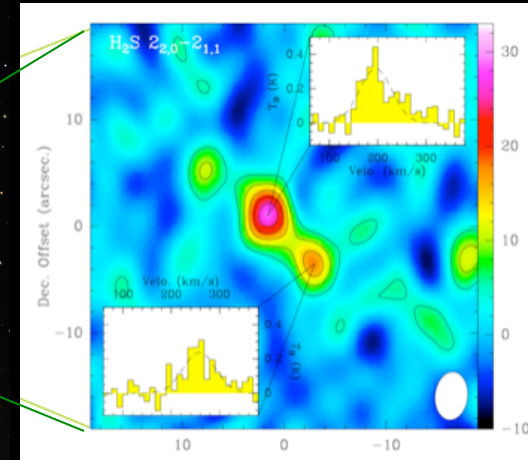
Observed power (E) $\rightarrow T(E = kT) \rightarrow$ Several corrections $\rightarrow T_B$ (Brightness T of the source)

6. Examples of Molecular Line Observations

NGC 253

Starburst galaxy (D~3.5 Mpc) in the Sculptor. Almost edge-on barred Sc galaxy
Optical: dominated by dust pattern ~ a normal spiral galaxy except the nucleus, where (probably) AGN is embedded.

Image Credit: D. Hager & E. Benson



SMA: H₂S (Minh et al. 2007)



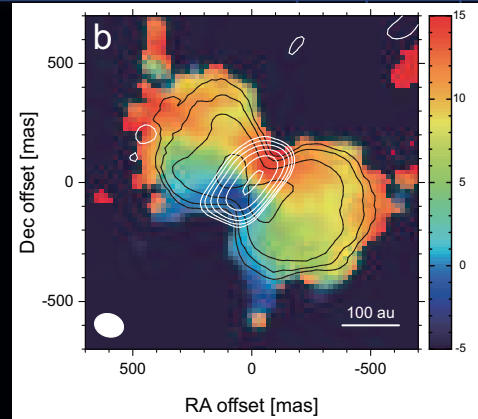
ALMA



484GHz Si¹⁸O line
490GHz continuum

Hirota et al. 2017

Motion of outflows



Star-forming Core in Orion

ALMA observations with Si¹⁸O and dust continuum (Hirota+ 2017)

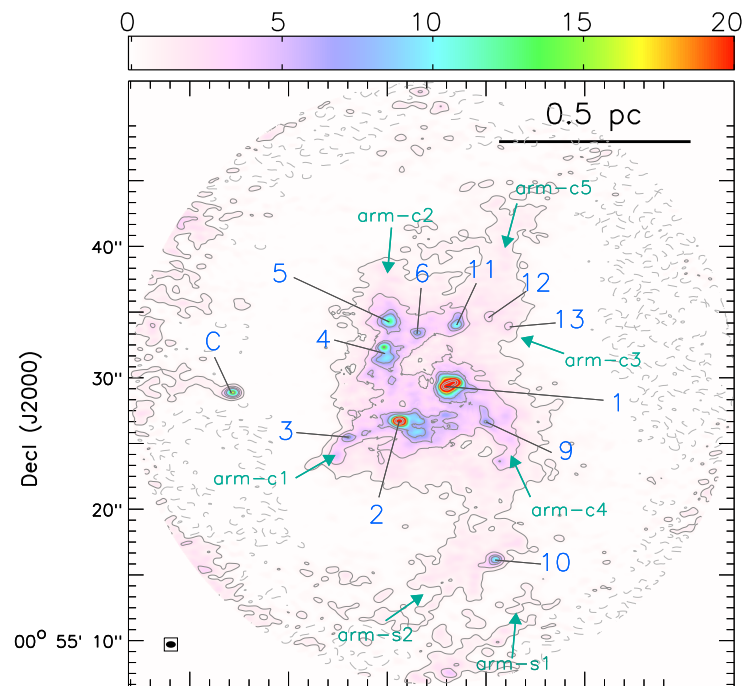
from K. Hada's slide



Massive Star-forming Region G33.92+0.11

- UC HII region, Distance ~ 7.1 kpc, $L_{bol}(\text{OB cluster}) \sim 2.5 \times 10^5 L_{sun}$, Mass $\sim 10^5 M_{sun}$ (in the ~ 5 pc area),
- Nearly face-on projection at an early evolutionary stage
- ALMA 12m + ACA : ~ 210 -230 GHz
- **2014** May: $\theta=0.6$ -0.8"; **2017** August: $\theta=0.1$ -0.2"
 ^{13}CS , CH_3OH , CH_3CN , OCS , H_2S , SO_2 , SiO , CN , C_3H_2 , ...

(1) **Dust continuum** – overall density tracer
 (2) **CS** – dense gas density, (3) **CH_3OH , CH_3CN** – hot core
 (4) **SiO** – shock/outflow, (5) **HDCS, DCN** – deuteration
 (6) **H_2S** – shock/high T , (7) **CN/HCN ratio** – PDR
 C_2D , $c\text{-C}_3\text{H}_2$, ...



Dust continuum image (free-free subtracted by model, ALMA: Liu et al. 2015)



(1) Continuum Emission from Dust

Thermal Dust Continuum: Gas (+ dust) distribution, Abundance, Mass, ..

T_{dust} : balance between grain heating and cooling

$$I_{\nu} \propto T_{dust} \pi a^2 Q_{ext} N_d$$

$$M_d \approx N_d \frac{4\pi}{3} a^3 \rho_d$$

$$Q_{ext} \sim \lambda^{-\beta}$$

$\beta = 0$: for a BB

$\beta = 1$: for amorphous material

$\beta = 2$: for metal and crystal

$\beta \approx 1.7$: $\sim$ ISM

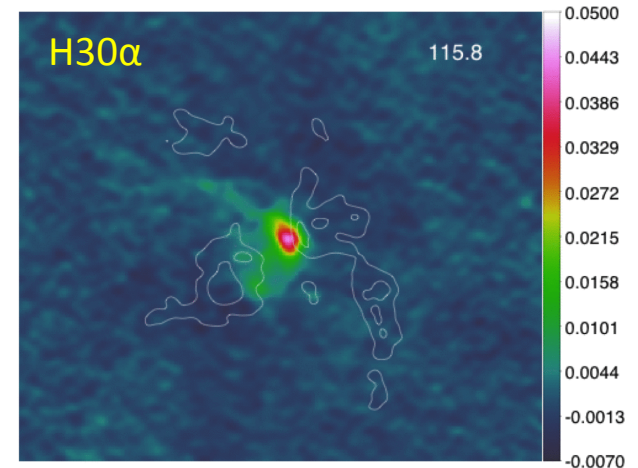
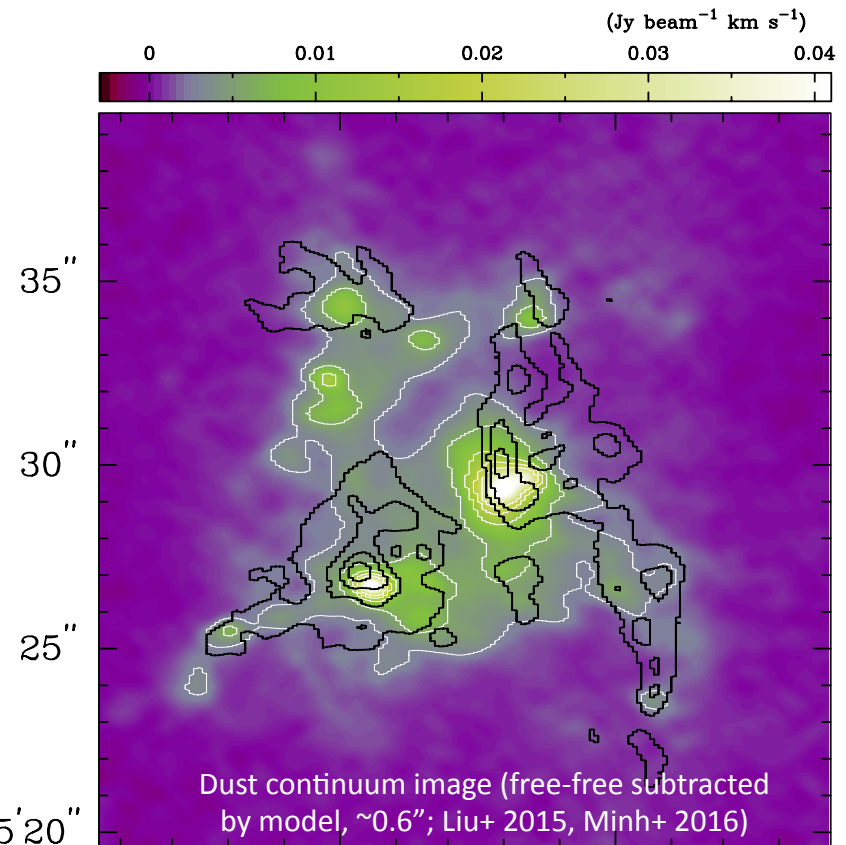
Observed Dust Continuum Flux

