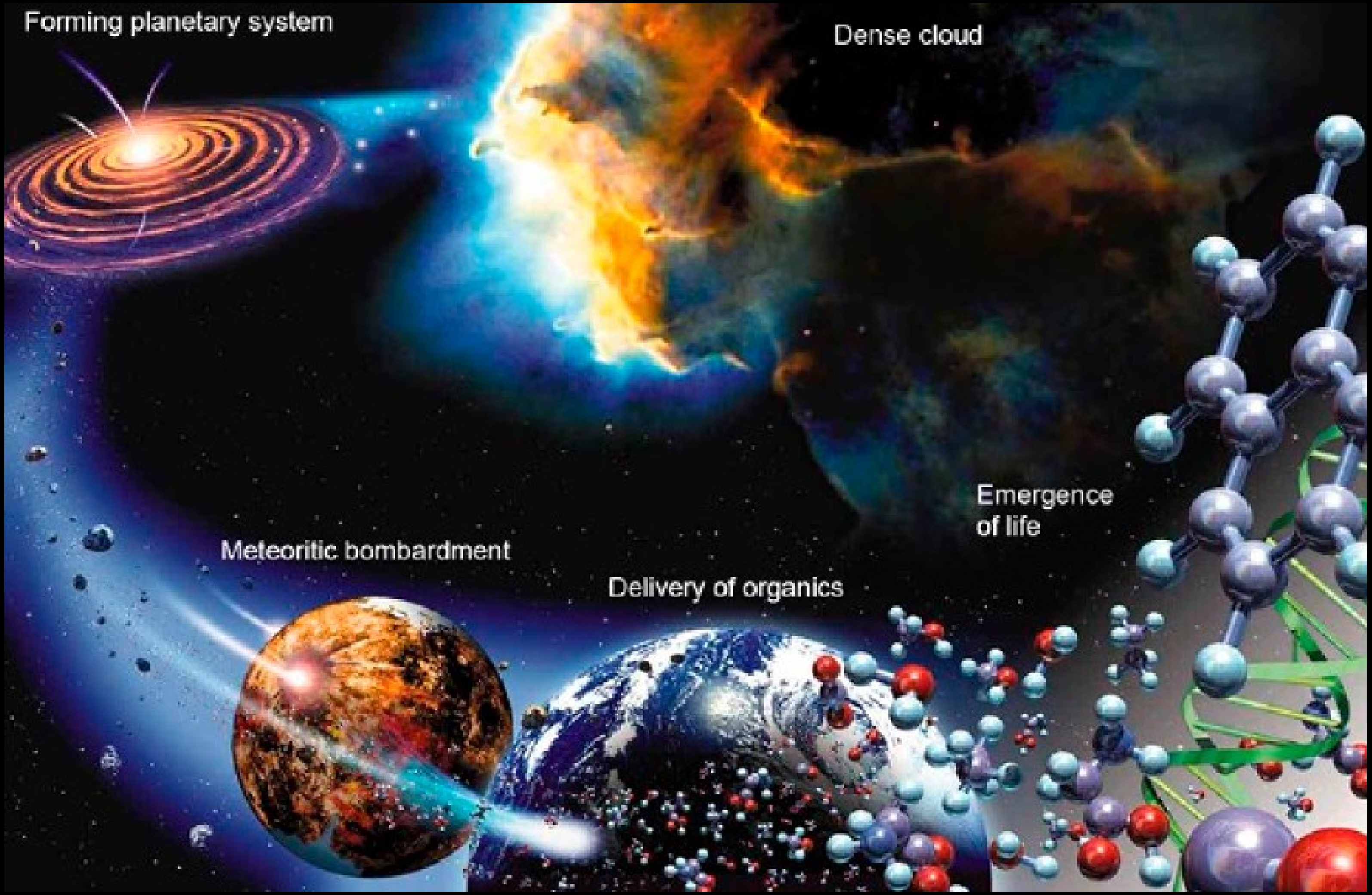
Master course: Astrochemistry I:

Lecture 5: Chemistry in shocked regions

Reading list:

Tielens Chap. 11

Water review (vD)
section 4.4



Dr. Helgi Rafn Hrodmarsson – UPEC – 2026-2027

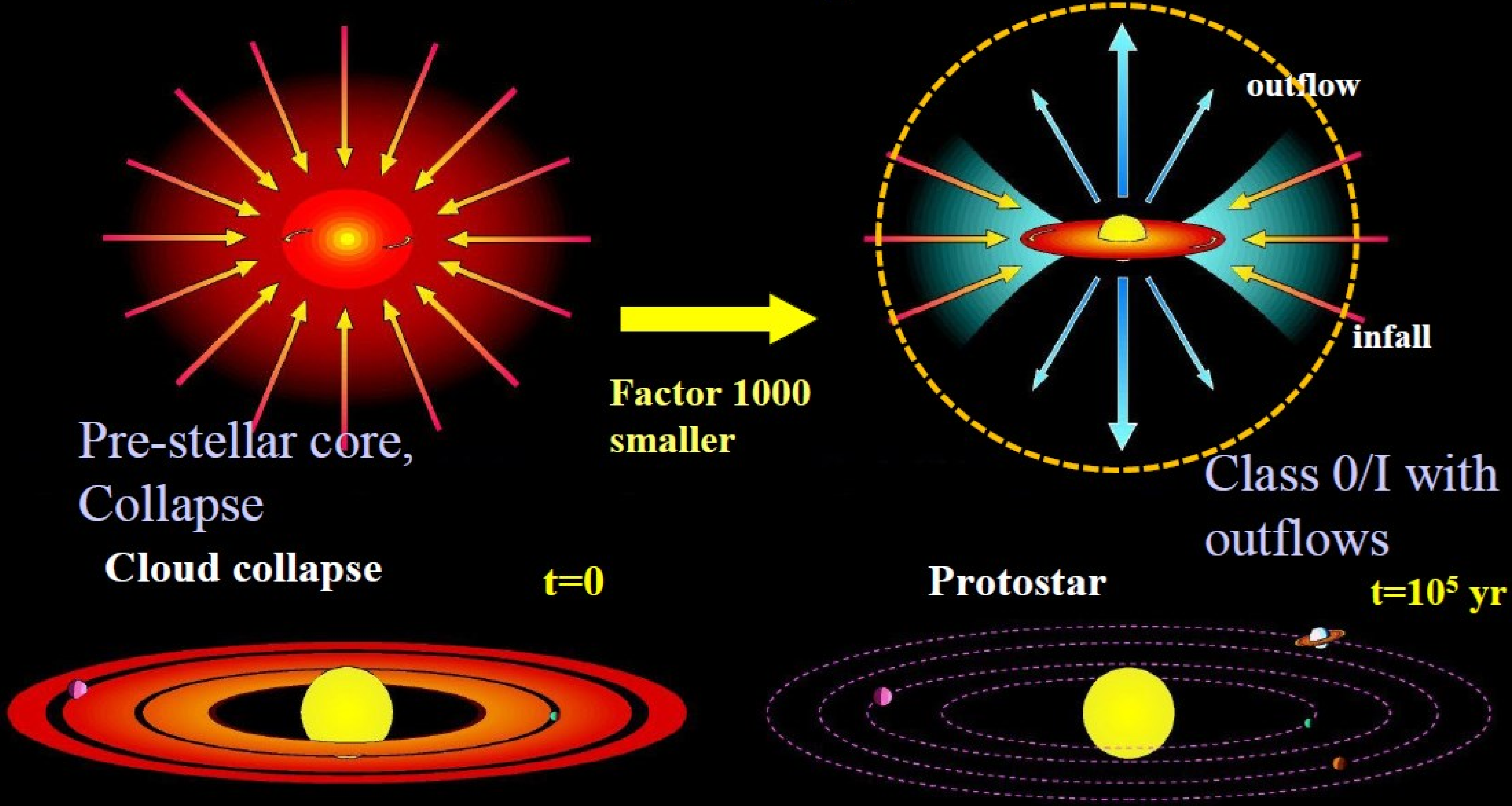
Outline

- Introduction
- J- vs. C-type shocks
- Chemistry in dissociative shocks
- Chemistry in non-dissociative shocks
- Comparison with observations
  - Supernova remnant: IC 443
  - Massive protostar: Orion-KL
  - Low-mass protostar: L1157
- Conclusions

5.1 Introduction

- A shock wave is a pressure-driven compressive disturbance propagating faster than ‘signal speed’.
- Shock waves produce an irreversible change in the state of a fluid
- Shocks are ubiquitous in the interstellar medium
  - Expanding H II regions
  - Supernova explosions
  - Stellar winds
  - Bipolar outflows
  - Accretion processes
  - Cloud-cloud collisions
  - …

Scenario for star- and planet formation



Pre-stellar core,
Collapse

Factor 1000
smaller

Class 0/I with
outflows

Cloud collapse t=0

Protostar $t=10^5$ yr

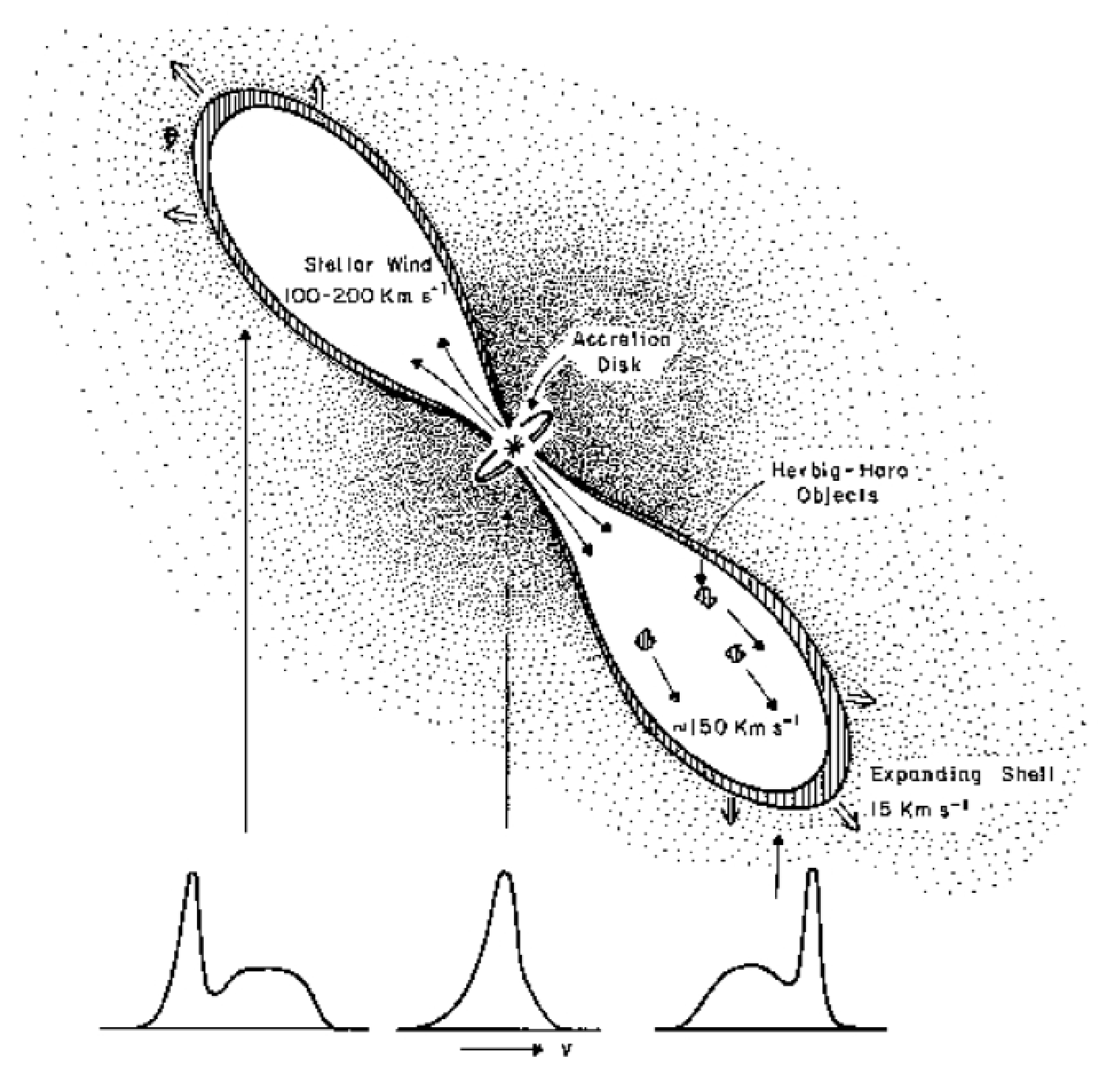
Class II

Protoplanetary disk $t=10^6$-10^6yr

Solar system $t>10^8$ yr

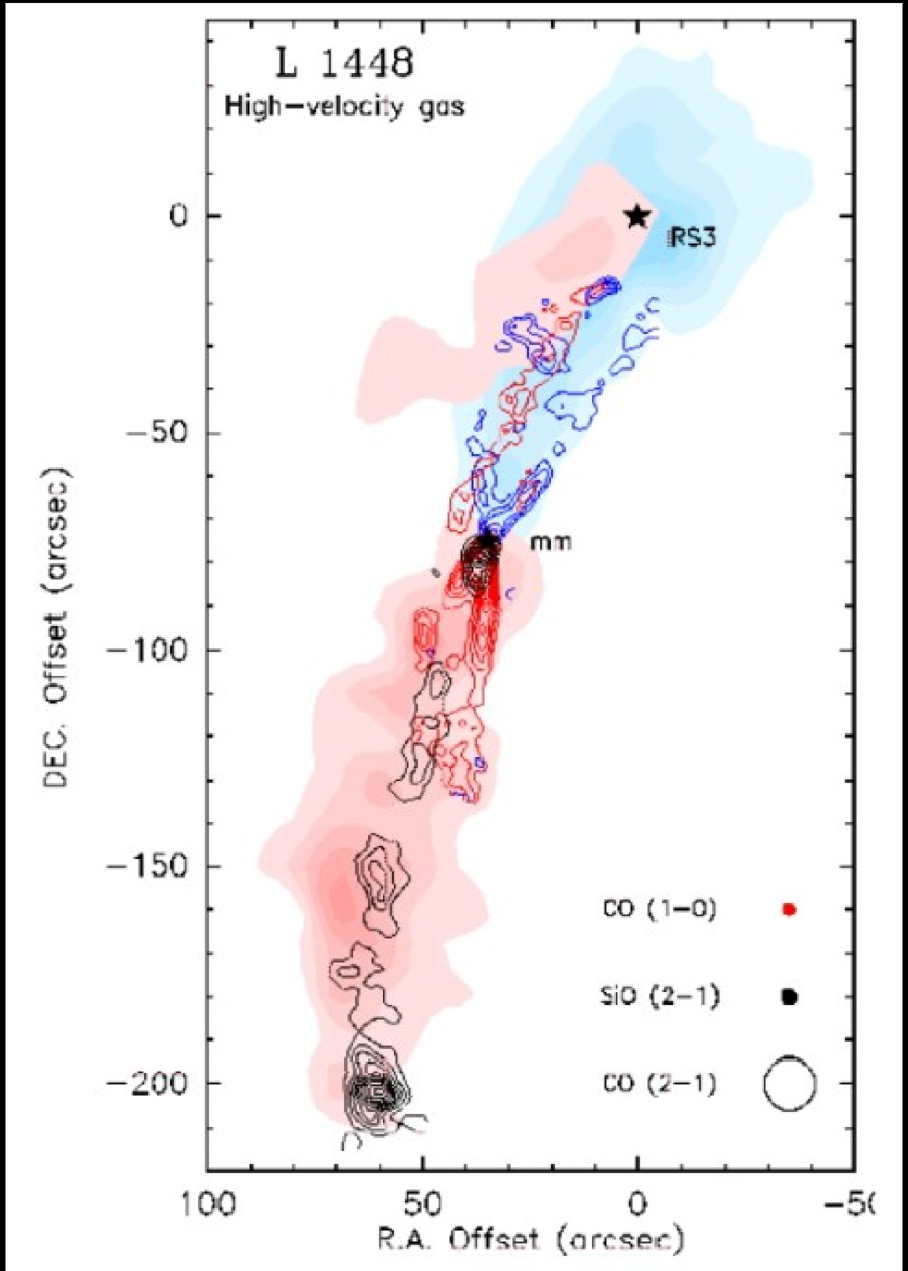
Fig. by M McCaughrean

Anatomy of bipolar outflows from protostars



Snell *et al.* 1980

Bipolar outflow from protostar



Outflows seen in molecular lines:

Molecular outflows

Bachiller & Tafalla 1999

Sound speed and Mach number

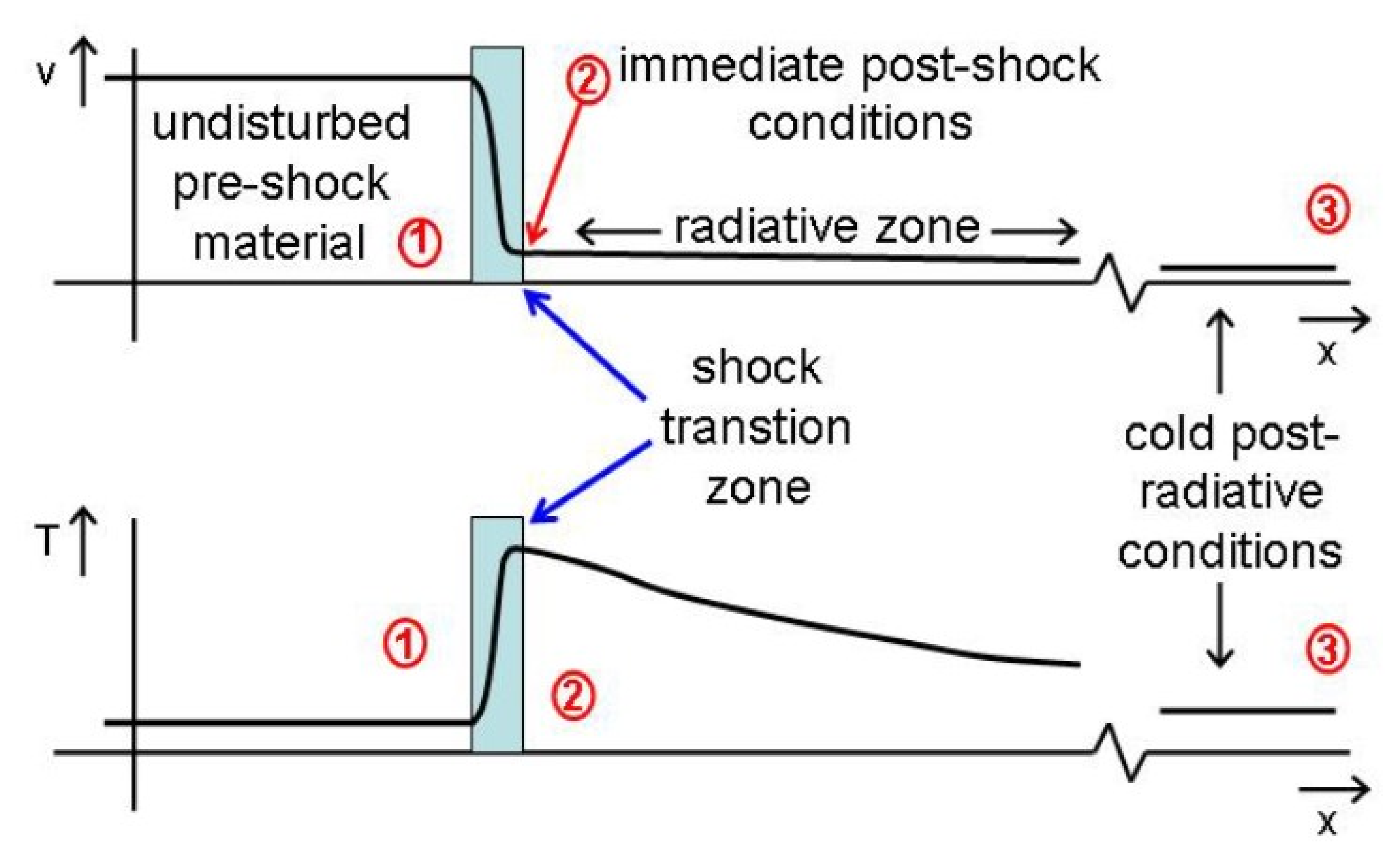
- ***Speed of sound:*** $C^2 \equiv \frac{dP}{d\rho}$
- $P = K\rho^{\gamma}$ with $\gamma = 5/3$ for adiabatic flow,

  $\gamma = 1$ for isothermal flow =>
- $C \propto \rho^{1/3}$ for adiabatic flow => speed of sound larger in denser gas
- $C \approx \sqrt{\frac{kT}{m}} \approx 1 \text{ km s}^{-1}$ for isothermal gas in ISM
- Above phenomena have $v_S \approx$ 5-100 km s^{-1} >> C => gas must be shocked
- ***Mach number:*** $\mathscr{M} \equiv$ ratio of shock velocity w.r.t. speed of sound, $\mathscr{M} \equiv v_S/C$

Shock jump conditions

- Adopt frame in which shock is stationary
- Consider plane-parallel shock: fluid properties depend only on distance x from shock;
- $v = v_x \perp$ shock
- Neglect viscosity, except in shock transition zone:
- Large v-gradient => viscous dissipation => transform bulk kinetic energy into heat => ***irreversible change*** (entropy increases)

Shock profile (shock frame)



- Shocks in dense molecular clouds are ***radiative*** => kinetic energy converted into radiation

Shock jump conditions (continued)

- Thickness of shock transition ≤ mean free path of particles
  - This is always << thickness of radiative zone (need collisions to get radiative cooling)
- Regard shock thickness as 0 => discontinuity
- Shock physics: find physical conditions at **2** (immediately behind shock) or **3** (in post-radiative zone) given those at **1** (pre-shock) and shock velocity v_S.

5.2 J- vs C-shocks

- Signal speeds in dense clouds:
- **Neutral speed of sound**
- $C_S \approx \left(\frac{5kT}{3\mu}\right)^{1/2} \approx 0.77\left(\frac{T}{100}\right)^{\frac{1}{2}} \; km\; s^{-1}$
- **Alfvén speed**
- $C_A \approx \left(\frac{B^2}{4\pi\rho}\right)^{\frac{1}{2}} \approx 1.8b\; km\; s^{-1}$
- With $B = {n_0}^{1/2} b$ microGauss and $\rho = \mu n_0$ = mass density
- Observations => $b \approx 1$
- Magnetosonic speed: $C_{MS} = ({C_S}^2 + {C_A}^2)^{1/2}$

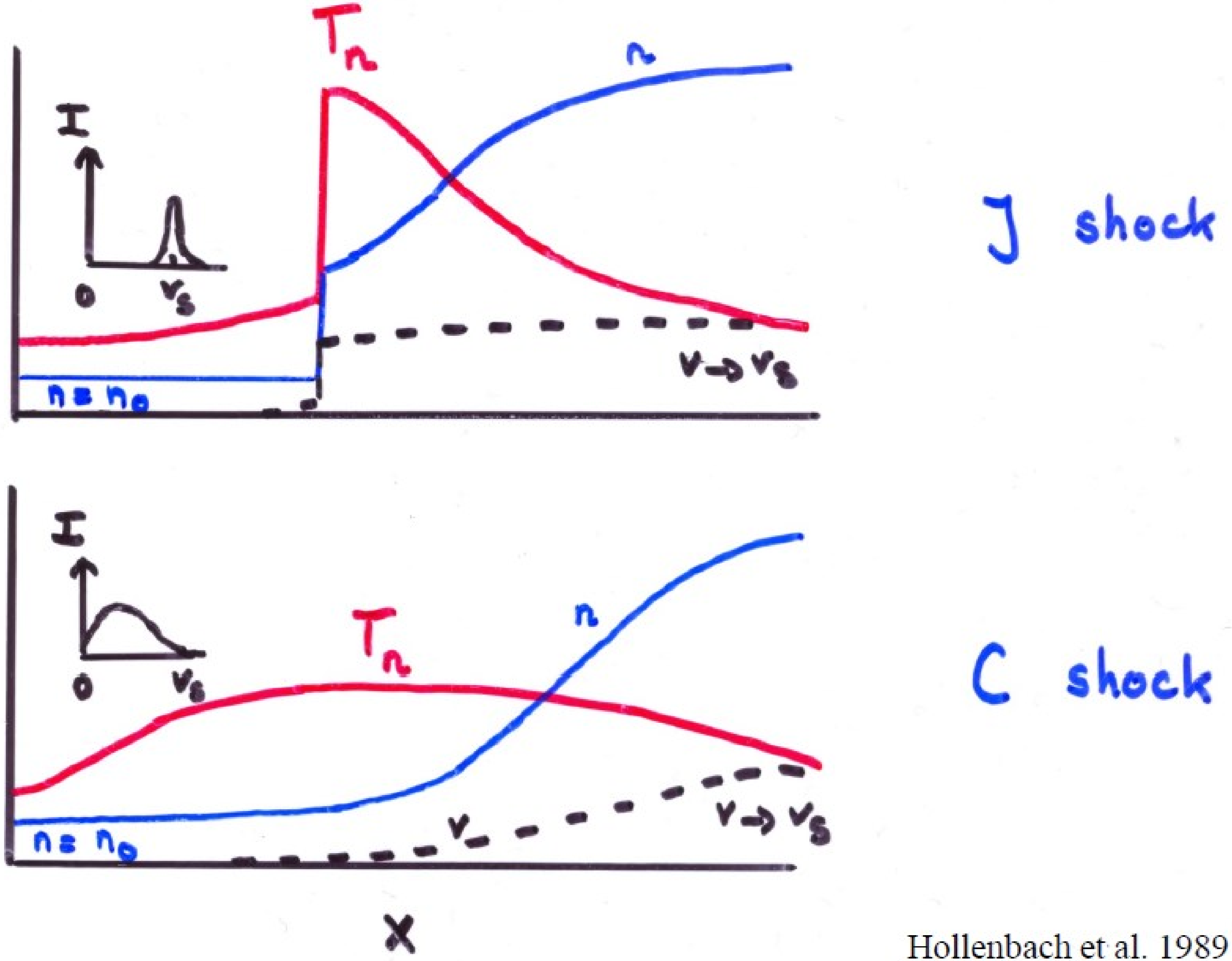
Signal speeds

- **Ion-Alfvén speed**
- $C_{iA} \left(\frac{B^2}{4\pi\rho_i}\right)^{1/2} = \frac{C_A}{y_i^{1/2}} \gg C_A$
- $y_i = \rho_i/\rho =$ ion mass fraction = 10^{-6}–10^{-8} in dense clouds
- Many shocks satisfy $C_S \le \underset{\overset{\uparrow}{\text{neutrals}}}{C_A} \le v_S \le \underset{\overset{\uparrow}{\text{ions}}}{C_{iA}}$
- => ion-Alfvén waves can transmit information of disturbance ahead of arrival; ions coupled to neutral by collisions

Two types of shocks

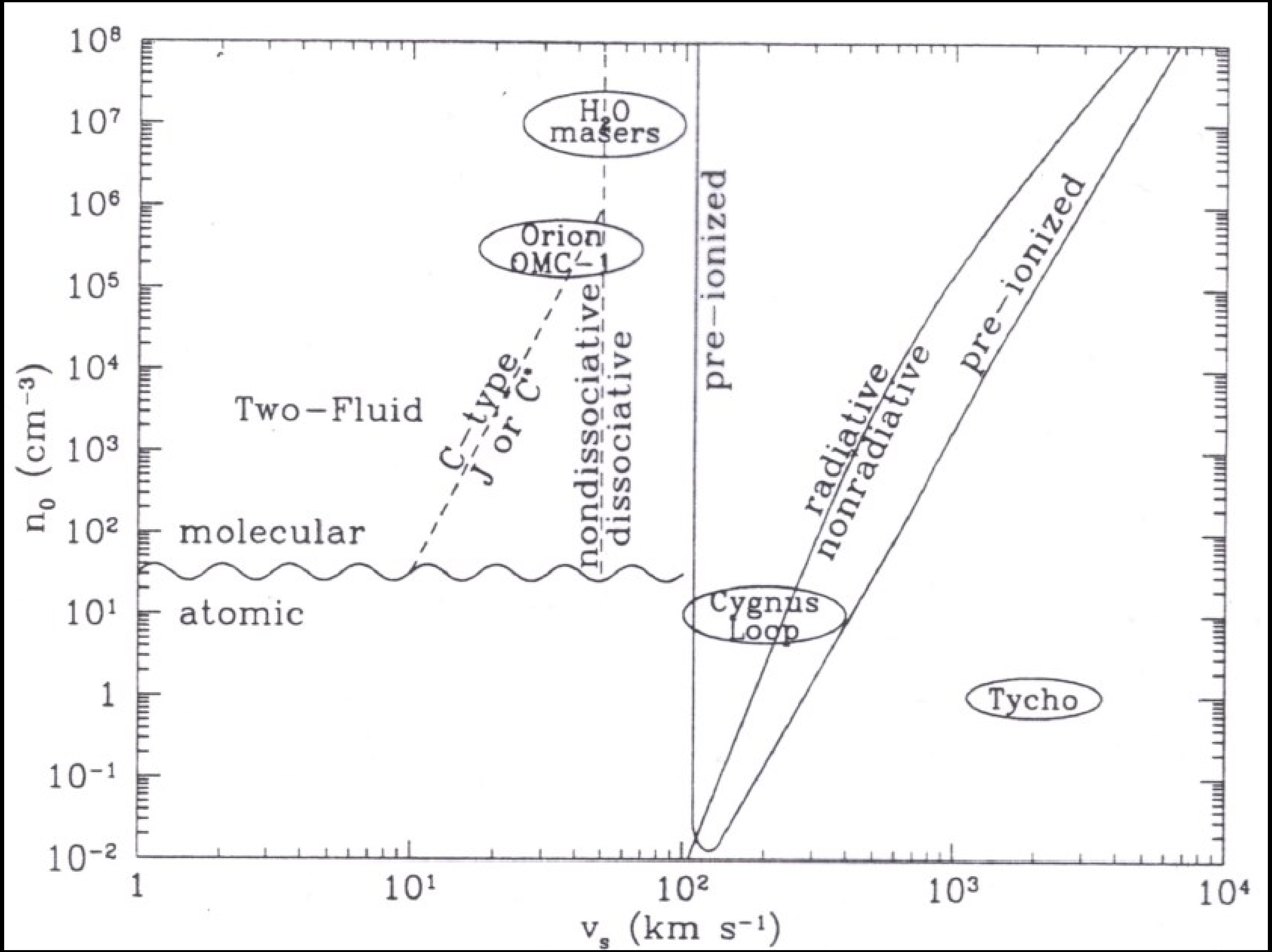
- ***J ("jump")-shocks:*** $v_S \geq 50$ km/s
  - Shock abrupt
  - Neutrals and ions tied into single fluid
  - T high: $T \approx 40\ (v_S/\mathrm{km\ s^{-1}})^2$
  - Most of radiation in ultraviolet
- ***C ("continuous")-shocks:*** $v_S \leq 50$ km/s
  - Gas variables (T, ρ, v) change continuously
  - Ions ahead of neutrals; drag modifies neutral flow
  - $T_i \neq T_n$; both much lower than in J-shocks
  - Most of radiation in infrared

J- vs. C-shocks



Hollenbach et al. 1989
Draine & McKee 1993, ARAA

Conditions for different shock types



Draine & McKee
1993

Chemical effects

- Endoergic reactions (*e.g.*, $O + H_2 \rightarrow OH + H$)
- Exoergic reactions with energy barriers
- Collisional dissociation (very high T, n only)
- Sputtering of icy grain mantles
- Sputtering of refractory grain cores to gas: Si
- Intense UV radiation field (I.E. Ly α)

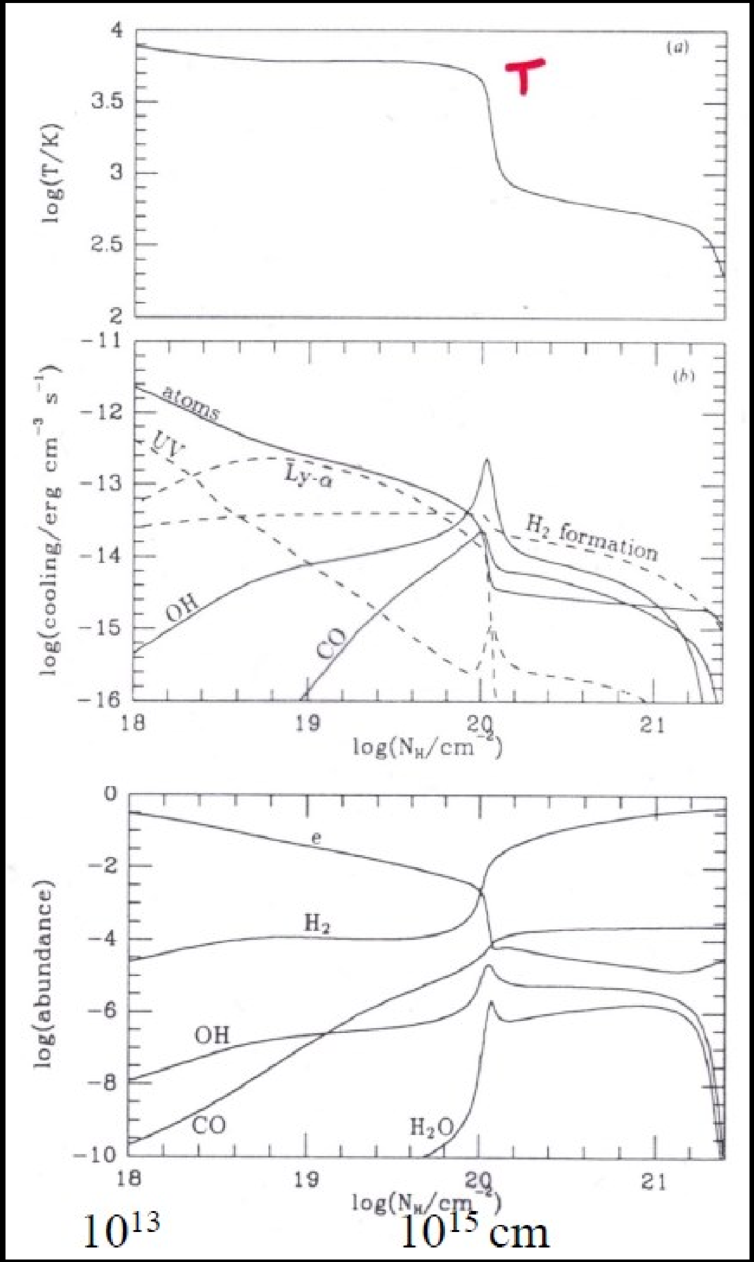
5.3 Chemistry in dissociative shocks

- Fast J-shocks destroy molecules, which re-form in the post shock gas
  - $v_S \geq 50$ km s^{-1} => dissociation of molecules into atoms
  - $v_S \geq 70$ km s^{-1} => ionization of atoms
  - $v_S \geq 80$ km s^{-1} => UV radiation destroys molecules ahead of shock

