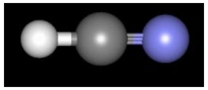


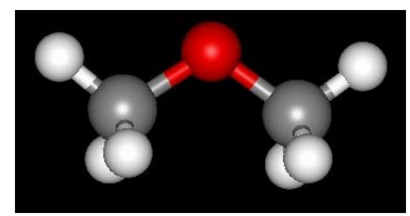
Astrochemistry
Lecture 5

Chemistry in shocked regions

Ewine F. van Dishoeck

Leiden Observatory

May-June 2022



Tielens Chap. 11
Hartquist & Caselli 1998
Water review Section 4.4

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

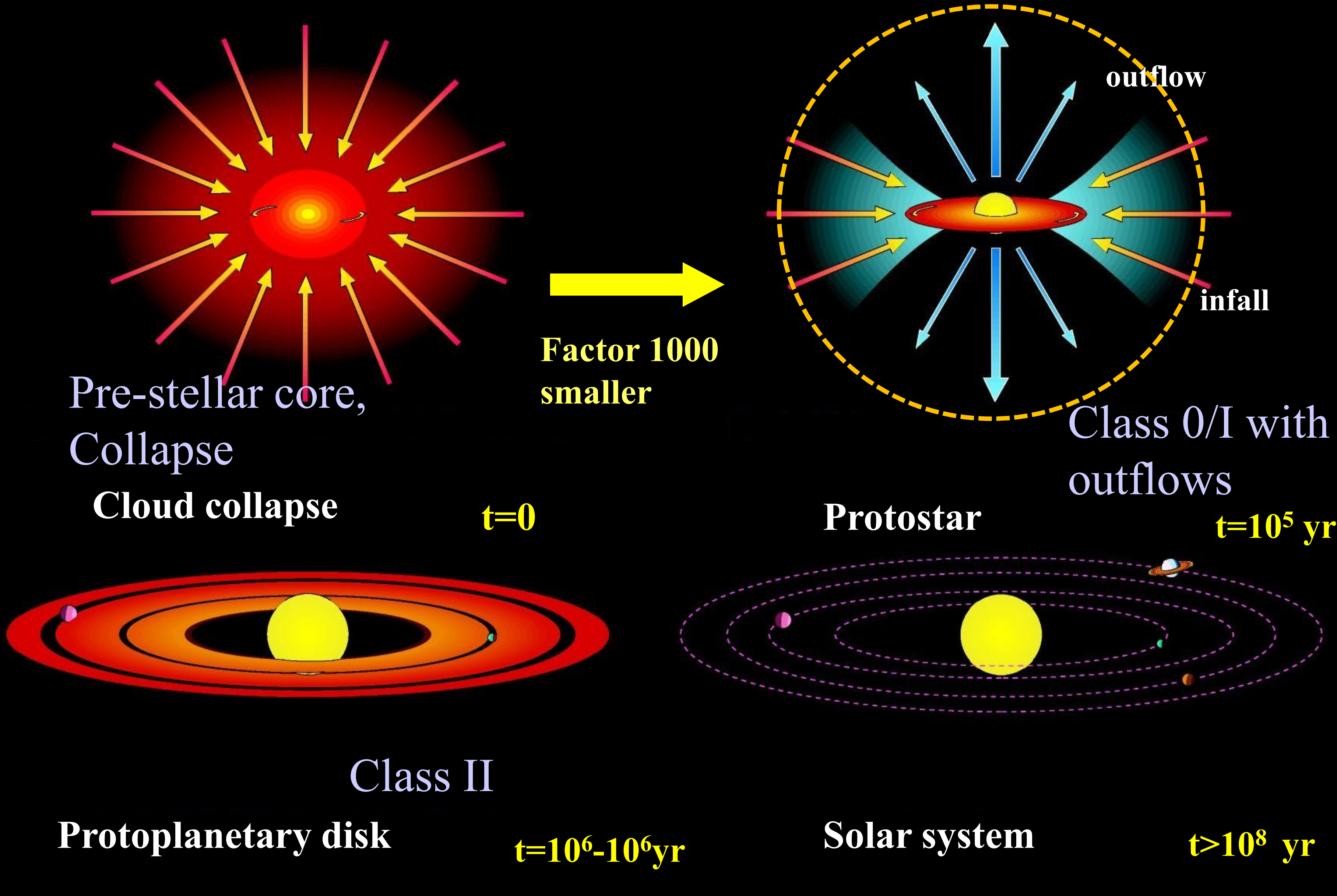
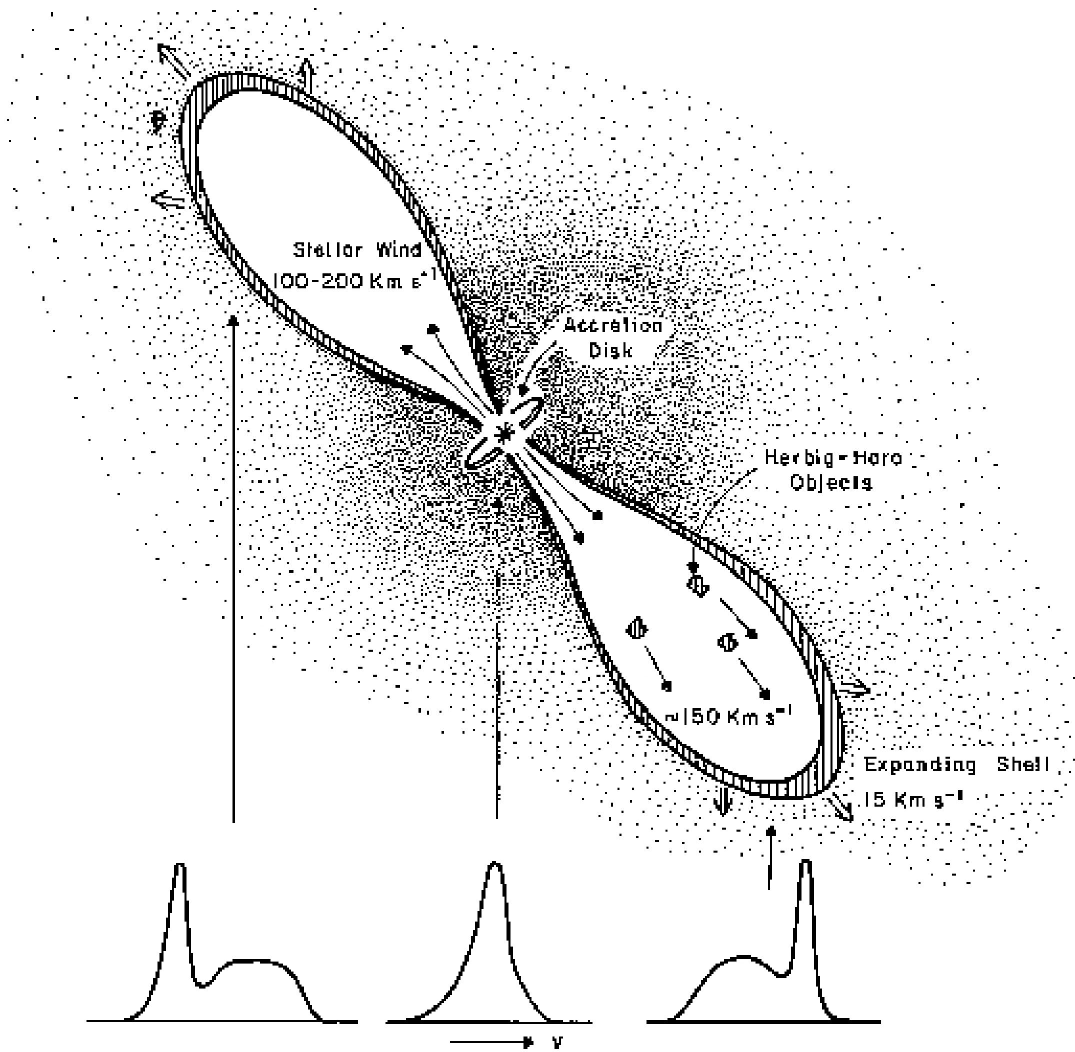