$\rightarrow (T_{dust}, Q, \text{Size, Distance..})$ **Dust Density, Dust Mass**

$\rightarrow (\text{Gas/Dust Ratio})$ **Gas Density, (Total) Gas Mass**

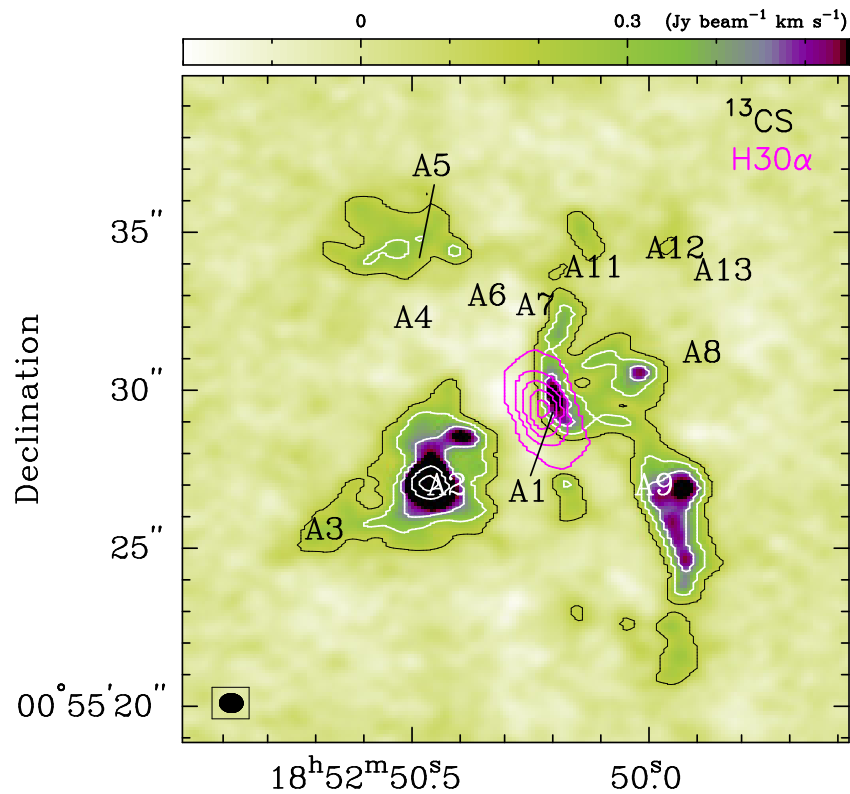
Declination

00°55'20"



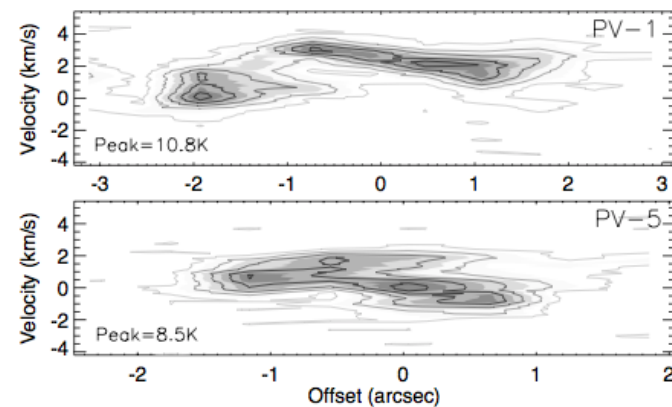
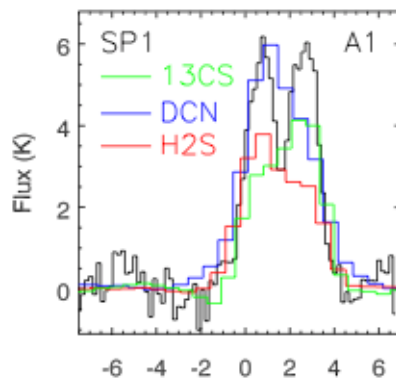
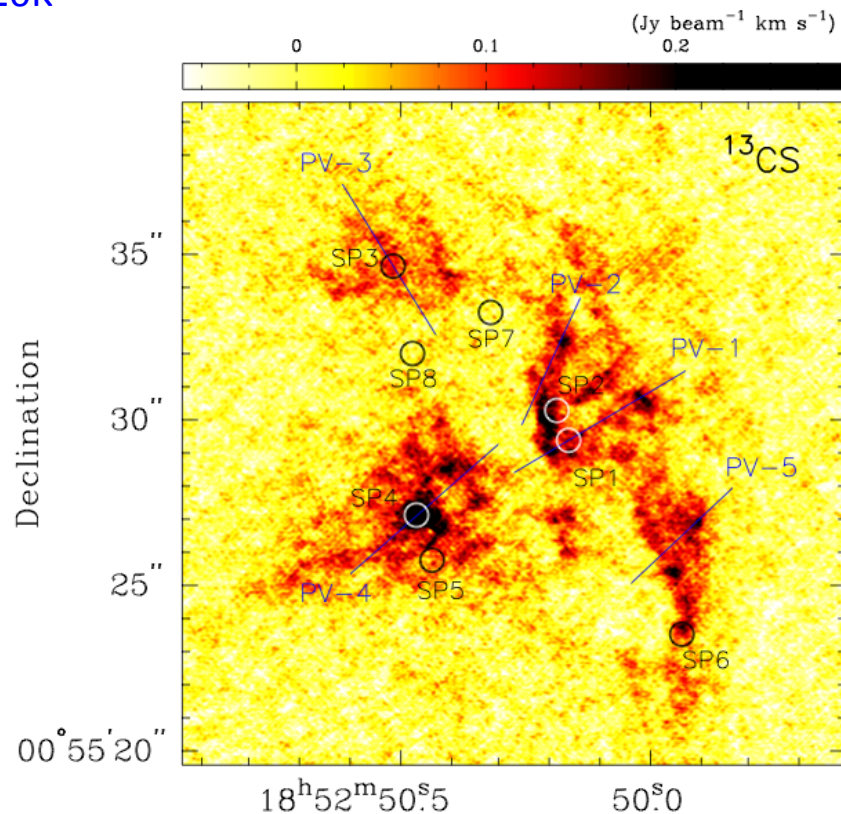
(2) CS

$$n_{\text{crit}} = 5.3 \times 10^6 \text{ cm}^{-3} \text{ for } ^{12}\text{CS 5-4 at 20K}$$