Shock structure

- Solve hydrodynamic equations subject to conservation of mass, momentum, and energy
- **Cooling**
  - Excitation of atoms, ions, and molecules
  - Gas-grain collisions
  - H_2 dissociation
  - H ionization
- **Heating**
  - Bulk motion => thermal energy
  - Radiation emitted by warm upstream gas
  - Exoergic chemical reactions
- Chemical composition determines cooling rate => solve hydrodynamic equations together with chemistry

Dissociative shock profile



$v_S = 80$ km s^{-1}

$n_0 = 10^5$ cm^{-3}

Neufeld 1990

Chemistry in dissociative shocks

- **$T \approx 10^5$ K** => collisional dissociation of molecules
  - $H_2 + H_2 \rightarrow H_2 + H + H$
  - $H_2 + H \rightarrow H + H + H$
  - $CO + H \rightarrow CH + O$ (reaction)
  - $CH + H \rightarrow C + H_2$ or $C + H + H$

Chemistry - continued

- **$T < 10^4$ K** => H_2 re-formation
  - Grains too hot => gas-phase processes (as in early universe)
  - $H + e^- \longrightarrow H^- + h\nu$ *slow*
  - $H^- + H \longrightarrow H_2 + e^-$ *fast*
  - This process dominates if $n(e)/n_H \geq 0.02$ and gives typically $n(H_2)/n_H \approx 10^{-3}$: small, but sufficient to cool the gas
- **$T \leq 3000$ K** => H_2 builds up rapidly
  - $O + H_2 \longrightarrow OH + H$
  - $OH + H_2 \longrightarrow H_2O + H$
  - $C^+ + OH \longrightarrow CO + H^+$

Chemistry - continued

- OH crucial intermediate in chemistry
  - $X + OH \rightarrow XO + H$
  - $X^+ + OH \rightarrow XO^+ + H$

  where X = Si, S, N, …
- SiO good shock diagnostic, especially if Si abundance is enhanced by destruction of grains

Chemistry - continued

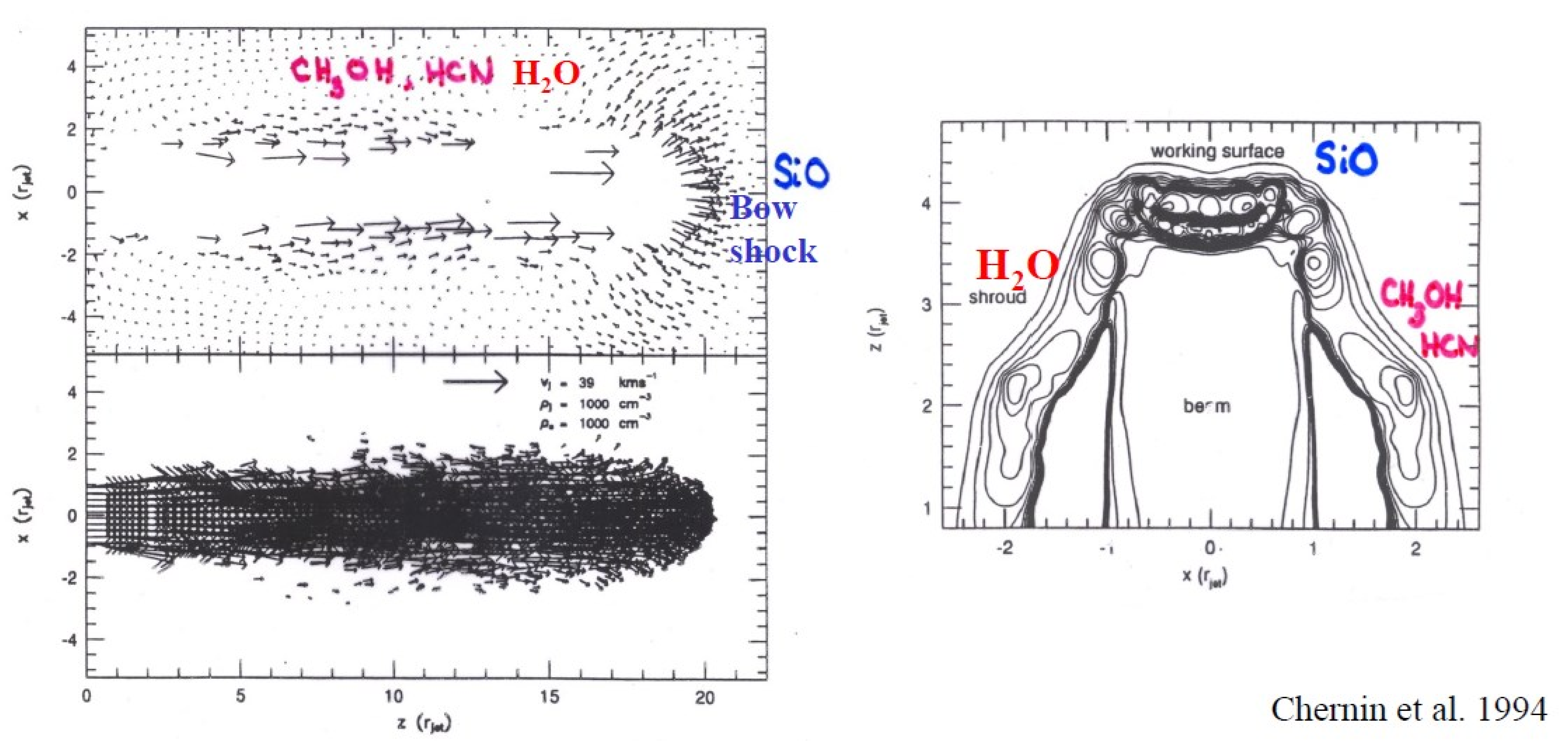
- Molecules can be destroyed by reverse reactions with H and by photodissociation. Much of shock energy emerges in Ly α 1216 Å line
  - OH, H_2O, …: can be dissociated by Ly α
  - H_2, CO, CN, …: cannot be dissociated by Ly α
  - H_2 ($v = 2$): can be pumped by Ly α => characteristic IR + UV spectrum
  - CO: can be dissociated by continuum from He ($2\ ^1S$) two-photon energy

Grain destruction

- **High-velocity J-shocks**
  - Thermal sputtering* of grain cores => local enhancements of gas-phase Si, Fe, …
- **Low-velocity C-shocks**
  - Non-thermal sputtering of grain cores and icy mantles
    - Uses different velocities, ions vs neutrals
    - Grains are charged → move with ions
  - Grain cores ($v_S \geq 25$ km s^{-1}) : enhanced Si, …
  - Grain mantles ($v_S \geq 10$ km s^{-1}): enhanced H_2O, CH_3OH, Sulfur? SiO_2?

*Sputtering = collisions of heavy atoms with grains liberating material

SiO formation and mantle release



Chernin et al. 1994

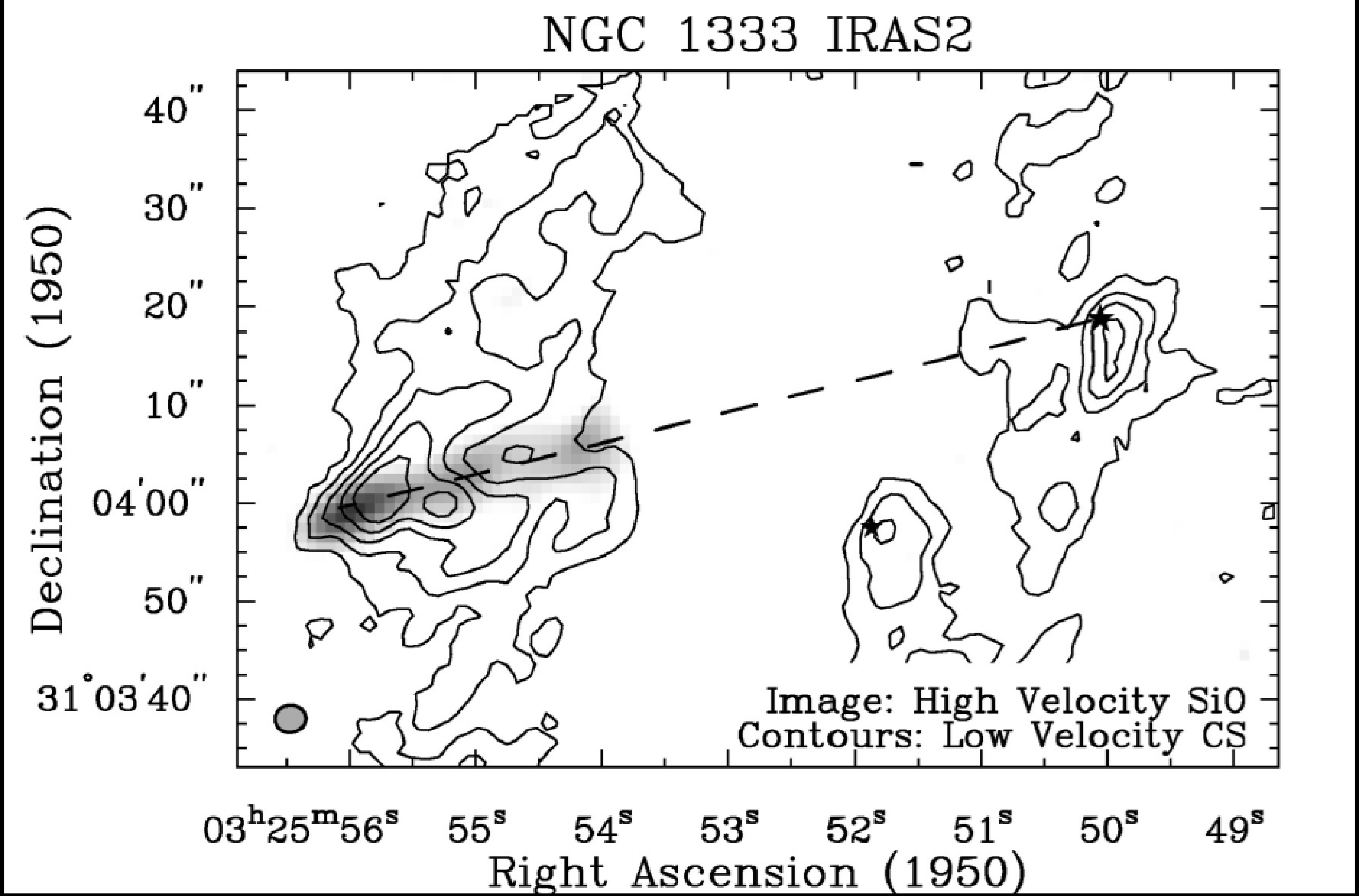
- Grain destruction at working surface of shock => Si released
- CH_3OH and H_2O released from icy grain mantles and entrained by less fast shocks

SiO as tracer of shocks: examples

- **NGC 1333 IRAS 2 (Class 0 protostar)**
  - Extremely collimated (<10^{16} cm width) SiO tip of CO outflow => bow shock
- **L1448-mm (Class 0 protostar)**
  - Extremely collimated SiO emission
  - Chain of high-velocity clumps up to 70 km s^{-1}
- **BHR 71 (Bok globule – dark nebulae)**
  - Widespread SiO emission => interaction wide-angle wind with surroundings?

SiO abundances enhanced by factors up to 10^6; detection rate high (≥ 50%) for deeply embedded ‘Class 0’ protostars, much lower (≤ 25%) for more evolved ‘Class I’ and ‘Class II’ young stellar objects

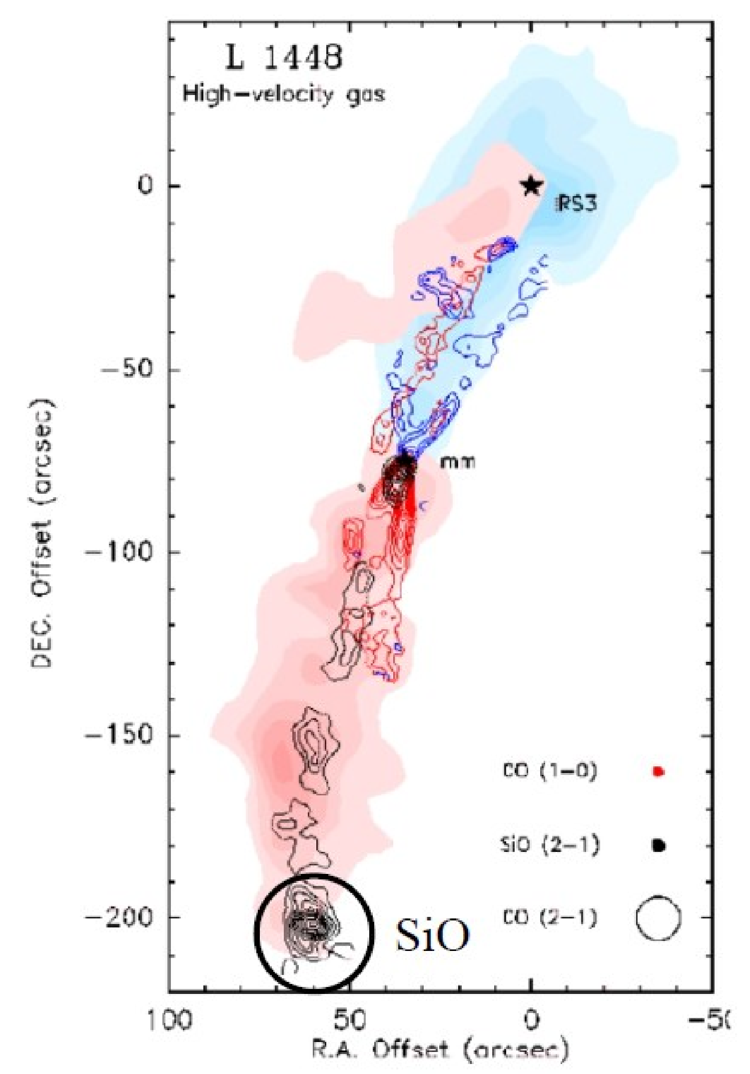
SiO at tip of jet



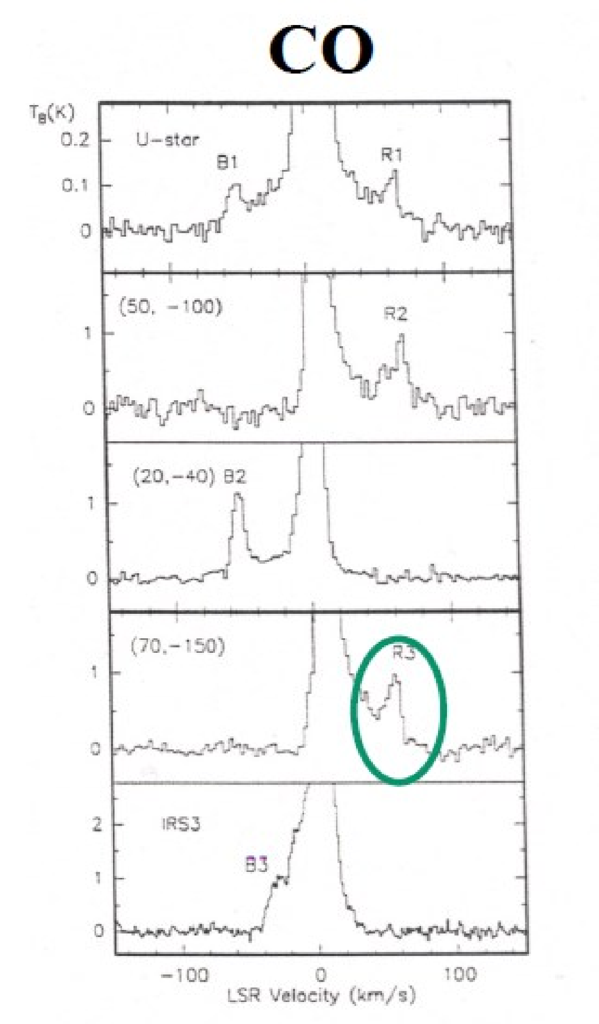
- **SiO traces deeply embedded, collimated outflows**