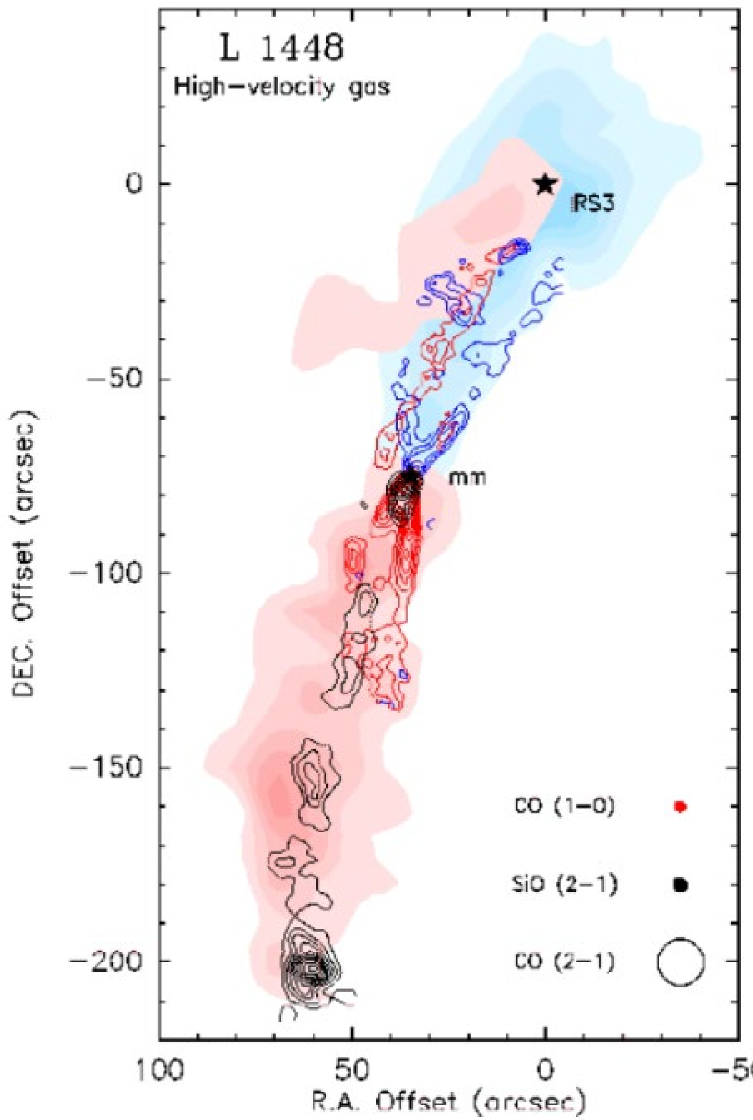
Fig. by M McCaughrean

Anatomy of bipolar outflows from protostars



Snell et al. 1980

Bipolar outflow from protostar



Bachiller & Tafalla 1999,
In Crete II

Outflows seen in molecular lines:

Molecular outflows

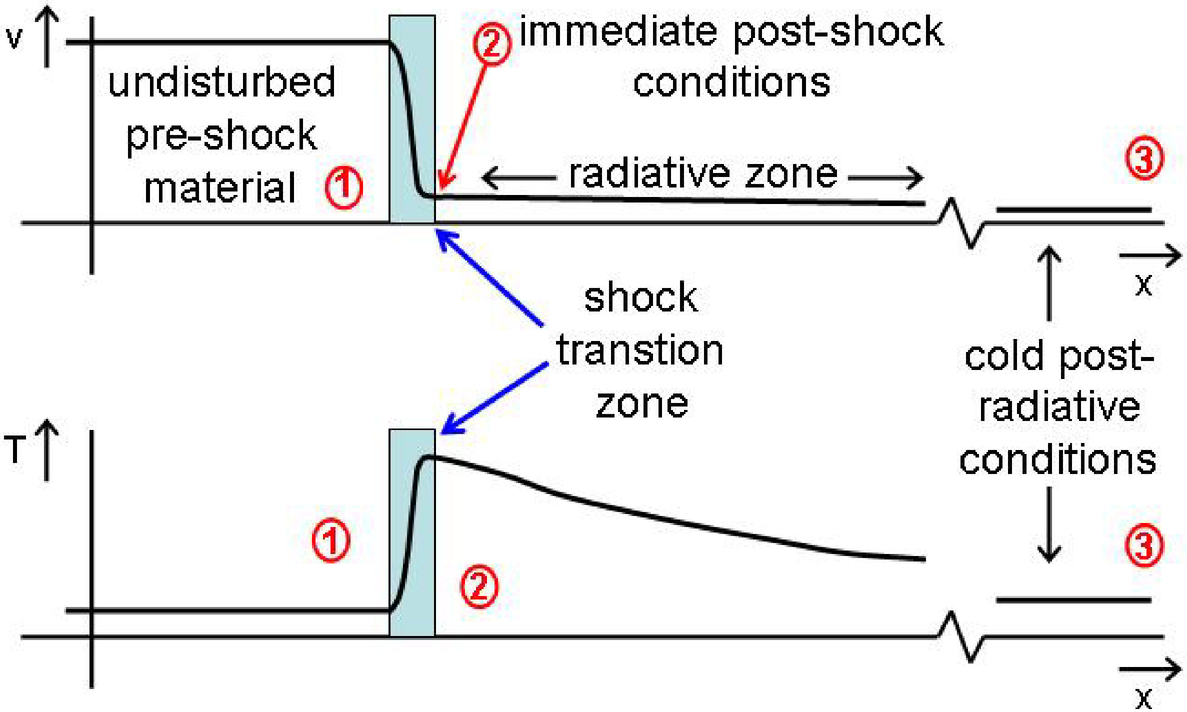
Sound speed and Mach number

- ***Sound speed:*** $C^2 \equiv \dfrac{dP}{d\rho}$
- $P = K\rho^{\gamma}$ with $\gamma = 5/3$ for adiabatic flow, $\gamma = 1$ for isothermal flow $\Rightarrow$
- $C \propto \rho^{1/3}$ for adiabatic flow $\Rightarrow$ sound speed larger in denser gas
- $C \approx \sqrt{\dfrac{kT}{m}} \approx 1 \text{ km s}^{-1}$ for isothermal gas in ISM
- Above phenomena have $v_S \approx 5\text{-}100 \text{ km s}^{-1} >> C$ $\Rightarrow$ ***gas must be shocked***
- ***Mach number:*** $\mathcal{M} \equiv$ ratio of shock velocity w.r.t. sound speed, $\mathcal{M} \equiv v_S/C$

Shock jump conditions

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

Shock profile (shock frame)



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

Shock jump conditions (cont'd)

- 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 $\Rightarrow$ 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 sound speed

$$C_s = \left(\frac{5kT}{3\mu}\right)^{1/2} \approx 0.77\left(\frac{T}{100}\right)^{1/2} \ \mathrm{km\,s^{-1}}$$

- Alfvén speed

$$C_A \approx \left(\frac{B^2}{4\pi\rho}\right)^{1/2} \approx 1.8b \ \ \mathrm{km\,s^{-1}}$$

with $B=n_0^{1/2}b$ microGauss and $\rho=\mu n_0$=mass density

Observations $\Rightarrow$ $b\approx 1$

Magnetosonic speed: $C_{MS}=(C_S{}^2+C_A{}^2)^{1/2}$

Signal speeds (cont'd)