Right Ascension
[Minh et al. 2016]

[Minh et al. to be submitted]



$n_{crit} \equiv \frac{A_{ij}}{C_{ij}}$ This equation only holds in the optically thin limit. If the transition becomes optically thick, the critical density is lowered by $1/\tau$, since part of the emitted photons are reabsorbed, with no net effect on the level populations.

$$C_{ij} = n_{col} K_{ij}$$

C_{ij} : Collision rate
 K_{ij} : Collision rate coefficient
(velocity integrated cross section)

(e.g.) LAMDA (Leiden Atomic and Molecular Database)
<https://home.strw.leidenuniv.nl/~moldata/>

Molecule	Transition	Frequency (GHz)	E_{upper} (K)	n_{crit}^a (cm^{-3})
CO	$1 \rightarrow 0$	115.271	5.5	4.1 (2)
	$2 \rightarrow 1$	230.538	16.6	2.7 (3)
	$3 \rightarrow 2$	345.796	33.2	8.4 (3)
	$4 \rightarrow 3$	461.041	55.3	1.9 (4)
	$7 \rightarrow 6$	806.652	154.9	9.4 (4)
CS	$2 \rightarrow 1$	97.981	7.1	8.0 (4)
	$3 \rightarrow 2$	146.969	14.1	2.5 (5)
	$5 \rightarrow 4$	244.936	35.3	1.1 (6)
	$7 \rightarrow 6$	342.883	65.8	2.9 (6)
	$10 \rightarrow 9$	489.751	129.3	8.1 (6)
CN	$2 \frac{5}{2} \rightarrow 1 \frac{3}{2}$	226.874	16.3	1.4 (6)
	$3 \frac{7}{2} \rightarrow 2 \frac{5}{2}$	340.248	32.7	6.0 (6)
HCN	$1 \rightarrow 0$	88.632	4.3	2.3 (5)
	$3 \rightarrow 2$	265.886	25.5	4.1 (6)

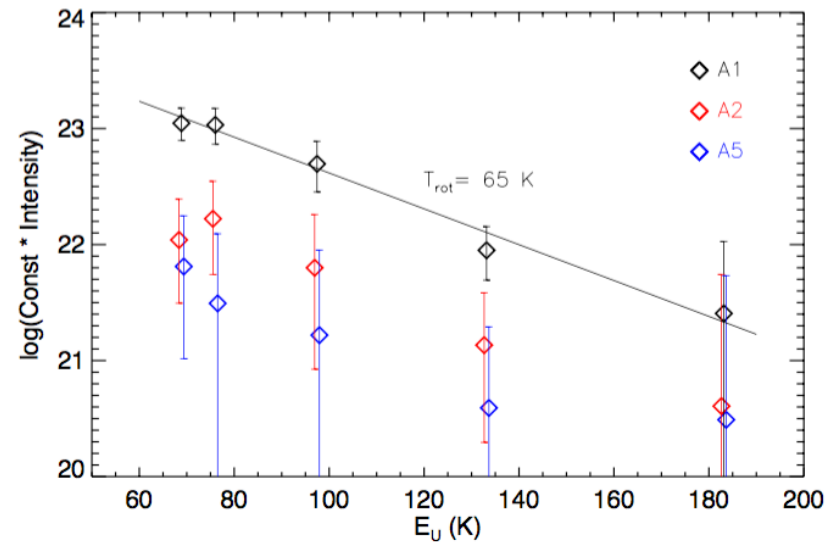
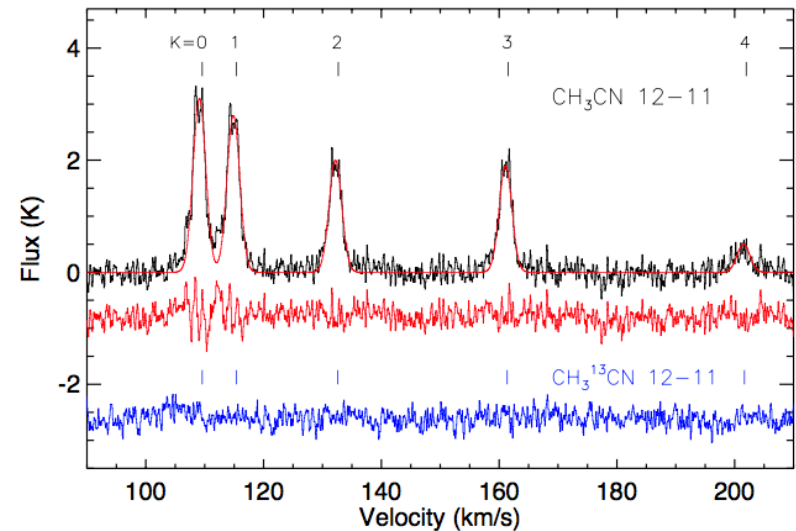
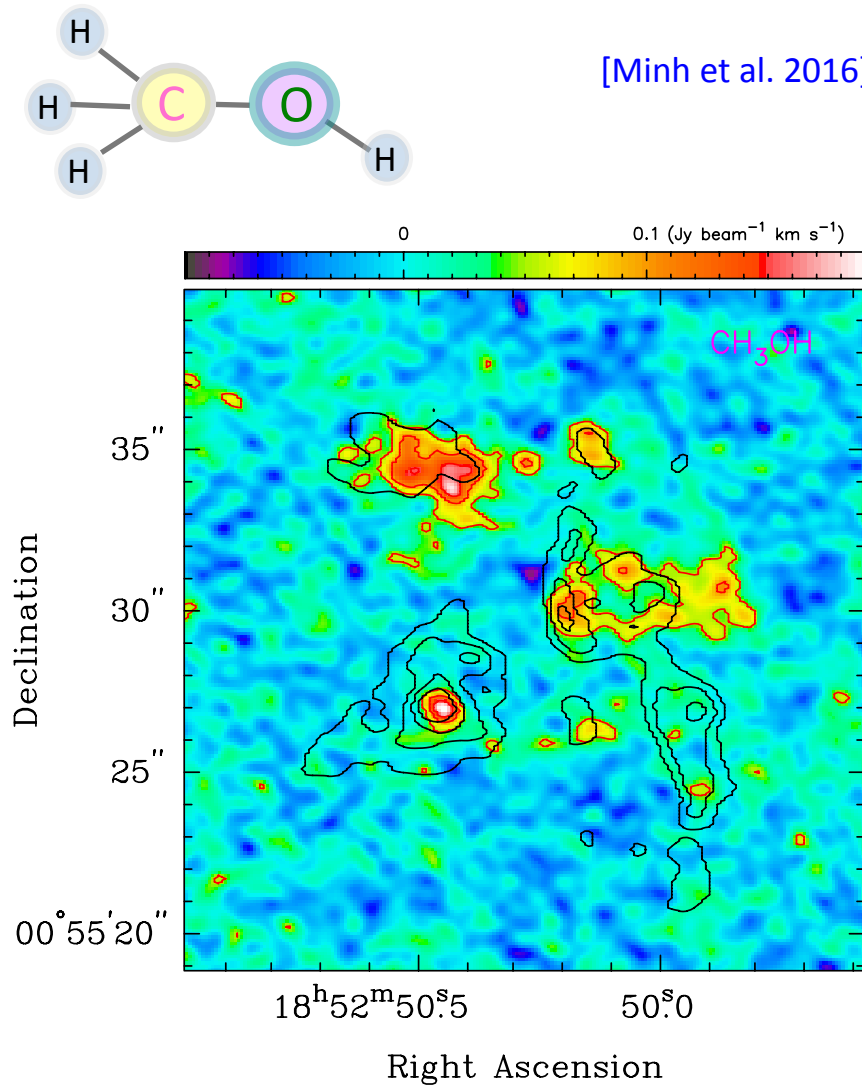
HCO ⁺	$4 \rightarrow 3$	354.506	42.5	8.5 (6)
	$1 \rightarrow 0$	89.189	4.3	3.4 (4)
	$3 \rightarrow 2$	267.558	25.7	7.8 (5)
H ₂ CO (para)	$4 \rightarrow 3$	356.734	42.8	1.8 (6)
	$2_{02} \rightarrow 1_{01}$	145.603	10.5	1.6 (5)
	$3_{03} \rightarrow 2_{02}$	218.222	21.0	4.7 (5)
	$5_{05} \rightarrow 4_{04}$	362.736	52.3	1.9 (6)
	$3_{22} \rightarrow 2_{21}$	218.476	68.1	2.3 (5)
H ₂ CO (ortho)	$5_{23} \rightarrow 4_{22}$	365.363	99.7	1.6 (6)
	$2_{12} \rightarrow 1_{11}$	140.840	21.9	1.0 (5)
	$2_{11} \rightarrow 1_{10}$	150.498	22.6	1.2 (5)
	$3_{12} \rightarrow 2_{11}$	225.698	33.5	4.5 (5)
	$5_{15} \rightarrow 4_{14}$	351.769	62.5	1.7 (6)
	$5_{33} \rightarrow 4_{32}$	364.340	158.4	1.3 (6)
	$2 \rightarrow 1$	86.847	6.3	1.3 (5)
SiO	$5 \rightarrow 4$	217.105	31.3	1.7 (6)
	$6 \rightarrow 5$	260.518	43.8	2.9 (6)
	$8 \rightarrow 7$	347.331	75.0	6.4 (6)
SO	$2_2 \rightarrow 1_1$	86.094	19.3	8.5 (4)
	$5_6 \rightarrow 4_5$	219.949	35.0	5.6 (5)
	$5_5 \rightarrow 4_4$	215.220	44.1	4.8 (5)
	$6_5 \rightarrow 5_4$	251.826	50.7	6.2 (5)
	$6_6 \rightarrow 5_5$	258.256	56.5	7.9 (5)
OCS	$8_9 \rightarrow 7_8$	346.528	78.8	2.0 (6)
	$8_7 \rightarrow 7_6$	340.714	81.2	1.5 (6)
	$8_8 \rightarrow 7_7$	344.310	87.5	1.8 (6)
	$18 \rightarrow 17$	218.903	99.8	5.1 (4)
	$20 \rightarrow 19$	243.218	122.6	7.0 (4)
	$21 \rightarrow 20$	255.374	134.8	8.1 (4)
	$22 \rightarrow 21$	267.530	147.7	9.4 (4)
	$28 \rightarrow 27$	340.449	237.0	1.9 (5)