van Dishoeck & Blake (1998)
Jørgensen et al. 2005

L 1448 outflow: CO vs SiO

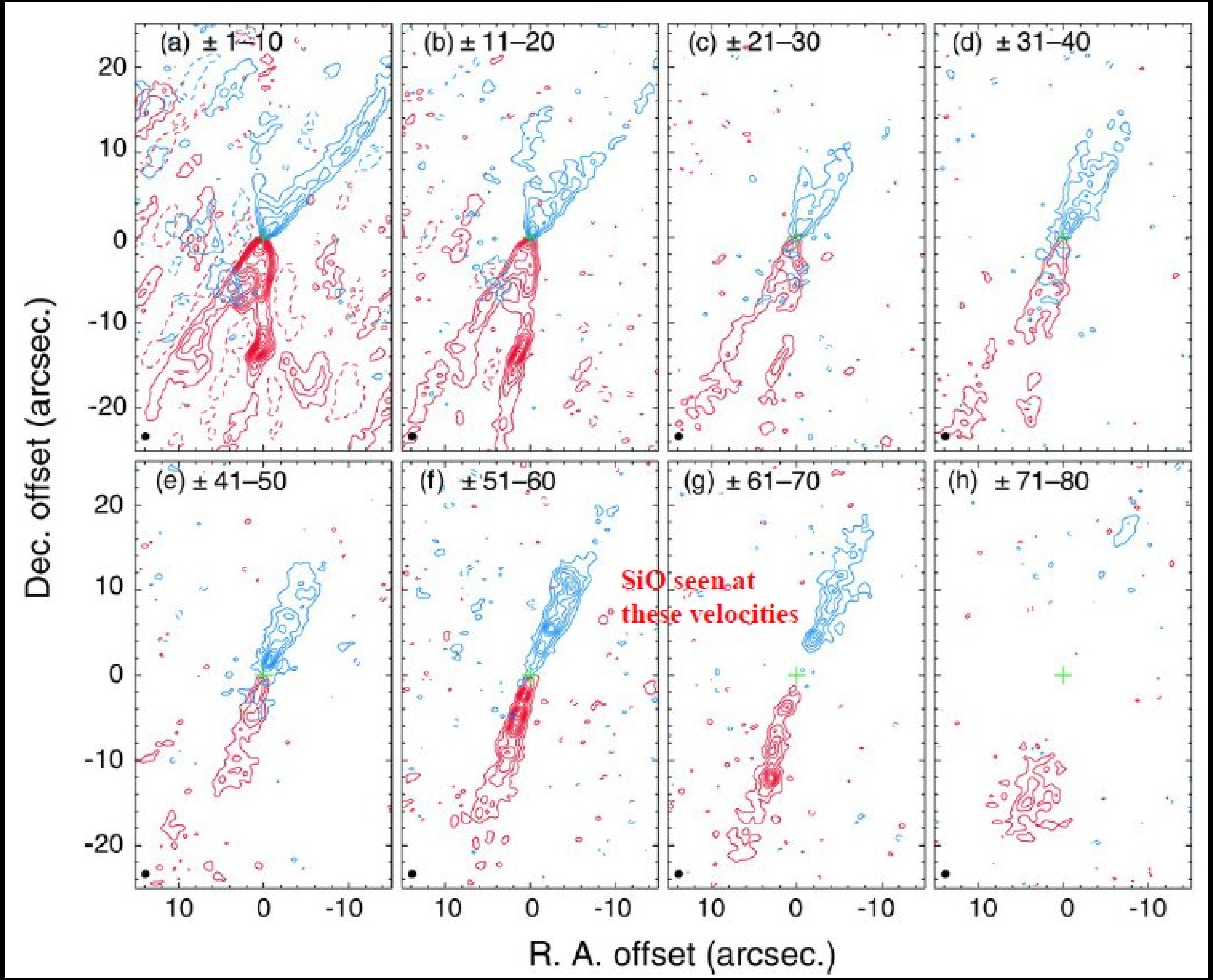


Bachiller et al. (1990, 1991)
Guilloteau et al. 1992



- Note high-velocity ‘bullets’ aka Extremely High Velocity (EHV) gas

Extremely High Velocity gas



SiO seen at these velocities

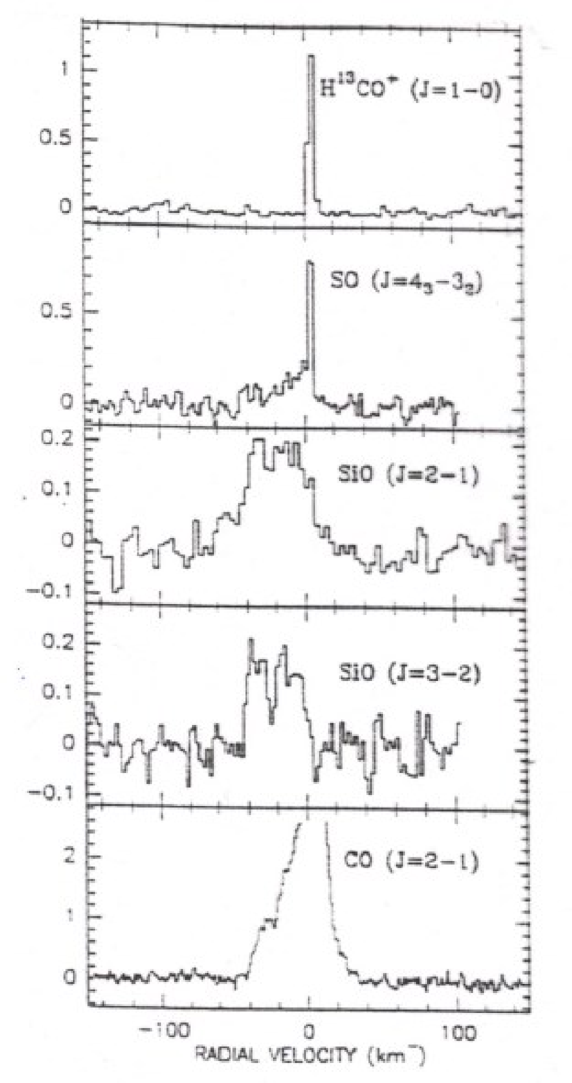
L1448mm
CO 3-2

Hirano et al. (2010)

- Low velocity gas coating outflow walls (shell shocks)
- High velocity gas in central jet; contains SiO and H_2O

High velocity SiO emission

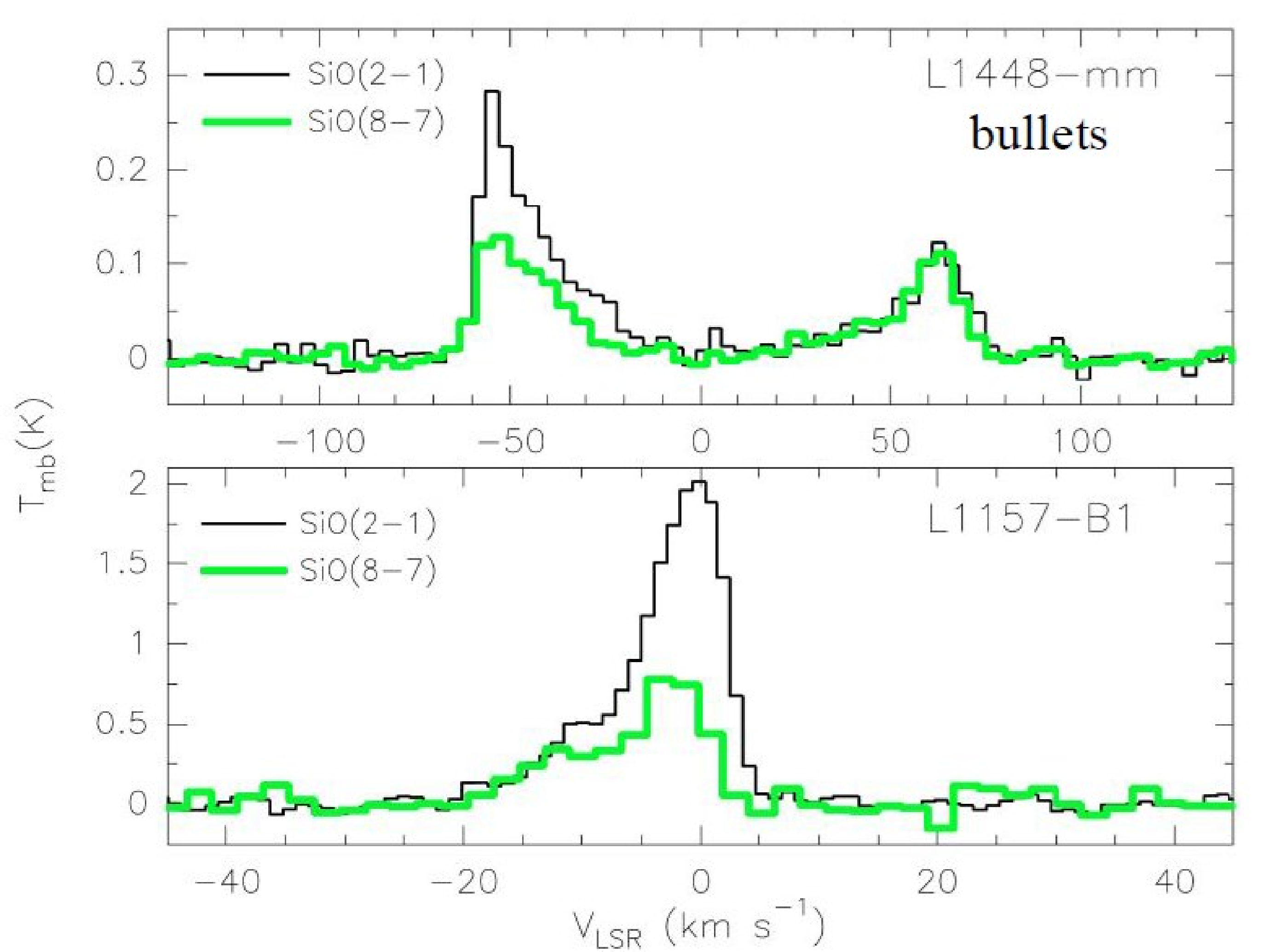
L1448mm



Narrow H^{13}CO$^+$
Broad and shifted SiO

- Quiescent gas: Si ≈ 10^{-6} wrt solar => heavily depleted
- Shocked gas: Si ≈ 10^{-2} wrt solar => increase due to grain destruction

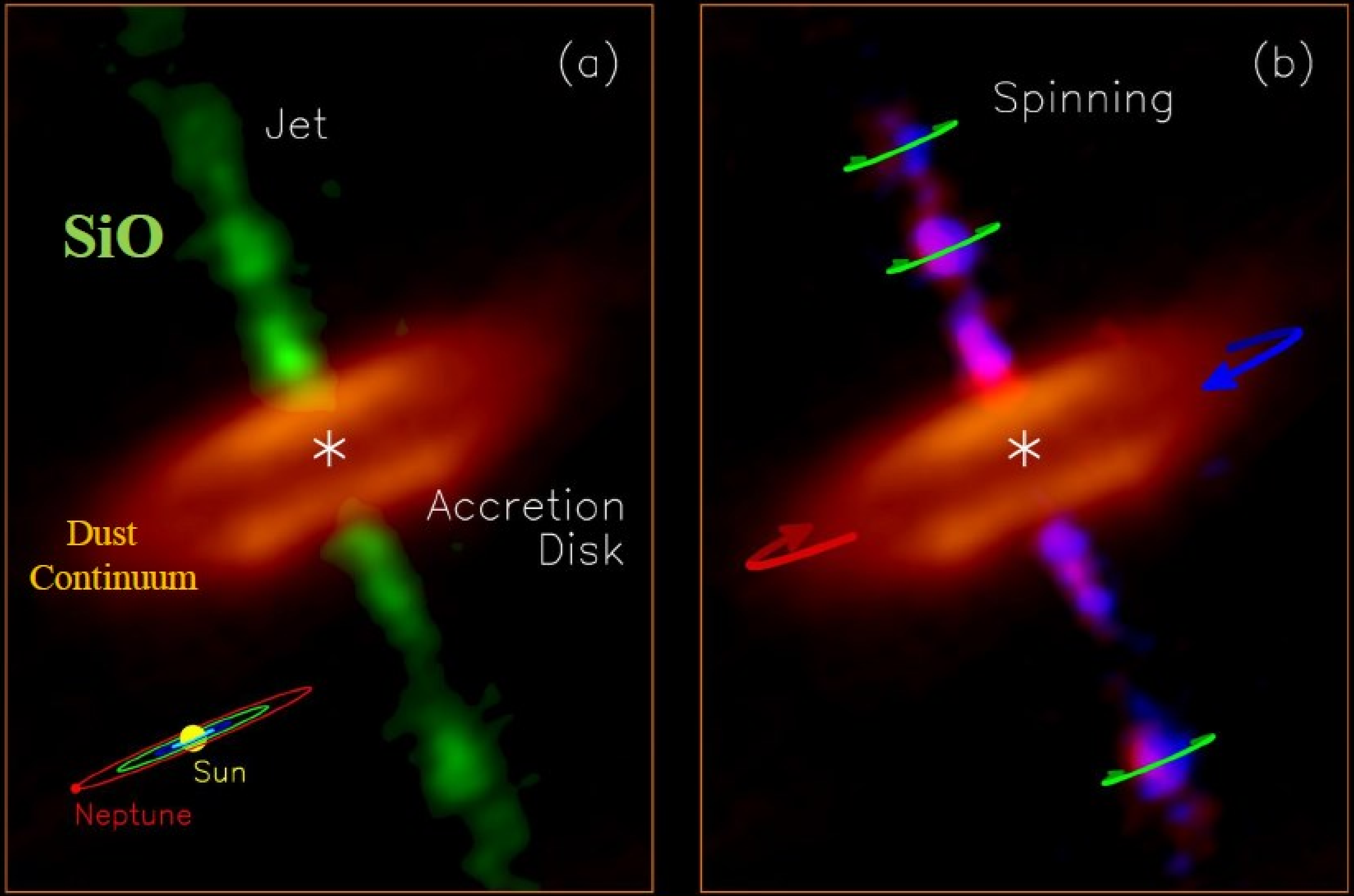
SiO profiles



Nisini et al. 2007

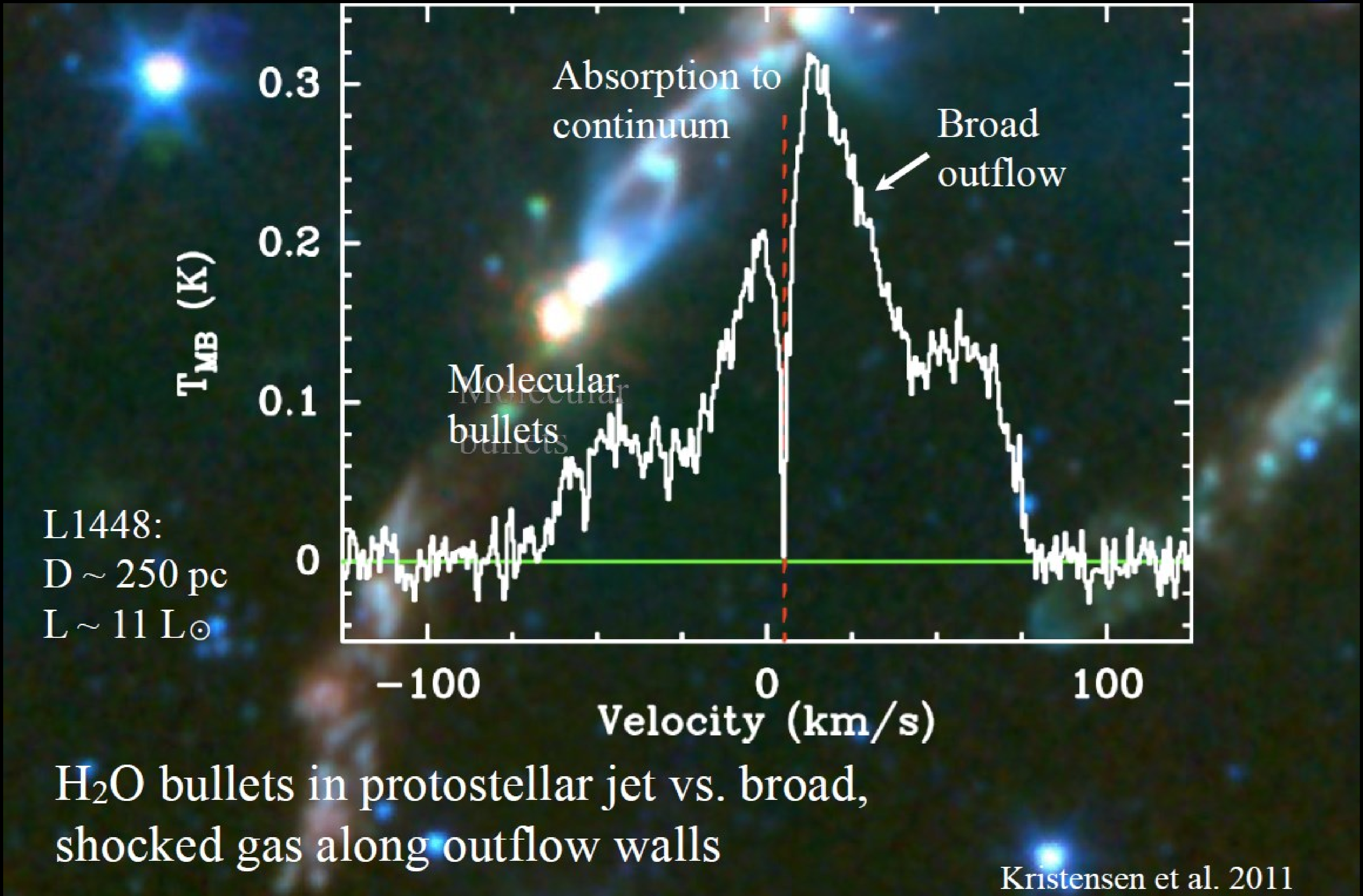
- SiO both in 'bullets' and in low-velocity shocks