- Ion-Alfvén speed

$$C_A = \left(\frac{B^2}{4\pi\rho_i} \right)^{1/2} = C_A / y_i^{1/2} >> C_A$$

$y_i = \rho_i / \rho$ = ion mass fraction = $10^{-6} - 10^{-8}$ in dense clouds

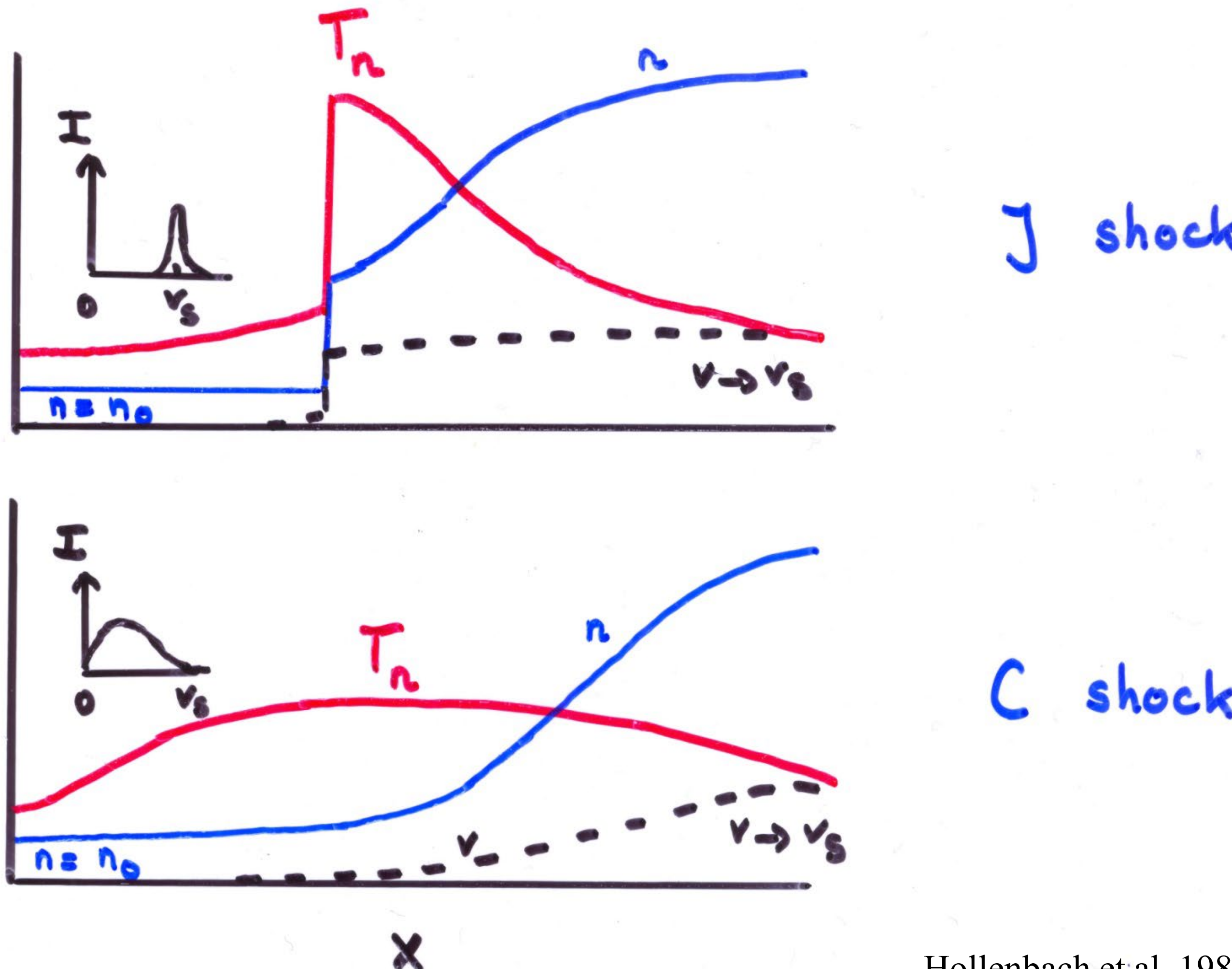
- Many shocks satisfy $C_S \leq \underset{\text{neutrals}}{C_A} < v_S < \underset{\text{ions}}{C_{iA}}$

- $\Rightarrow$ ion-Alfvén waves can transmit information of disturbance ahead of arrival; ions coupled to neutral by collisions