^a Calculated for $T_{kin} = 100$ K in the optically thin limit.

(3) CH₃OH and CH₃CN

Saturated, hot core species trace star-forming dense cores

[Minh et al. 2016]



$$R = \text{CH}_3\text{OH} / \text{CH}_3\text{CN}$$

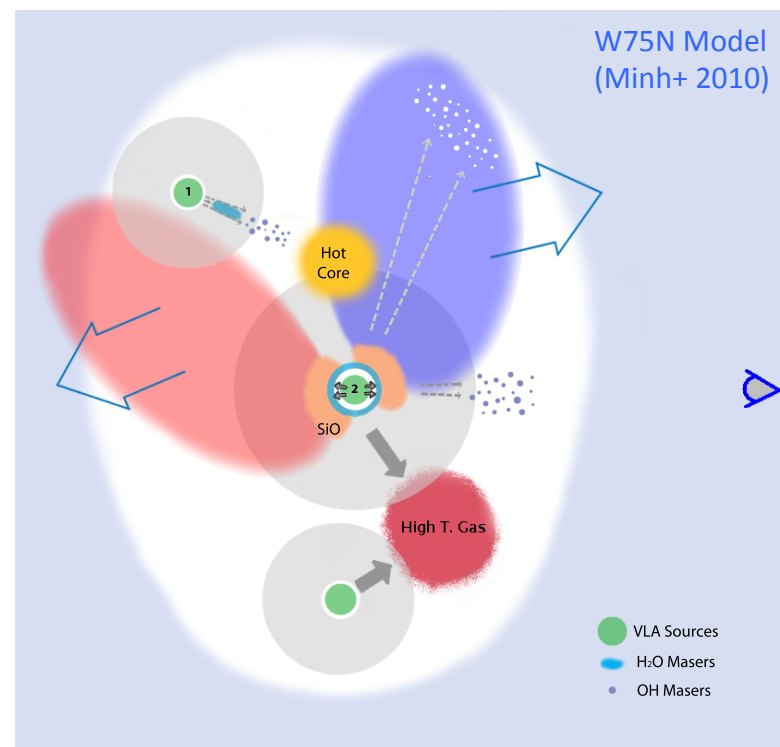
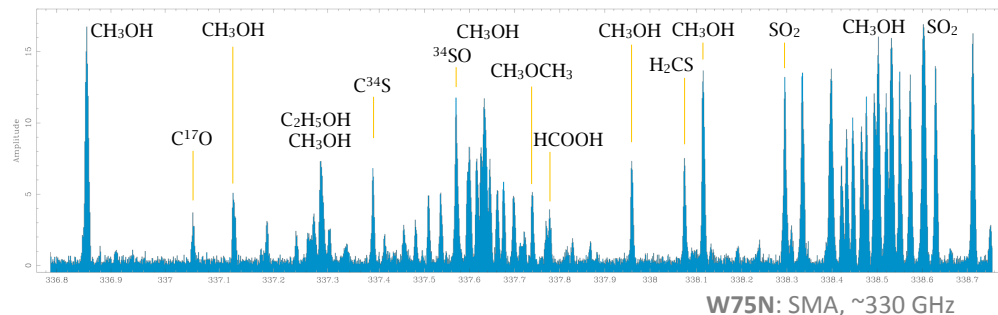
$$R = 5: \text{A1} \rightarrow \sim 10^5 \text{ yrs} ; R = 24: \text{A2, A5} \rightarrow \sim 10^4 \text{ yrs}$$

Hot Core

- Represent one of the earliest stages in the evolution of massive stars.
- Appear immediately after the formation of a protostar but before the protostar has sufficient power to ionize all of the surrounding gas.
- small ($10^{-2} - 10^{-1}$ pc), dense ($\geq 10^7$ H₂ cm⁻³), and relatively warm (≥ 100 K) gas cores
- exist in the vicinity (≤ 0.1 pc) of newly formed massive stars
- believed to be the remnants of the cloud that collapsed in the process of forming the massive star
- Hot cores have rich chemistry: especially in saturated molecules $\leftarrow$ from the evaporation of ice mantles frozen-out onto the grains during the cloud collapse

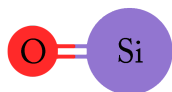
Various molecular lines detected in the hot cores provide unique tools for understanding the very early phase of star-forming processes.