HH211: textbook example jet + disk



Lee et al. 2017

Water ‘bullets’ in a low-mass protostar



L1448:
D ~ 250 pc
L ~ 11 L$_\odot$

H_2O bullets in protostellar jet vs. broad, shocked gas along outflow walls

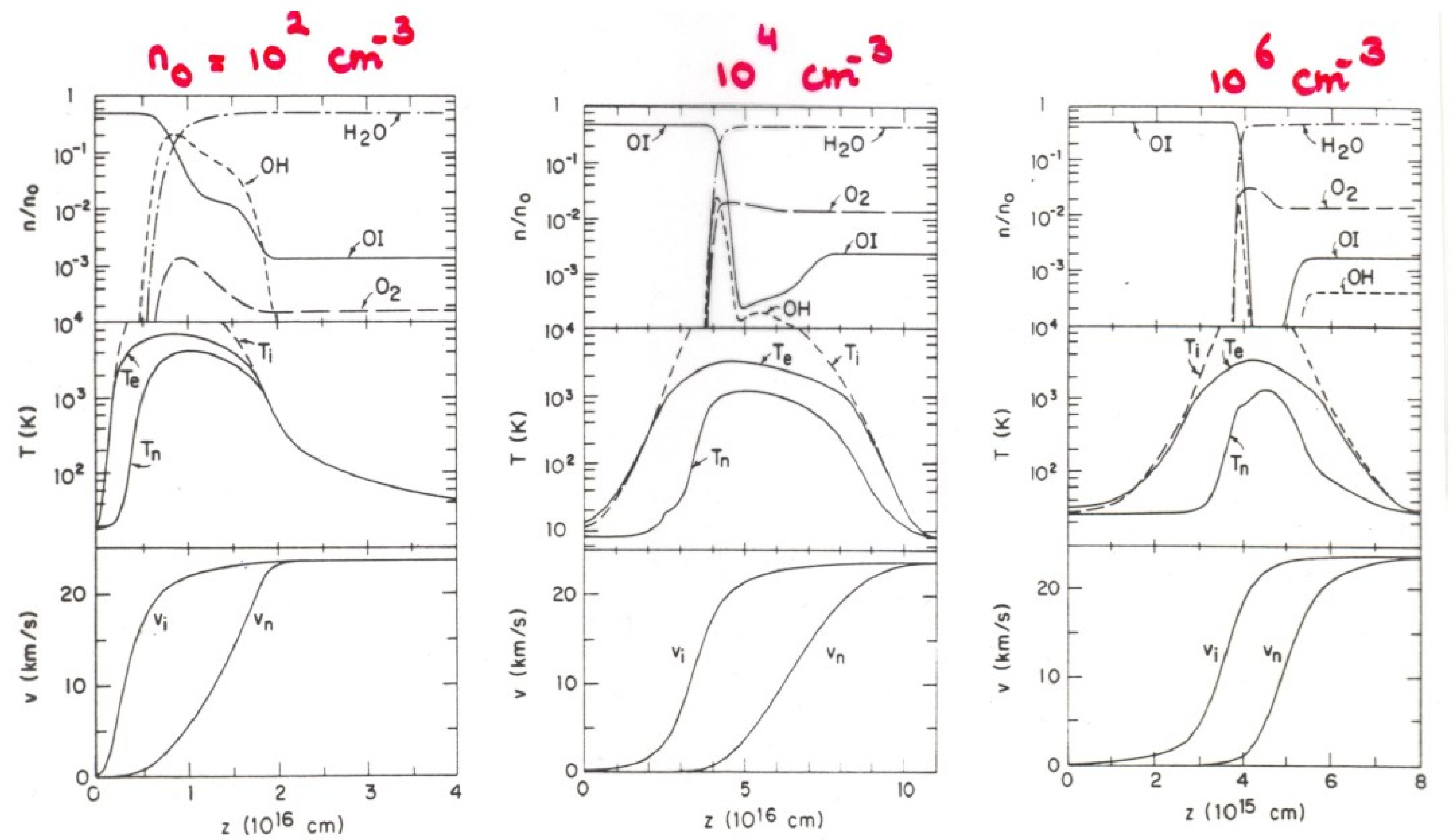
Kristensen et al. 2011

5.4 Chemistry in non-dissociative shocks

- Molecules survive shocks. Typical temperatures **$T \approx$ 1000-3000 K**
  - $O + H_2 \rightarrow OH + H$
  - $OH + H_2 \rightarrow H_2O + H$

  - $C^+ + H_2 \rightarrow CH^+ + H$

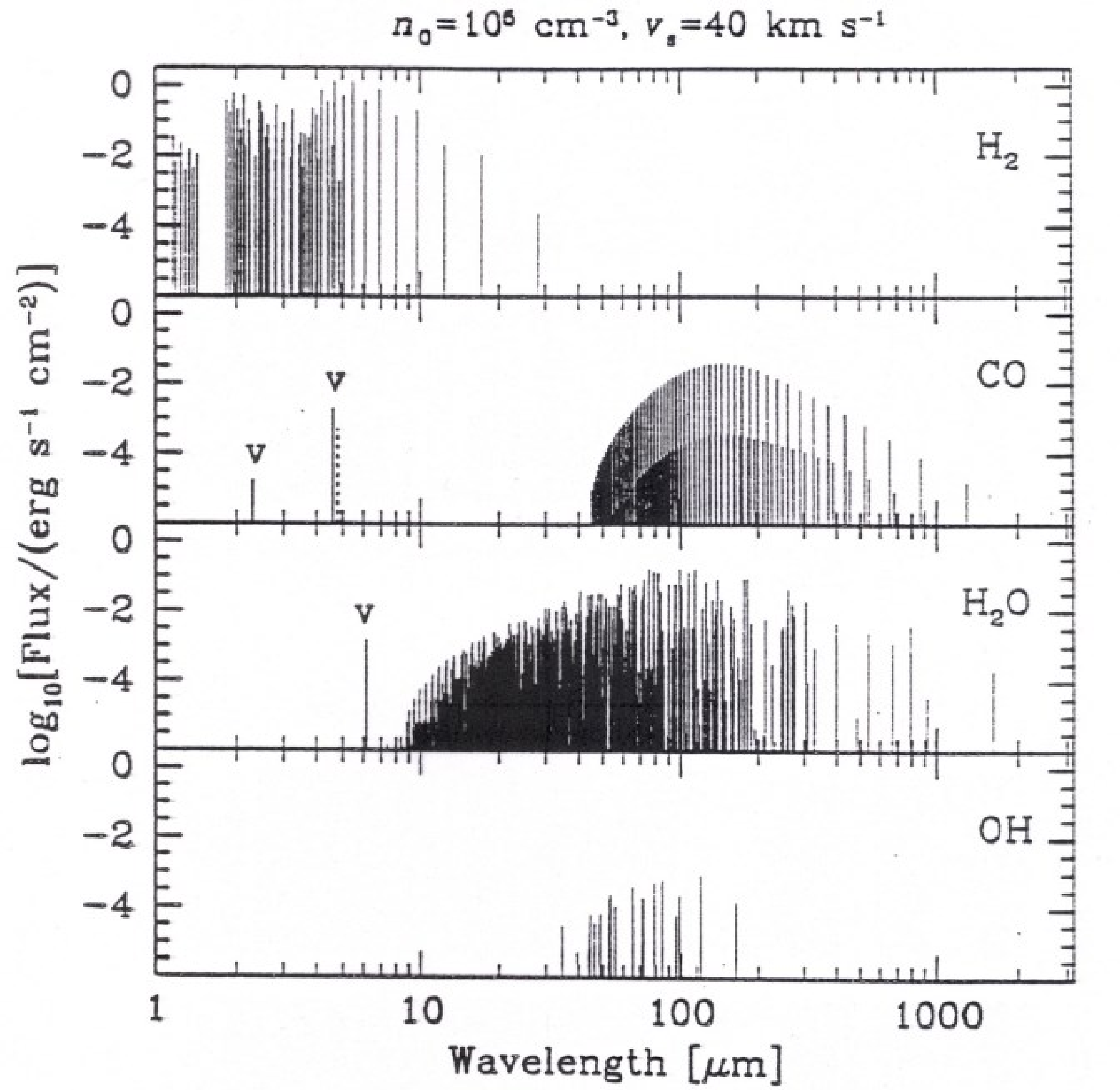
Shock profiles: $v_S = 25$ km s^{-1}



- Note different velocities of ions and neutrals
- CH^+ also enhanced in low-density shocks

Draine et al. (1983)

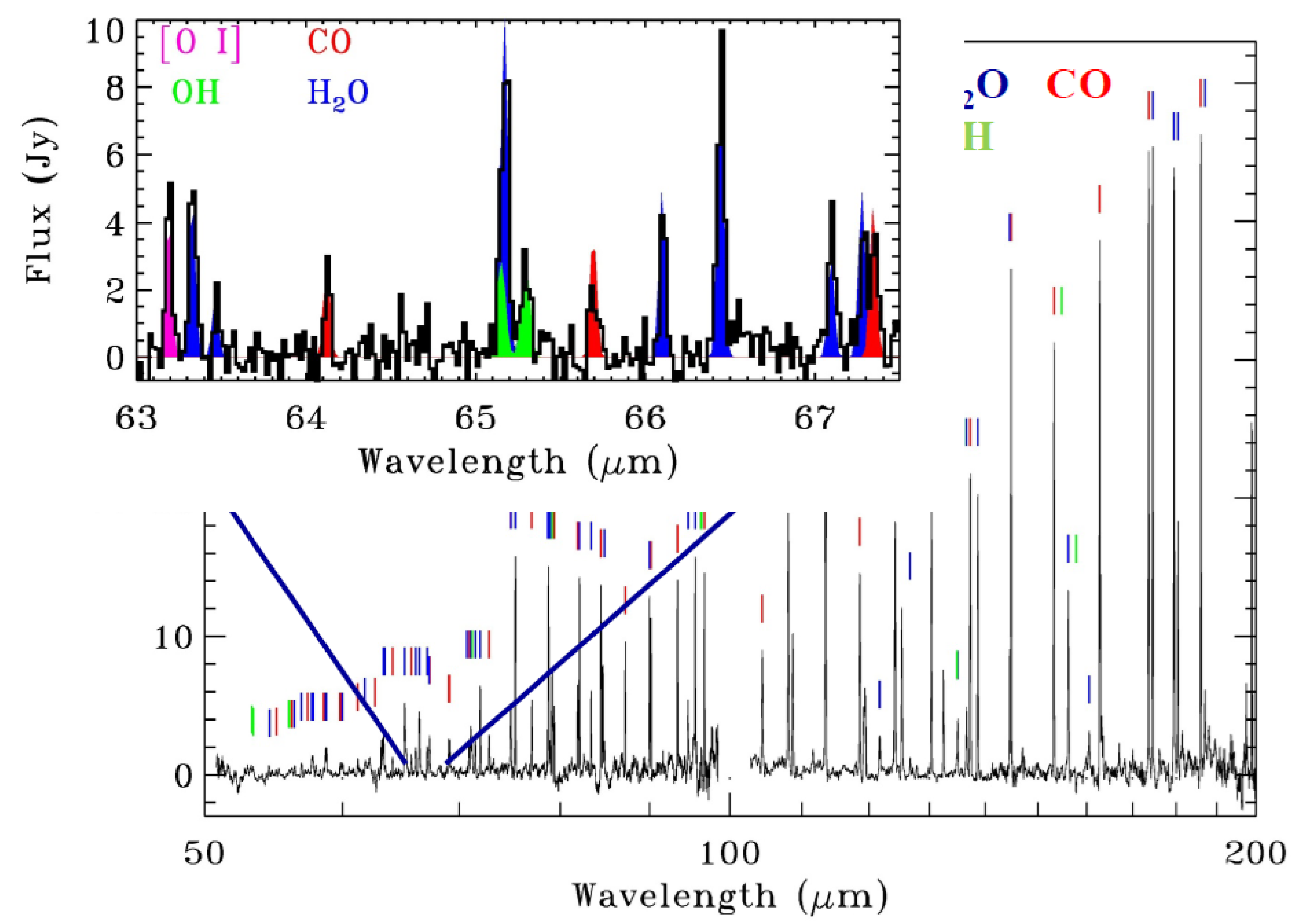
C-shock emission



- Note strong far-IR emission => ***Herschel!***

Kaufman & Neufeld (1996)

Herschel-PACS spectroscopy of shocks: Hot H_2O, OH and CO



Low-mass protostar

NGC1333
IRAS4B
(cont. subtr.)

Herczeg et al. (2012)

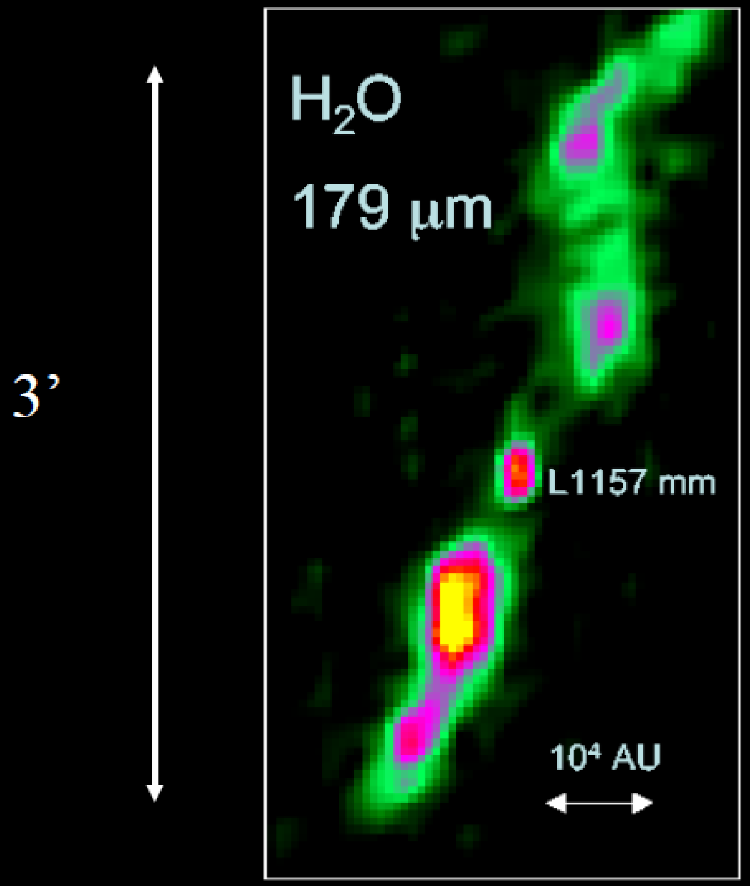
General trends models

- **Oxygen**
  - O, OH, H_2O enhanced
- **Carbon**
  - H_2CO? (from $CH_3 + O \rightarrow H_2CO + H$)
- **Sulfur**
  - H_2S
  - SO, SO_2
- **Silicon**
  - SiO
- **Nitrogen**
  - NH_3, HCN?

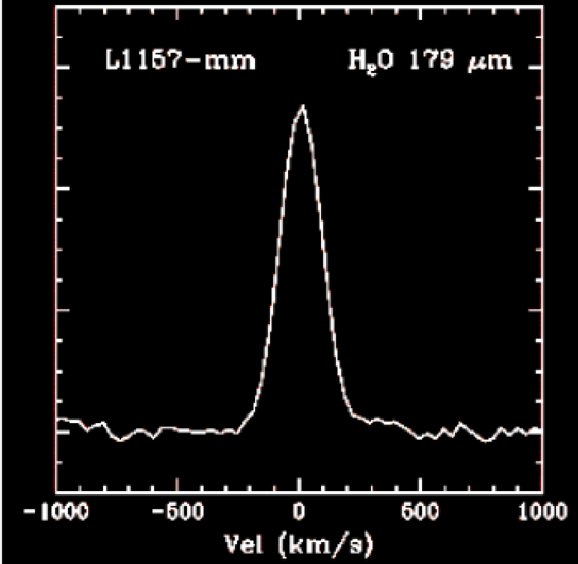
Note that model results depend sensitively on H/H_2 and C/CO ratios in pre-shocked and shocked gas

H_2O as tracer of shocks

Herschel-PACS image of water in proto-stellar systems



L1157-mm outflow
$D = 440$ pc, $L_{bol} = 11$ L_o



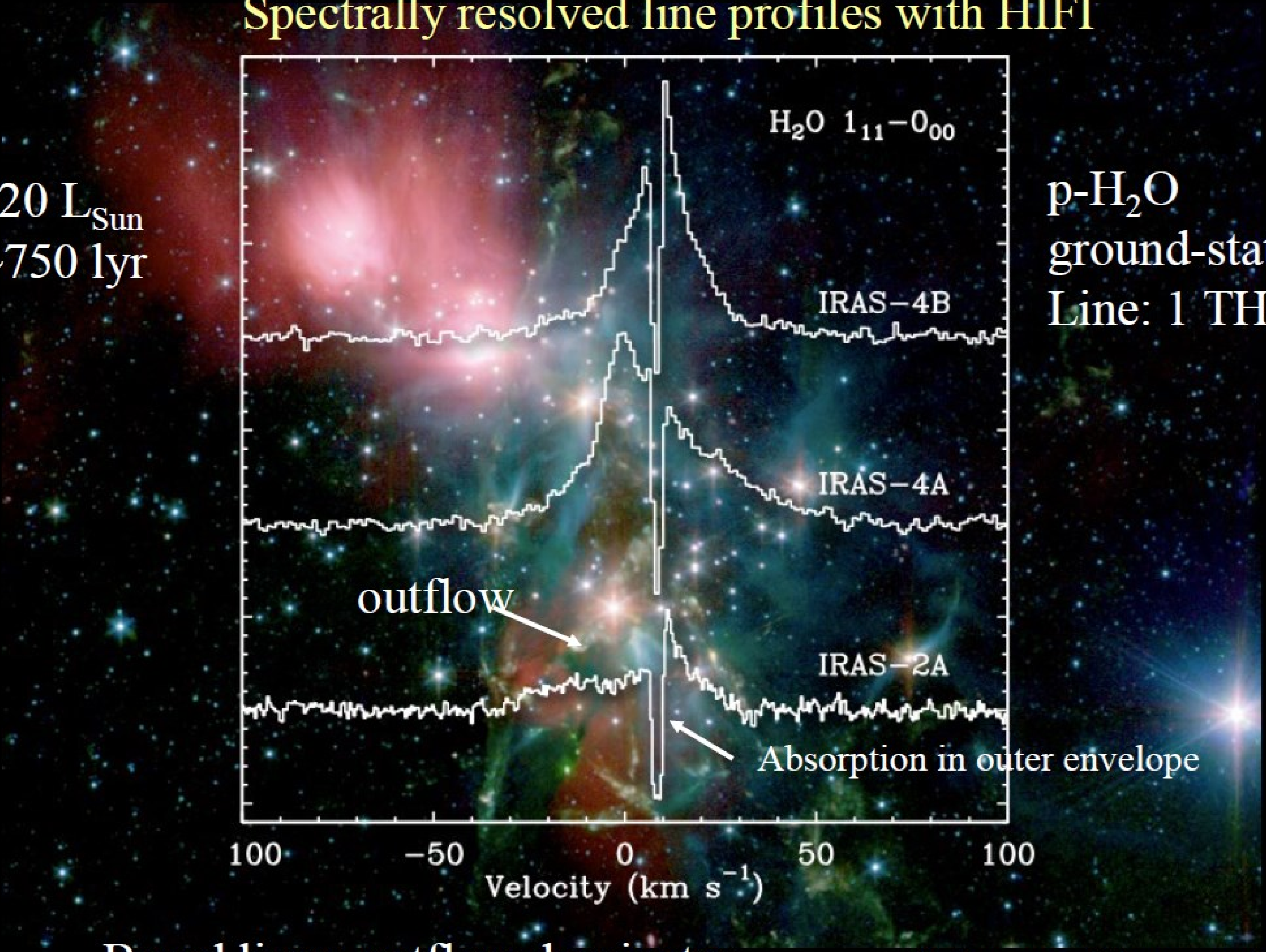
Nisini et al. 2010

- Water traces ‘hot spots’ where shocks dump energy into cloud

Low-mass protostars: NGC 1333

Spectrally resolved line profiles with HIFI

L~20 L_{Sun}
D~750 lyr



outflow

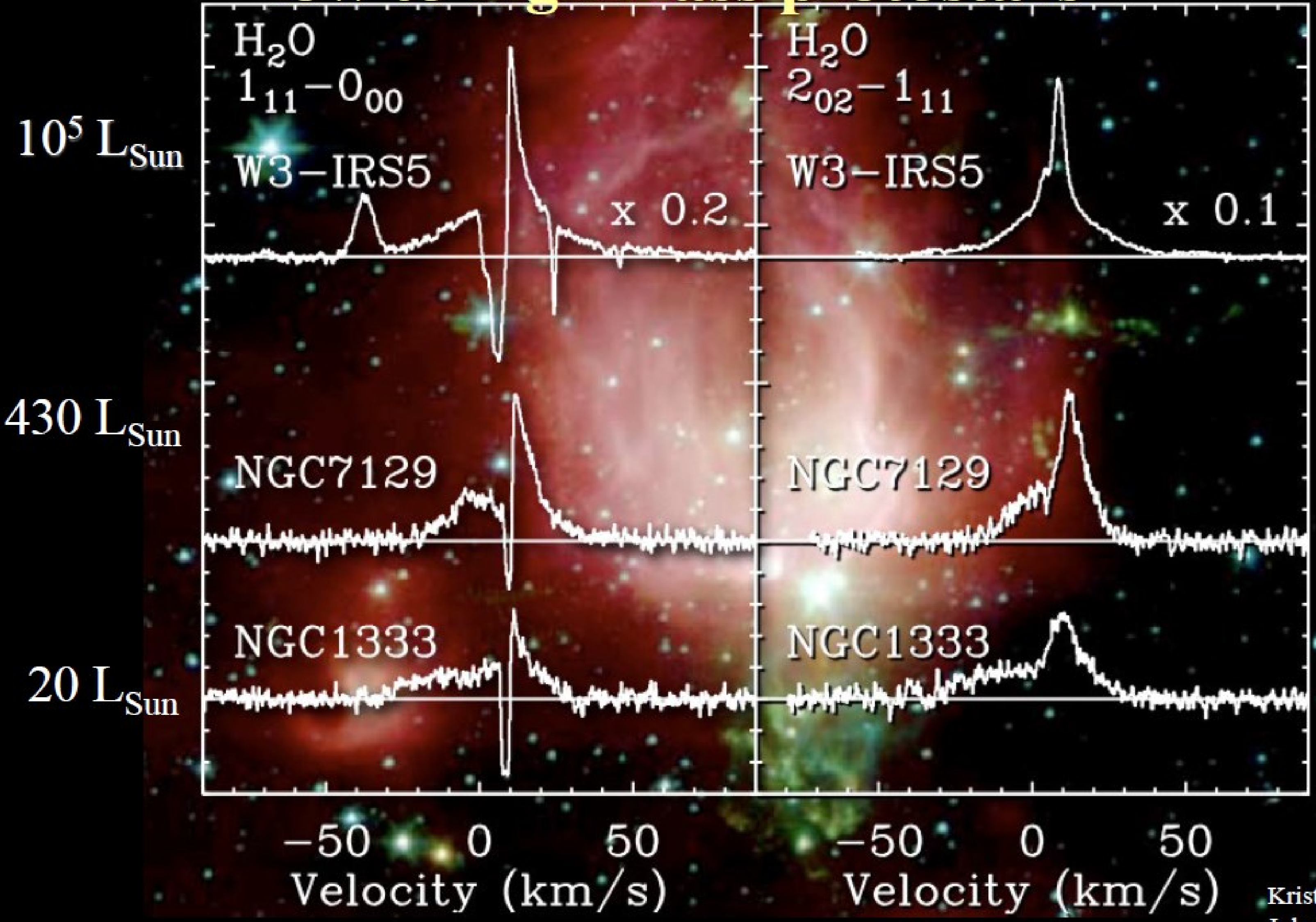
Absorption in outer envelope

p-H_2O
ground-state
Line: 1 THz

Broad lines: outflow dominates

Kristensen, Visser et al. 2010

Shocked H_2O lines: low to high mass protostars



Kristensen et al. 2010
Johnstone et al. 2010
Chavarria et al. 2010

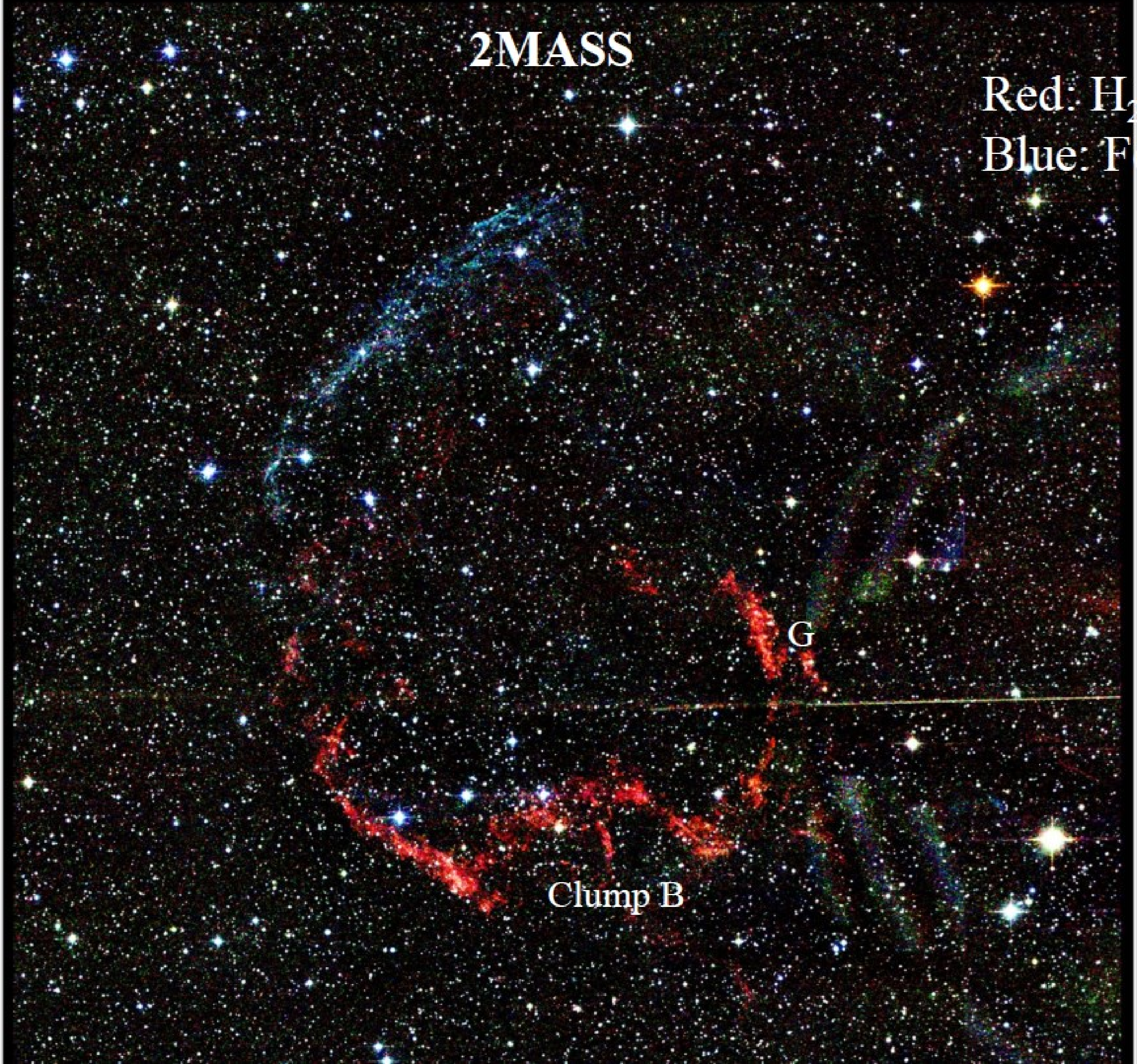
Note similar profiles

5.5 Comparison with observations

a. IC 443

- Best studied and nearest (1500 pc) example of interacting supernova remnant with a molecular cloud
- Observations at optical, infrared, radio, X-ray => several shell-like regions, shocked molecular gas in sinuous, flattened ring seen in H_2 2 μm, IRAS 100 μm, …
- Many molecules show broad, asymmetric shocked line profiles. Data cannot be fit by single *J*- or *C*-shock but requires multiple *T*, *n* components

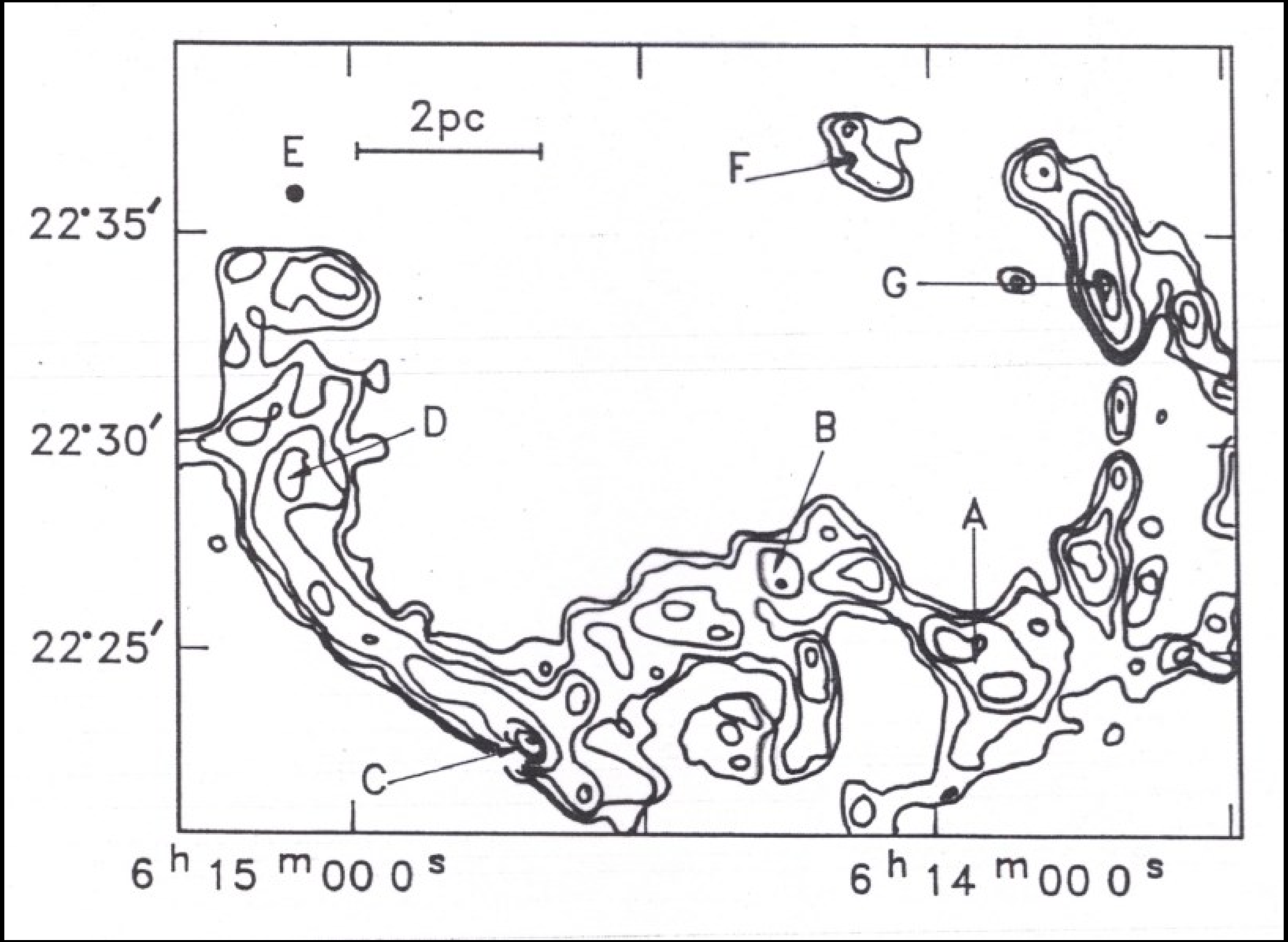
The Supernova Remnant IC 443



2MASS

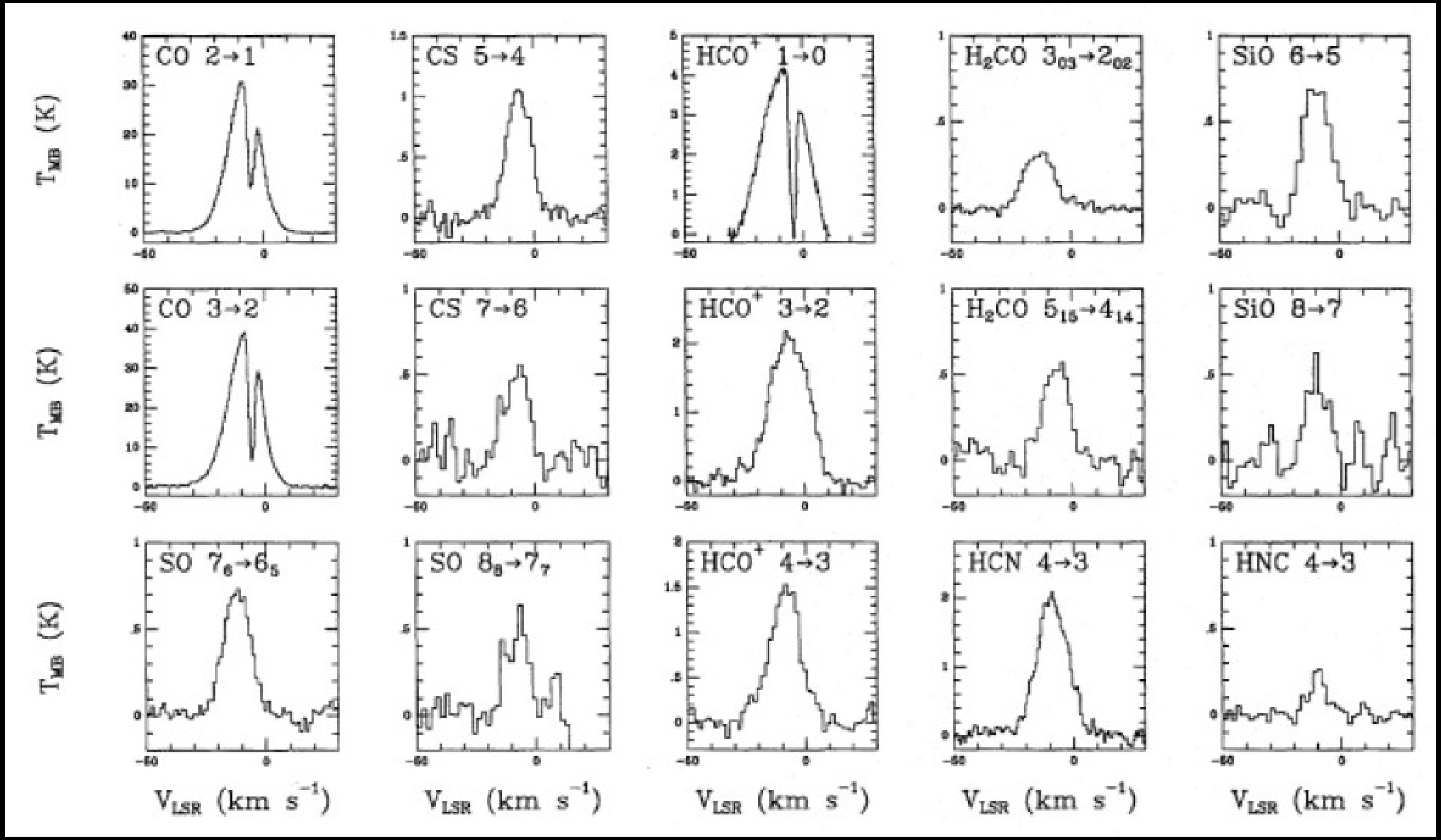
Red: H_2 2.12 μm
Blue: Fe II

Shocked H_2 emission



Burton 1987

IC 443 clump G spectra

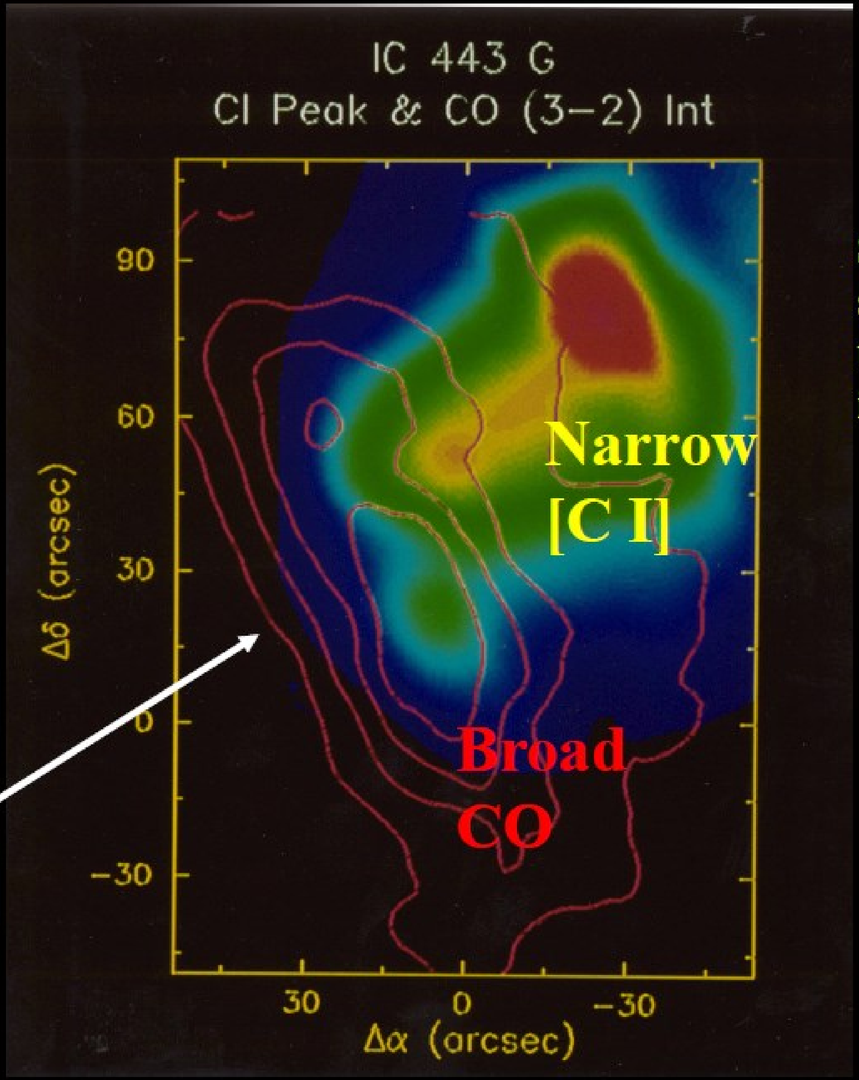


van Dishoeck et al. (1993)