Observations of Massive Star-forming Region, W75N



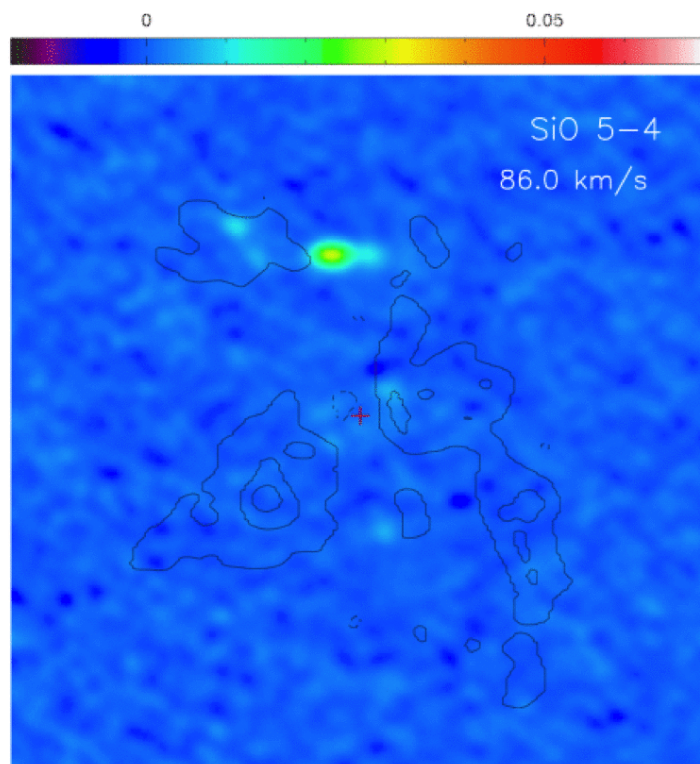
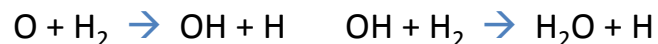
(4) SiO

Shock (outflow) tracer



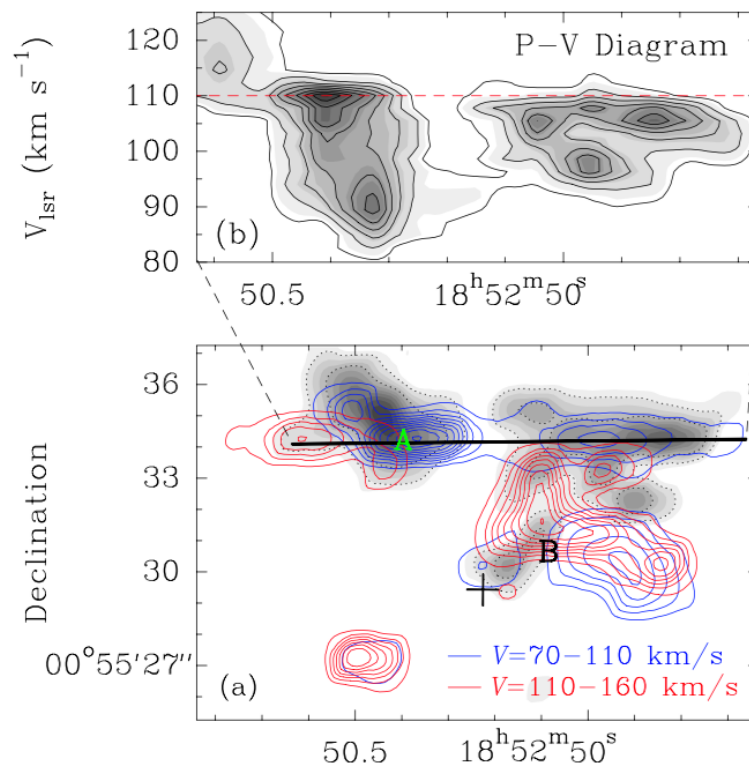
Si-containing species ← grain destruction, sputtering, ..

SiO chemistry: shocks



SiO in G33.92+0.11: **Outflows**

[Minh et al. 2016]



(5) HDCS, DCN

Deuteration: H_2D^+ and HD_2^+
 CH_2D^+

[Minh et al. 2018]

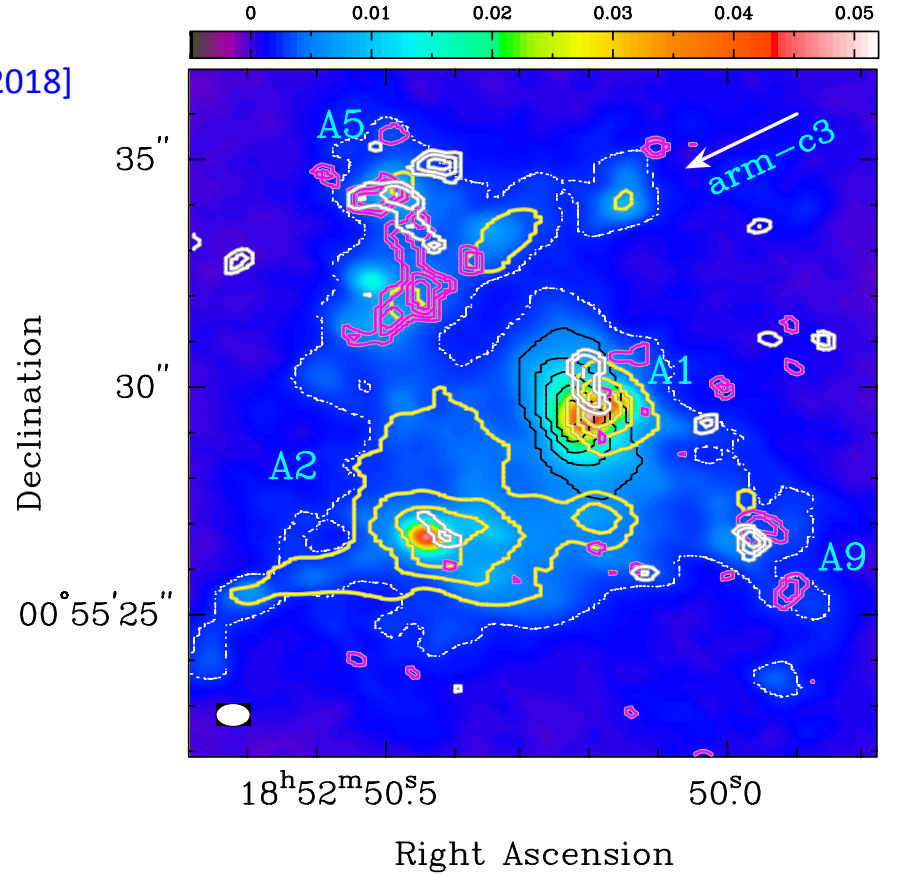
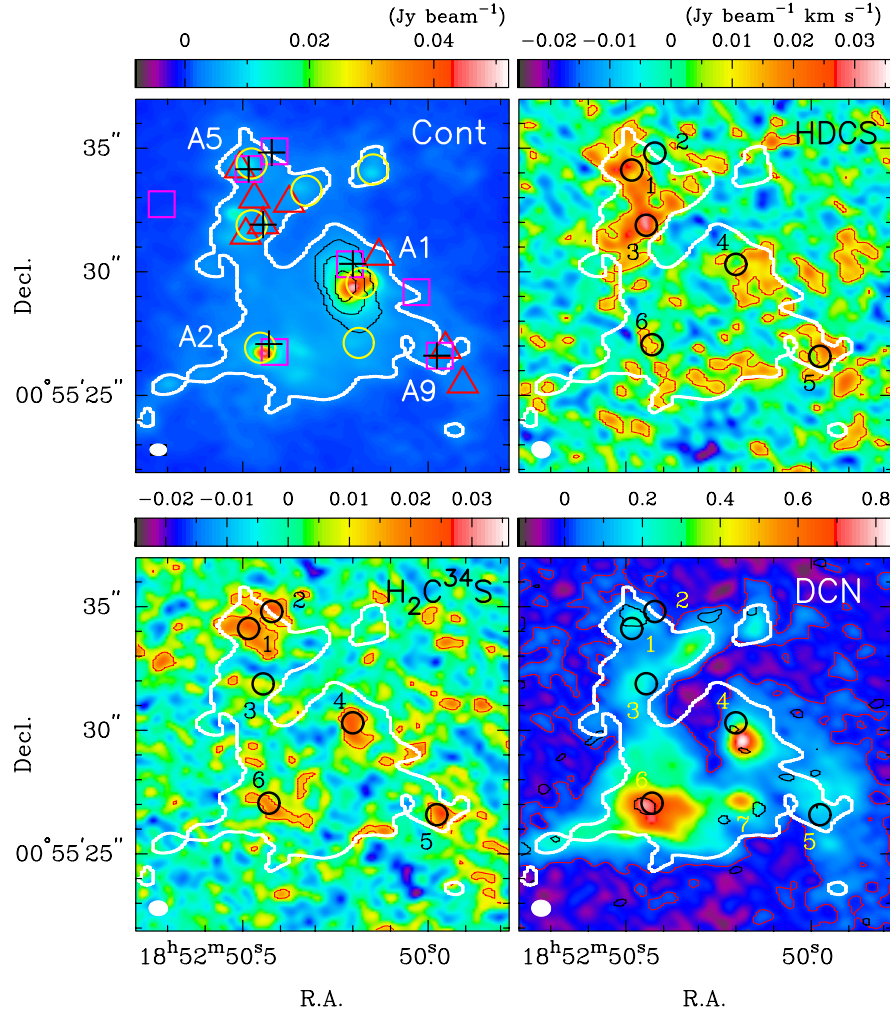
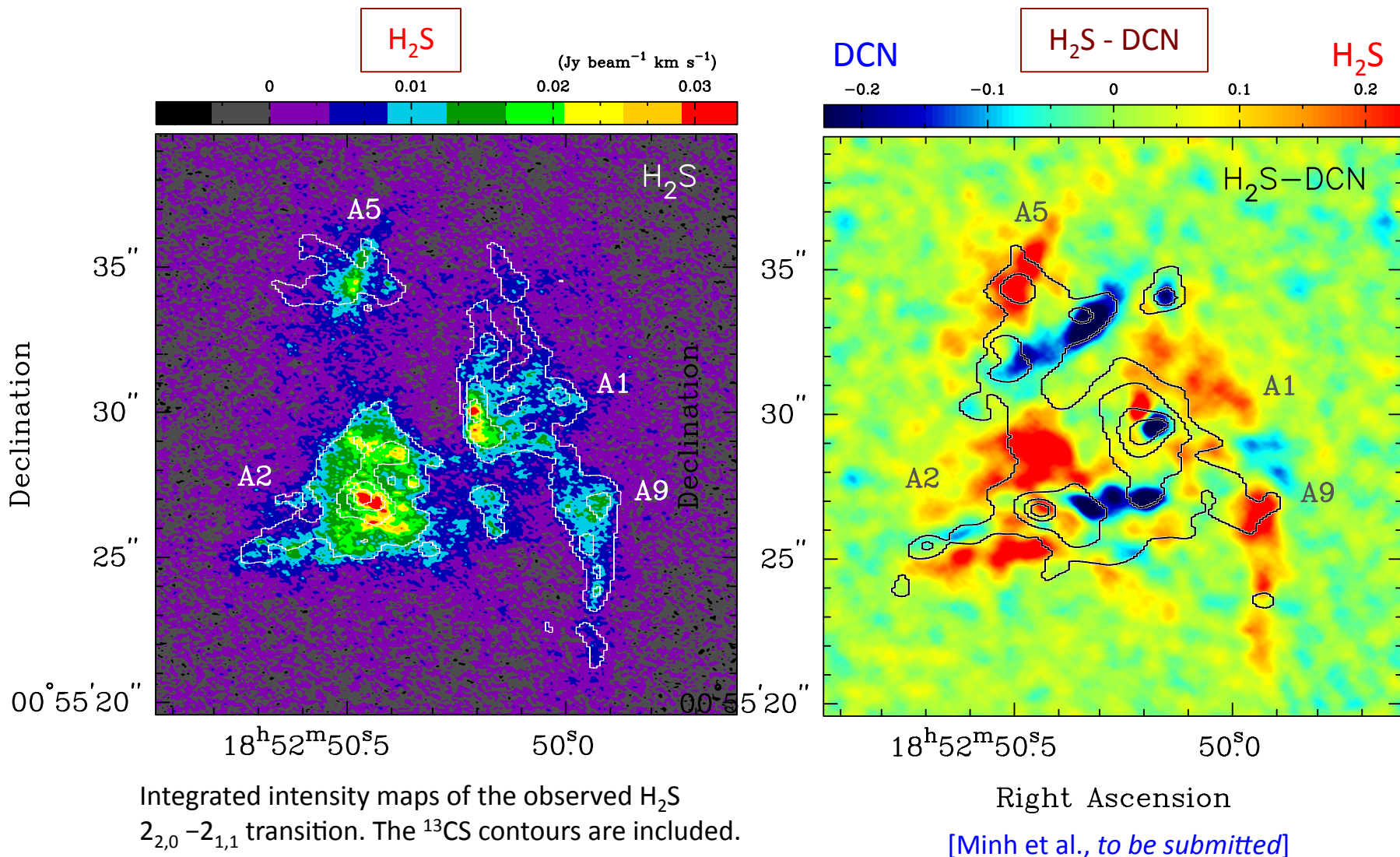


Table 2: Abundances of the observed species.