- Note broad profiles, characteristic of shocked gas
- But abundances not much changed compared with quiescent gas (except SiO)

(Strong lines do not necessarily imply higher abundances; can also be higher density)

IC 443 G: radiative precursor



Strong narrow [C I] 492 GHz seen ahead of shock due to photodissociation of CO in pre-shock gas

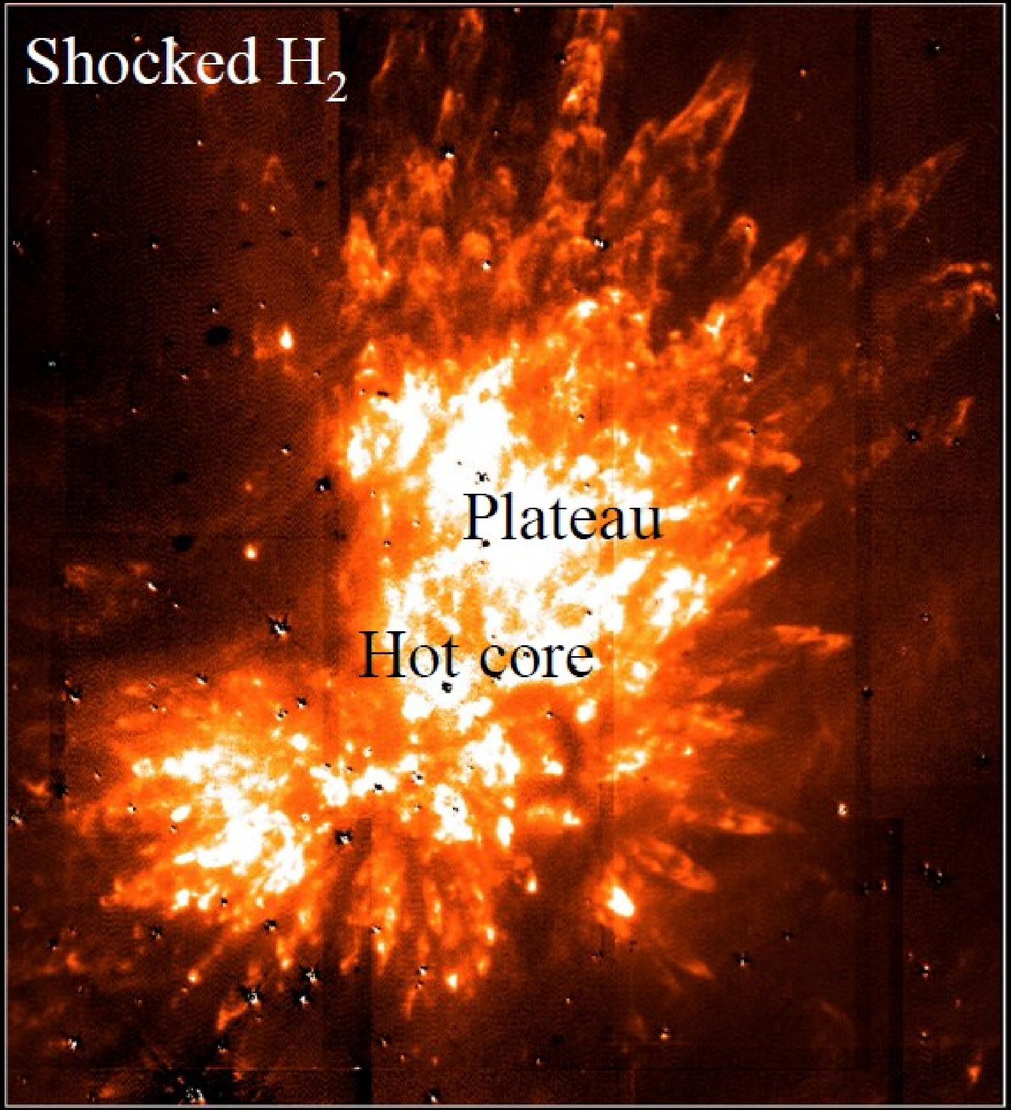
Color: narrow [C I]
Contours: shocked CO

Keene et al. 1994

Conclusions IC 443

- Most molecules (including HCO^+, HCN, CS) show no significant abundance enhancements in shock; only SiO shows clear increase
- Lack of enhancements may be due to high H/H_2 ratio (=> back reactions important) and/or radiation field from shock
- Evidence for radiative precursor seen in strong [C I] emission upstream from shock

b. Orion/KL shock



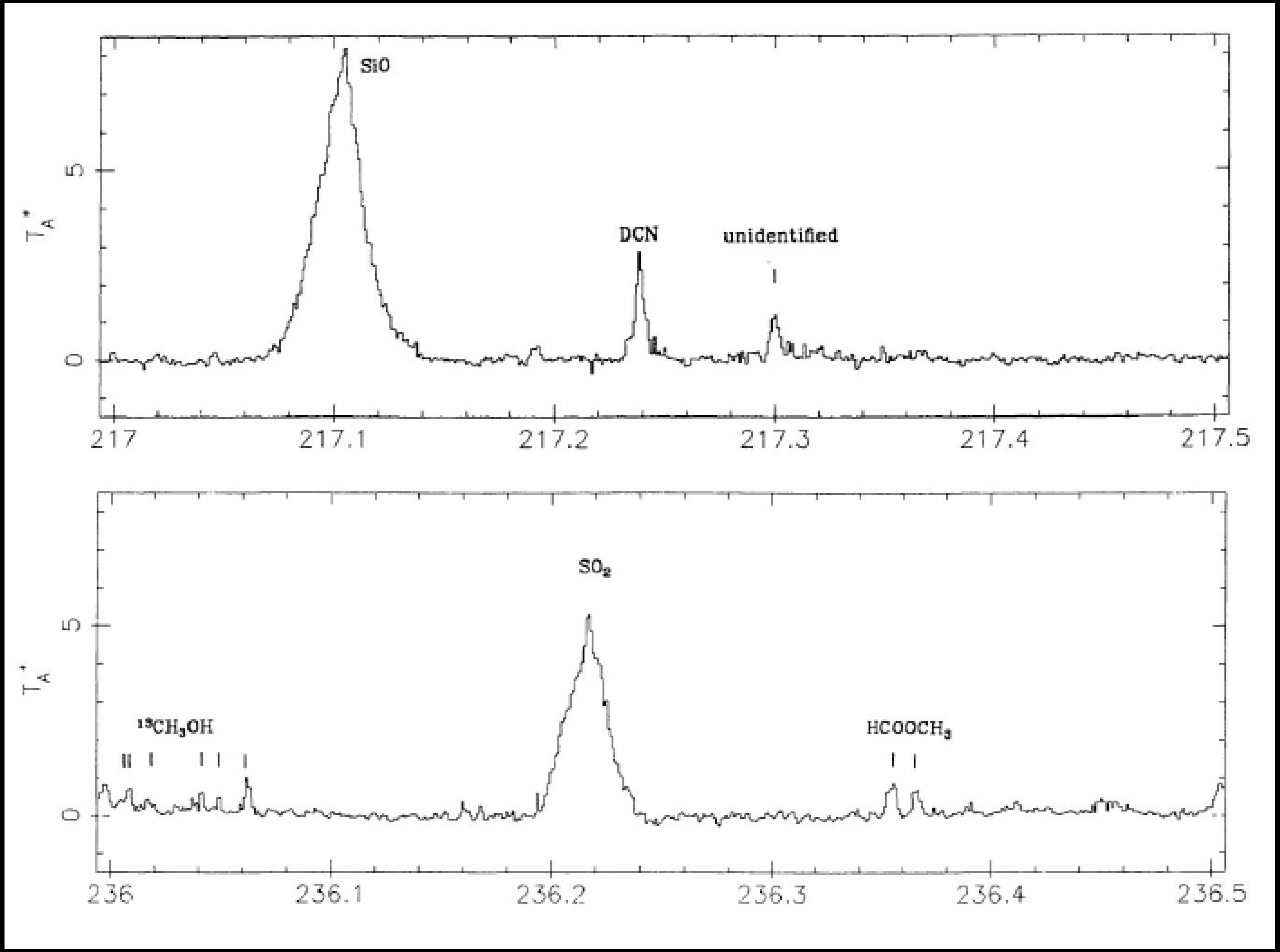
Orion KL

CISCO (H_2 (v=1-0 S(1)) – Cont)

Subaru Telescope, National Astronomical Observatory of Japan

January 28, 1999

Orion/KL shock



Sutton et al. (1985)

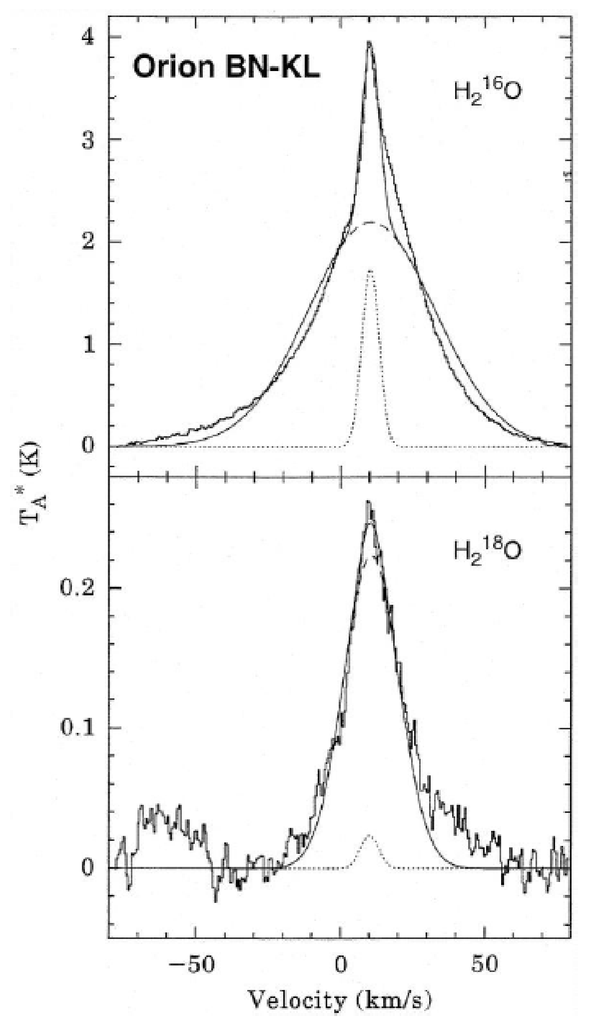
- Plateau region in Orion shows very broad lines (ΔV up to 100 km s^{-1}) in SO, SO_2, SiO… Abundances enhanced by factor > 100 compared with quiescent ridge

Orion abundances

	Plateau	**Ridge**
SO	5(-7)	≤1(-9)
SO_2	5(-7)	≤3(-9)
SiO	1(-7)	≤3(-10)

- Orion pre-shock density (~10^5 cm^{-3}) much higher than in IC 443 (~10^3 cm^{-3})
- Prominent water emission observed (Melnick et al. 2010)

Orion H_2O and $H_2{}^{18}O$ profiles



Melnick et al. (2000)

SWAS observations:
Ground state 557 GHz
o-H_2O 1_{10}-1_{01}

Note broad line
profiles, even for $H_2{}^{18}O$
=> shock

Abundance ~10^{-4}
=> Most O driven into H_2O

- Note: other shocks show a much lower H_2O abundance by factor 10-100
- → UV irradiated shocks where H_2O is photodissociated

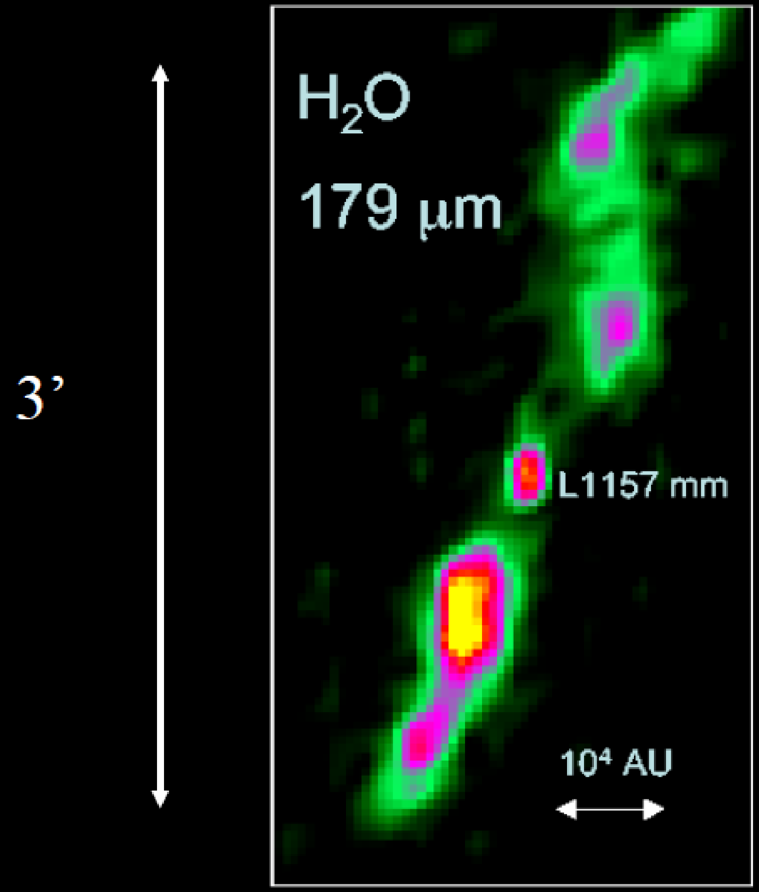
Karska et al. (2014, 2018)

c. L 1157

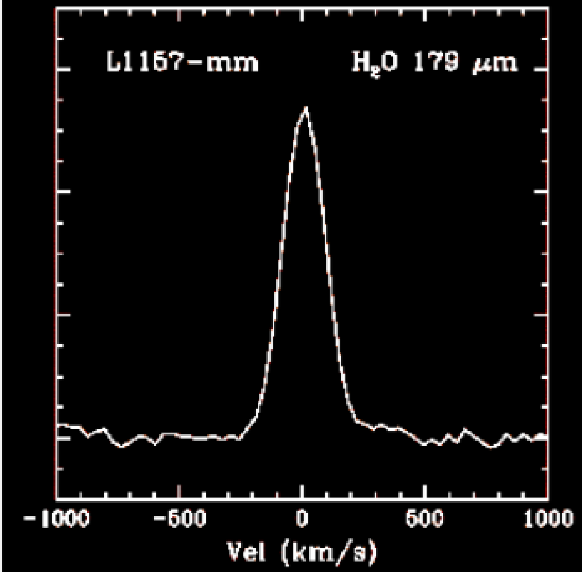
- Highly collimated outflow driven by Class 0 deeply embedded protostar, ~11 $L_\odot$, d = 440 pc
- Shock vs. quiescent gas revealed by profiles
  - **Quiescent gas: $C^{18}O$, N_2H^+, $H^{13}CO^+$, DCO^+**
  - **Shocked gas: SiO, CH_3OH, H_2O, CS, H_2CO, …**
    - **Recently: SO^+, HCS^+, $HOCO^+$**
- Significant abundance enhancements for SiO ($\geq 10^4$) and CH_3OH (10^2–10^3), but much less / no enhancements for other species => grain destruction and release of icy mantles