Pos. ^a	DCN (cm ⁻²) [%]	HDCS (cm ⁻²) [%]	H ₂ C ³⁴ S (cm ⁻²) [%]	¹³ CS (cm ⁻²) [%]	DCN H ₂	H ₂ CS H ₂	HDCS H ₂ CS	DCN HDCS
1 (A5)	0.8(13) [29]	2.9(13) [32]	3.5(13) [25]	2.0(13) [14]	1.5(-10)	1.4(-8)	0.028	0.40
2 (A5)	0.3(13) [30]	0.8(13) [47]	3.0(13) [29]	2.2(13) [14]	0.5(-10)	1.1(-8)	0.014	0.32
3	0.9(13) [29]	2.5(13) [31]	1.1(13) [29]	-	-	-	0.117	0.35
4 (A1)	1.3(13) [29]	1.0(13) [40]	3.6(13) [25]	4.7(13) [14]	1.1(-10)	0.6(-8)	0.013	1.35
5 (A9)	0.7(13) [29]	1.4(13) [39]	3.0(13) [30]	5.8(13) [14]	0.5(-10)	0.4(-8)	0.023	0.49
6 (A2)	2.9(13) [29]	1.2(13) [36]	2.5(13) [72]	7.8(13) [14]	1.5(-10)	0.3(-8)	0.025	2.38

(6) H_2S

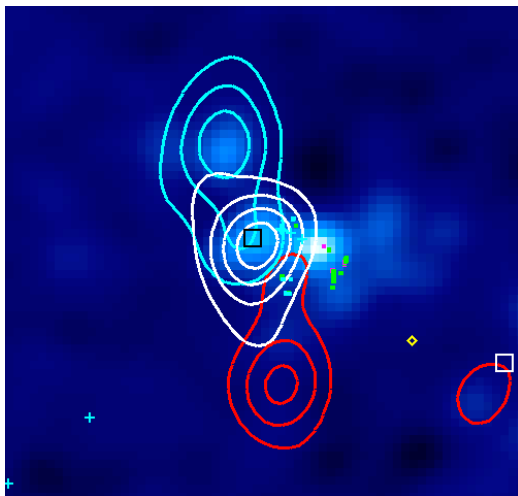
Sulfur is highly depleted in the dense quiet ISM (but not depleted in the diffuse medium). The sum of the detectable S-bearing molecules in cold molecular cloud is only a very small fraction of the elemental S abundance.



Sulfur Chemistry in Massive Star-forming Regions

- Sulfur is highly depleted in the dense quiet ISM (but not depleted in the diffuse medium).
- The major reservoir of S in cold molecular clouds is a long standing and unresolved problem.
The sum of the detectable S-bearing molecules in cold molecular cloud: only a very small fraction of the elemental S abundance.
- The chemical models - the main reservoir of sulfur is H_2S on grain mantles: injecting H_2S into the gas phase $\rightarrow \text{S} \rightarrow \text{SO} \rightarrow \text{SO}_2$ (Their abundance ratios are function of time.)
- But *ISO*: low solid H_2S (mantle H_2S cannot exceed $\sim 10^{-7} / \text{H}_2$), OCS is the only S-bearing species firmly detected on granular surface, but relatively low fractional abundance of 10^{-7} (Palumbo et al. 1997)

Probably not in the form of H_2S , but OCS or H_2CS ? in solid state of grain mantle...



H_2CS outflow in DR21(OH)

[Minh et al. 2011]

two possibilities to interpret:

- Evaporation of H_2CS directly from the mantle $\rightarrow$ **solid H_2CS**
- H_2CS formation from the evaporated S in the shocked gas

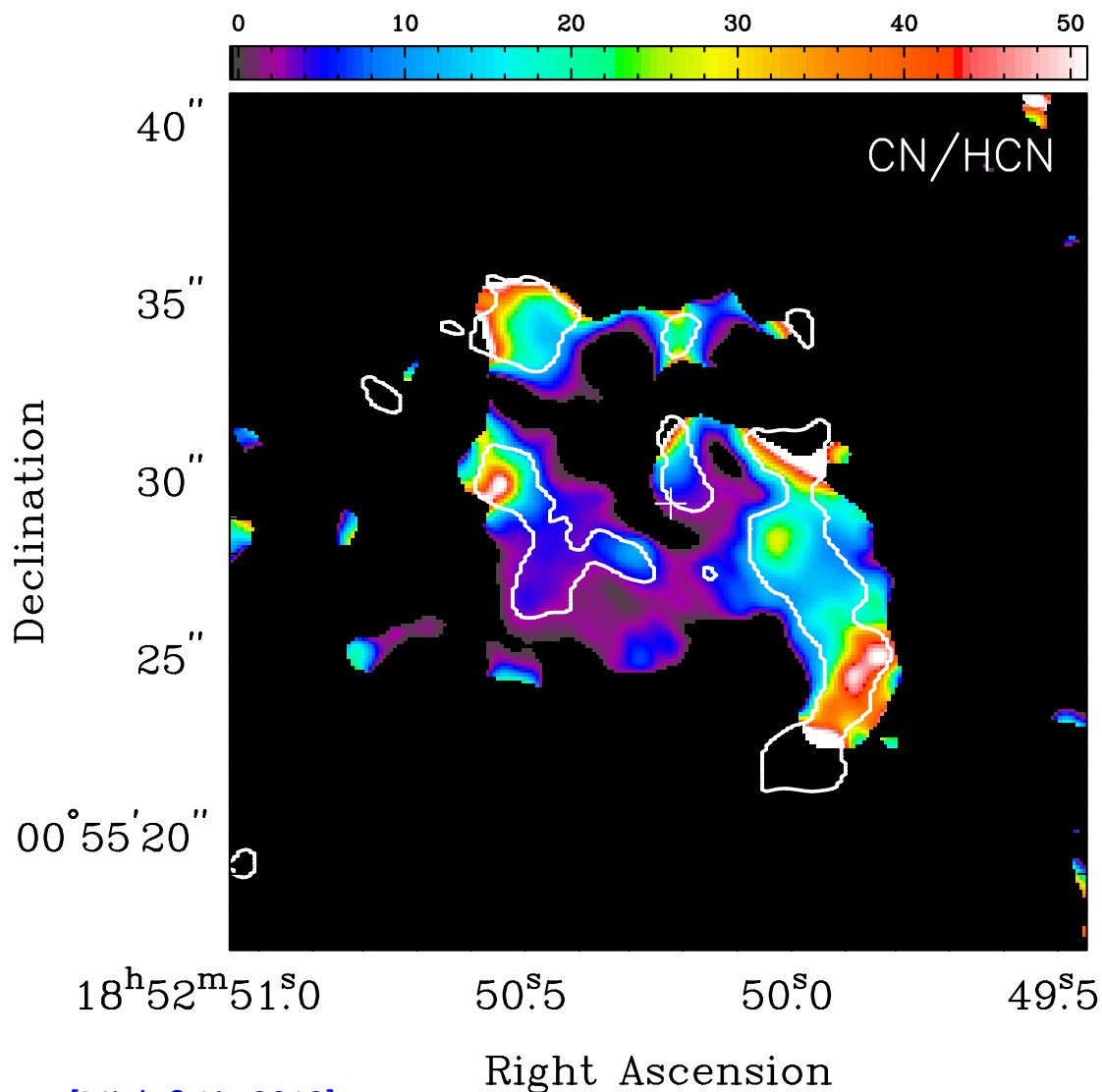
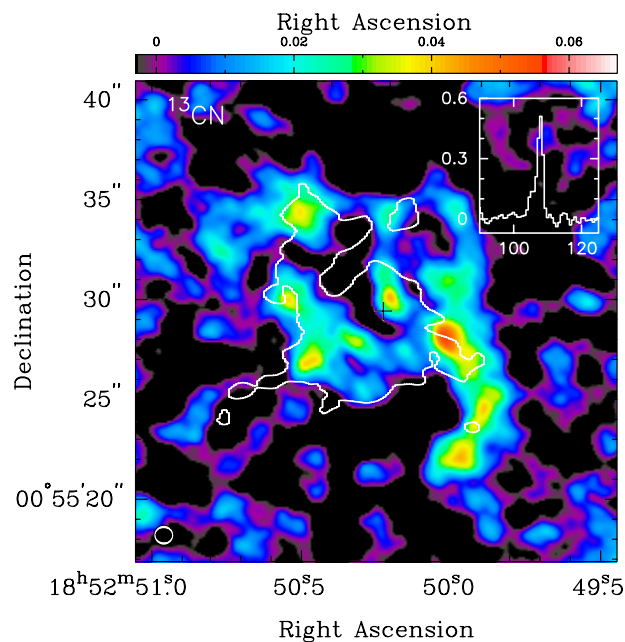
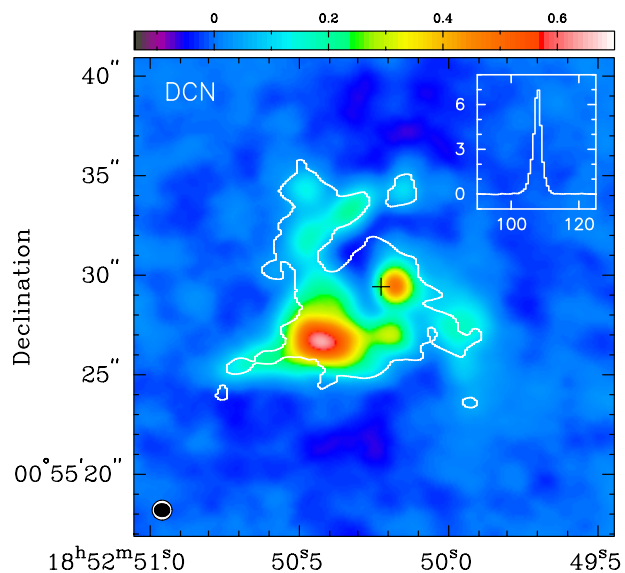
Depleted S or CS $\rightarrow$ OCS or H_2CS ?

Hydrogenation or oxygenation ?

MM1b - no H_2CS emission: very early time species?

(7) CN/HCN Ratio

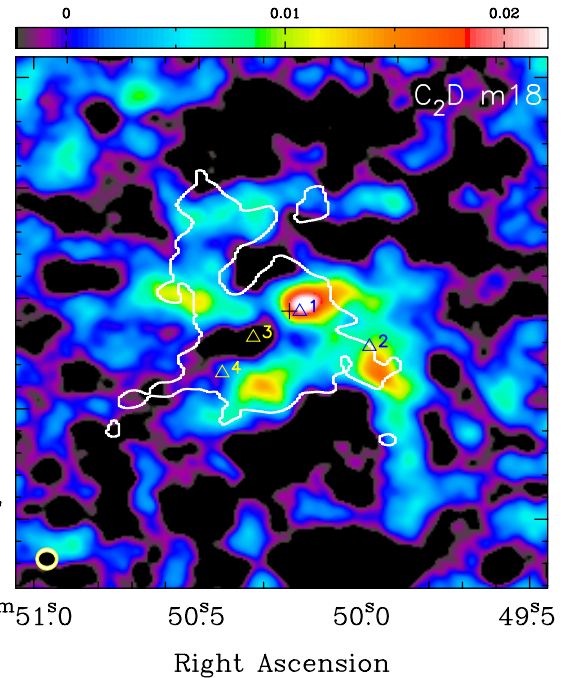
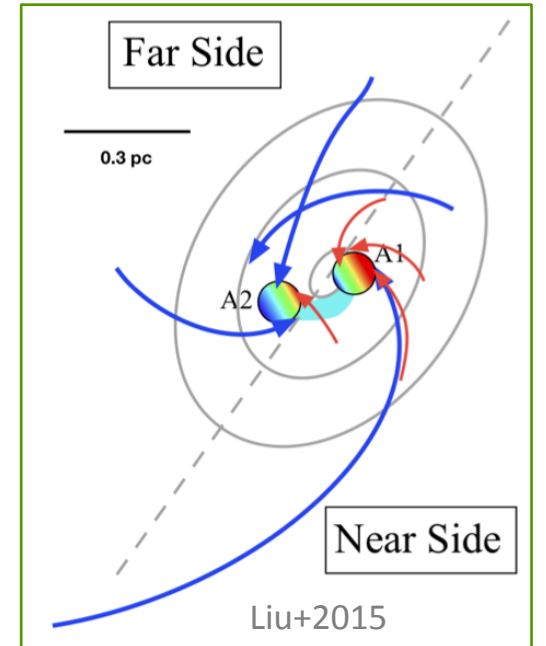
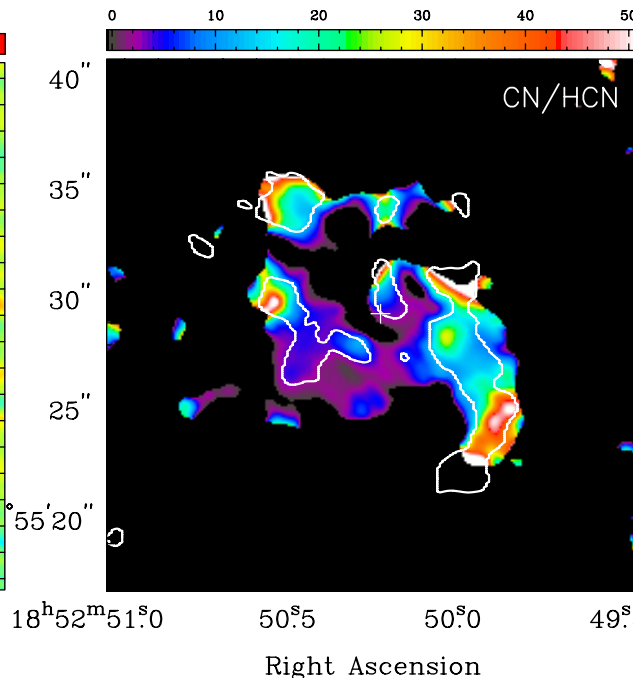
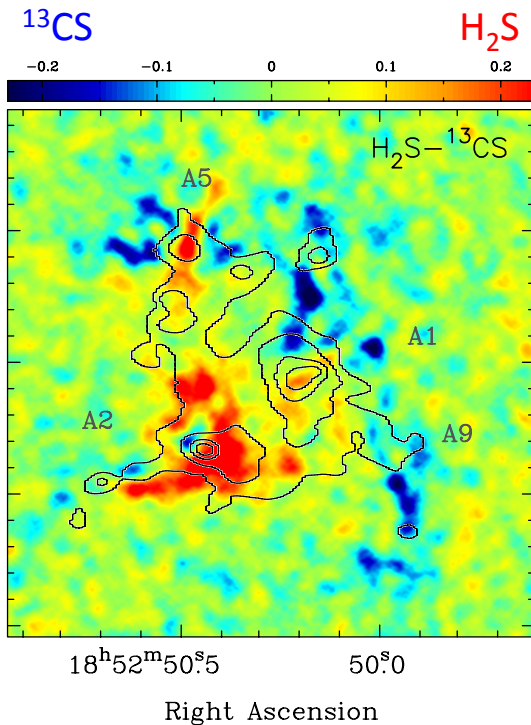
$$\text{CN} \leftarrow \text{HCN} + (uv)$$



[Minh & Liu 2019]

G33.92+0.11 Summary

- A highly complex massive star-forming region largely influenced by still accreting ambient gas
- Sequential formation of massive star clusters
- Triggered by intermittent accreting gas
- Coexist of distinct gas components: dense star-forming cores, turbulent gas, accreting warm gas, pristine cold dense gas, ..
- Chemical evolutionary time scale $\approx$ free-fall time scale



7. Summary

Radio Telescopes and interstellar molecular lines are powerful tools to understand the universe.