H_2O as tracer of shocks

Herschel-PACS image of water in proto-stellar systems



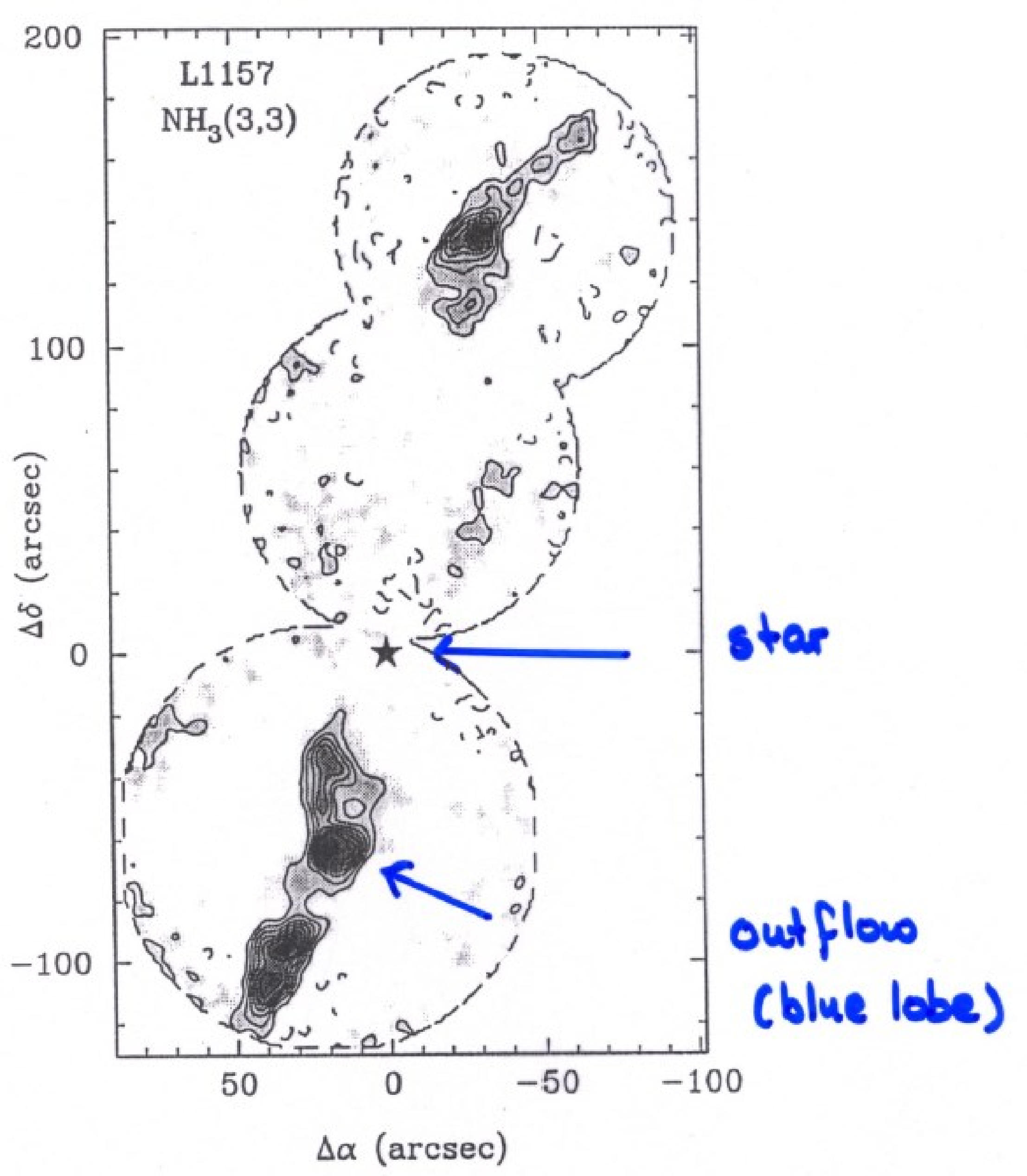
L1157-mm outflow
$D = 440$ pc, $L_{bol} = 11\ L_o$



Nisini et al. 2010

Water traces ‘hot spots’ where shocks dump energy into cloud

L 1157 shock



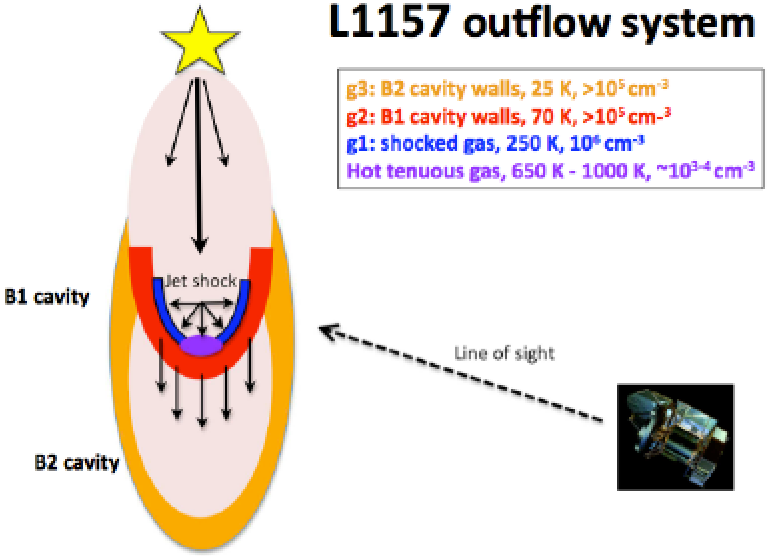
star

outflow (blue lobe)

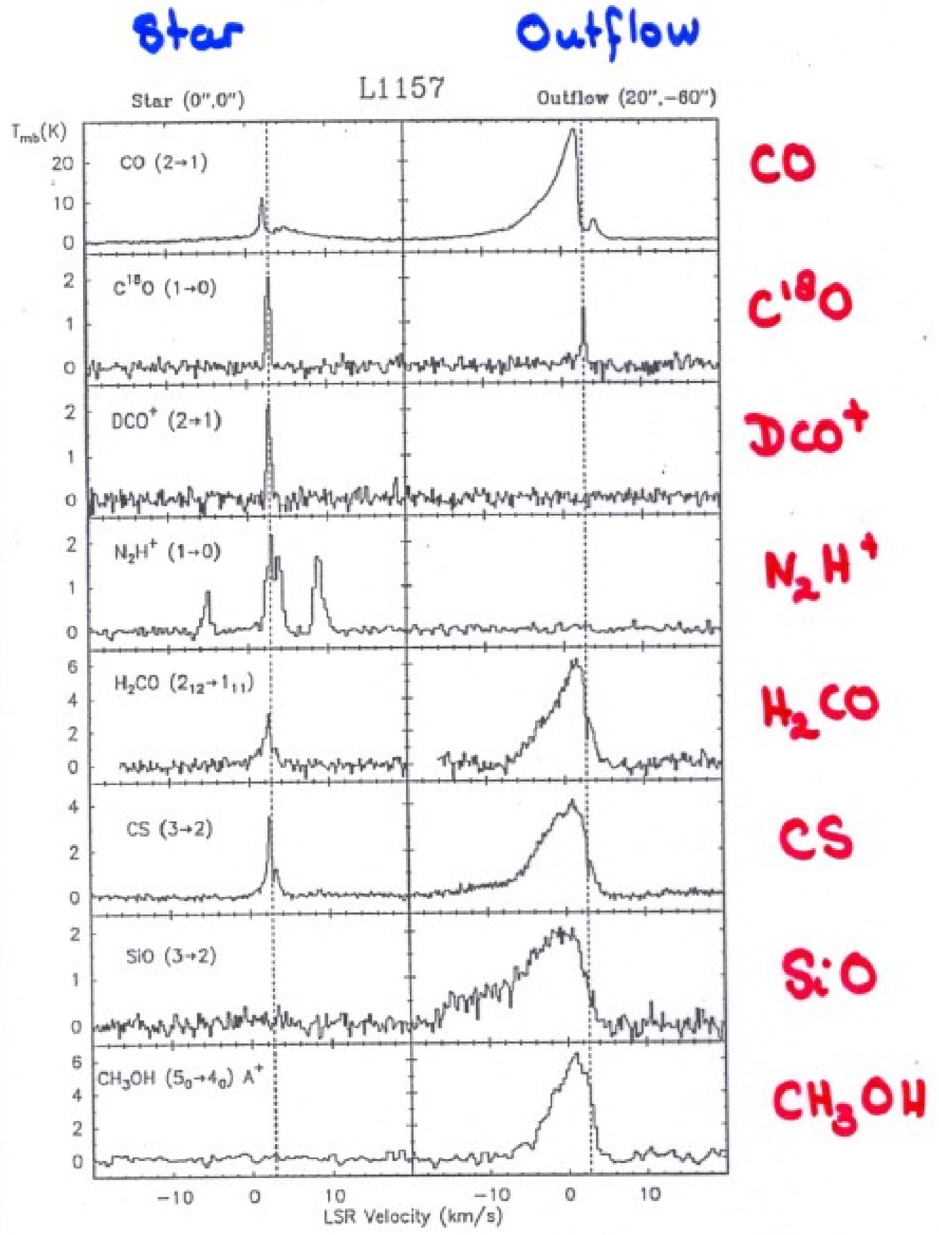
Grain surface product: NH_3

Bachiller (1997)

L 1157 line profiles

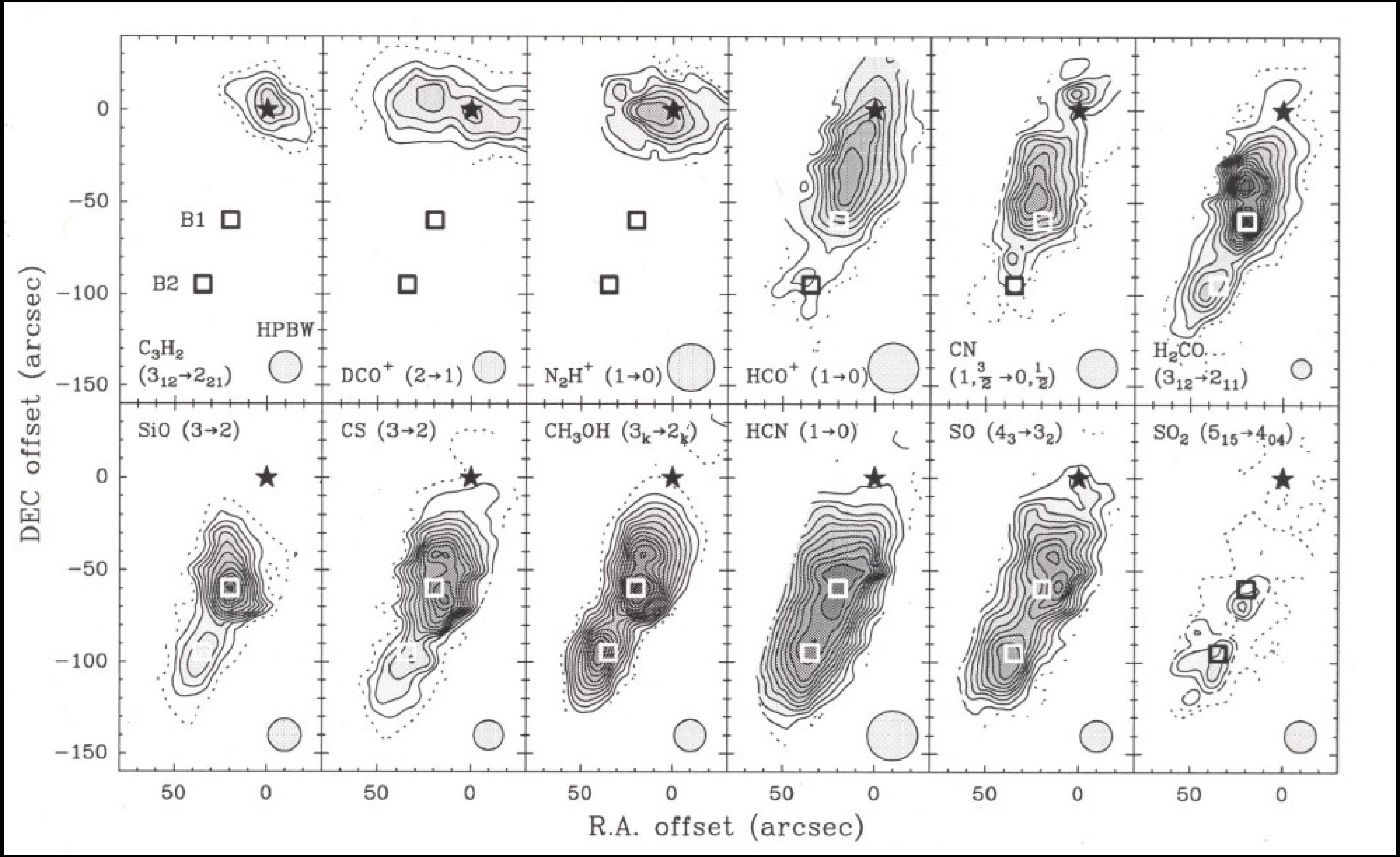


Busquet, Benedettini, LeFloch et al.
2012-2014



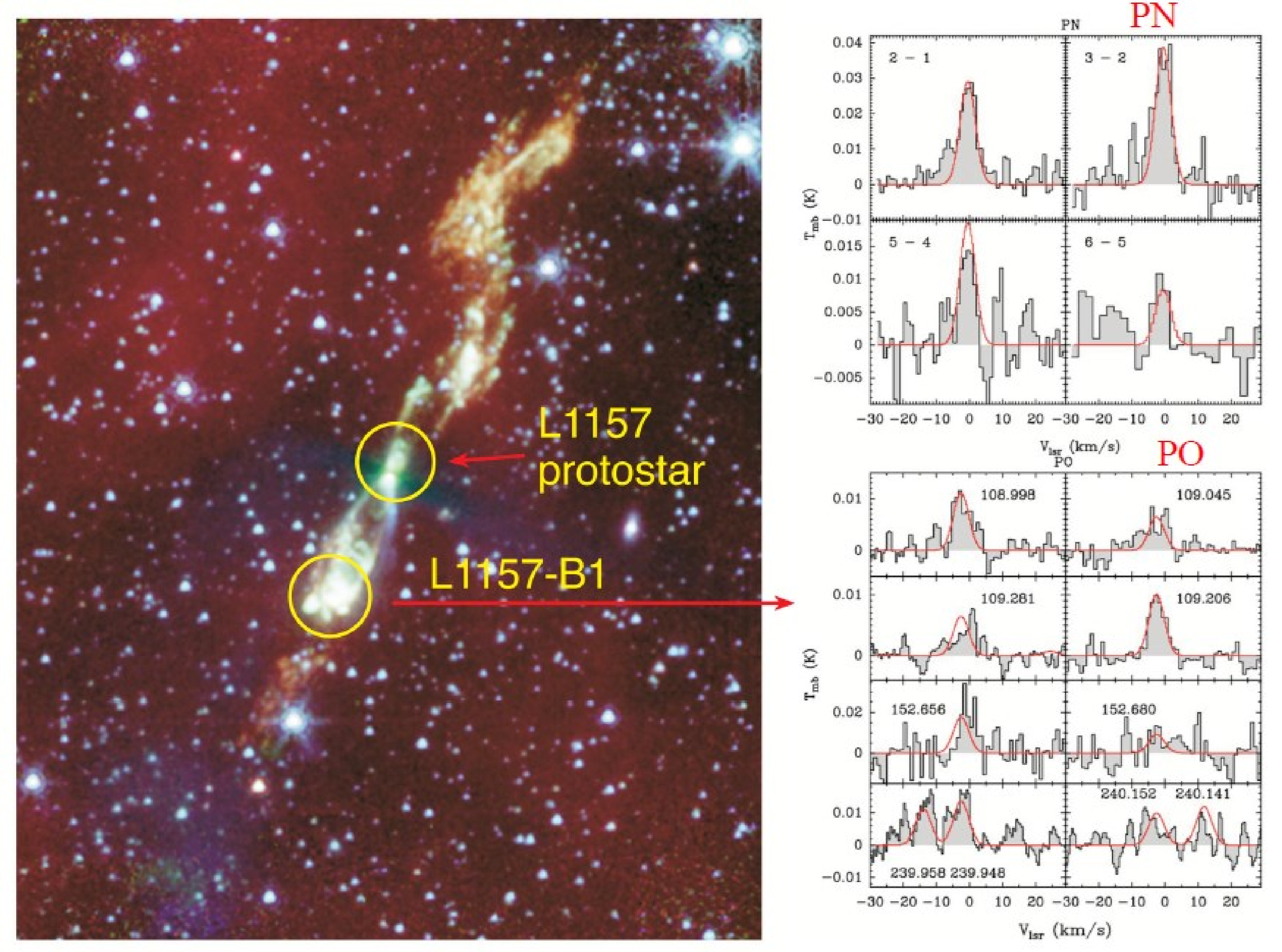
Bachiller (1997)

L 1157 southern (blue) lobe



- Note: different molecules peak at different locations: time dependence

Rich chemistry in L 1157 B1



- Complex organics, phosphorous molcules, ...

Lefloch et al. (2017)

5.6 Summary Lecture 5

- Detailed physical models of shocks in molecular clouds exist; ***J*-, *C*-, *C**- shocks**. Observations suggest, however, that in most cases a single shock does not apply.
- Chemistry investigated in detail in dissociative and non-dissociative shocks. Chemistry in *C*-shocks needs to take account of UV radiation in shock and pre-shocked gas created by fast *J*-shock.
- Grain sputtering => clear observational diagnostics: **SiO**
- Bipolar outflows around YSOs release grain mantles, enhancing **CH_3OH** and other grain mantle components
- High temperature chemistry drives most O into **H_2O** in dense shocks in Orion
  - Evidence for new class of UV-irradiated shocks with lower H_2O abundances in most protostars