Two types of shocks

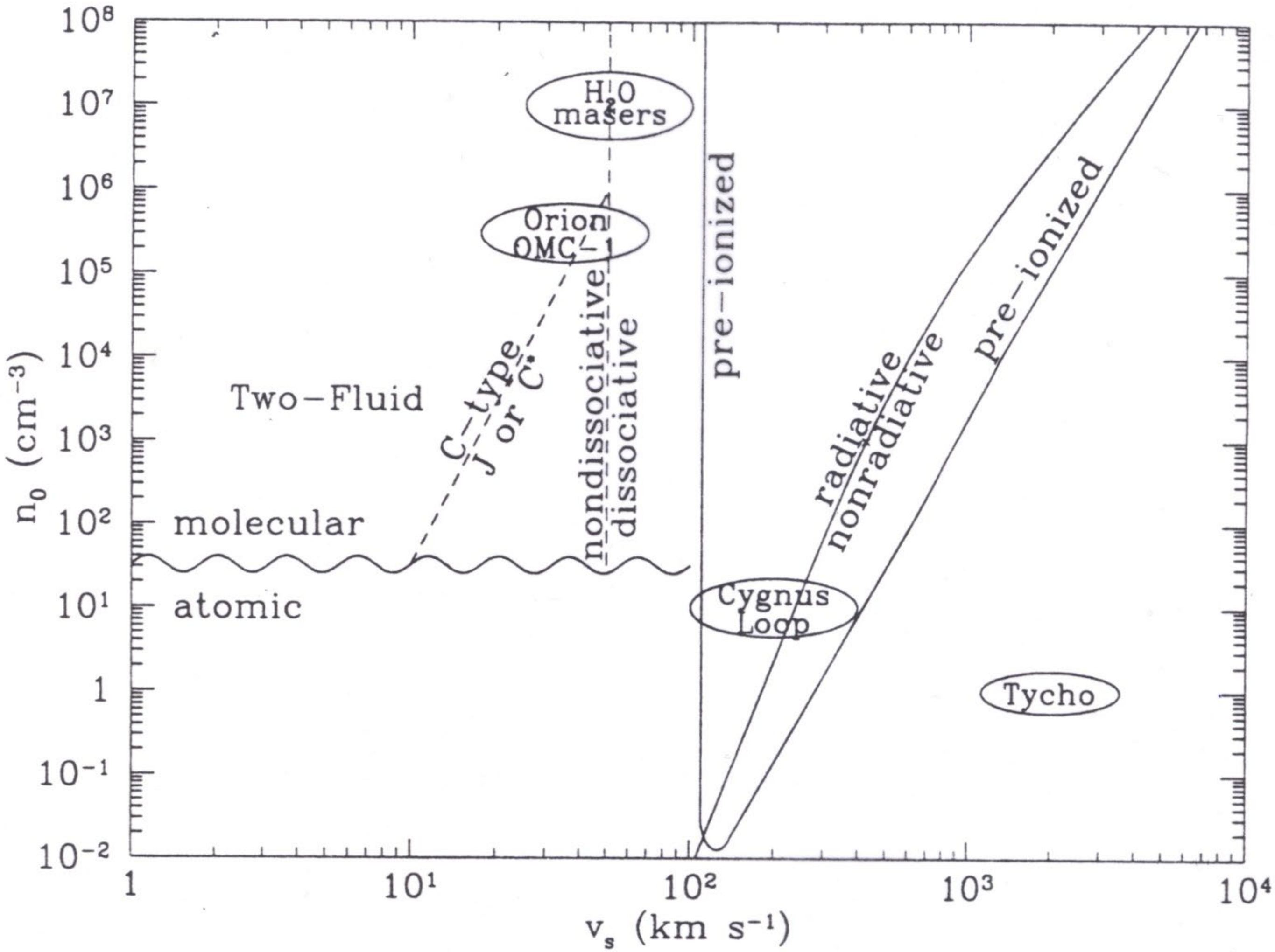
- ***J ("jump")-shocks:*** $v_S \geq 50$ km/s
  - Shock abrupt
  - Neutrals and ions tied into single fluid
  - T high: $T \approx 40\ (v_S/\mathrm{km\ s^{-1}})^2$
  - Most of radiation in ultraviolet
- ***C ("continuous")-shocks:*** $v_S \leq 50$ km/s
  - Gas variables (T, ρ, v) change continuously
  - 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 icy grain mantles
- Sputtering refractory grain cores to gas: Si
- Intense UV radiation field (i.p., Ly α)

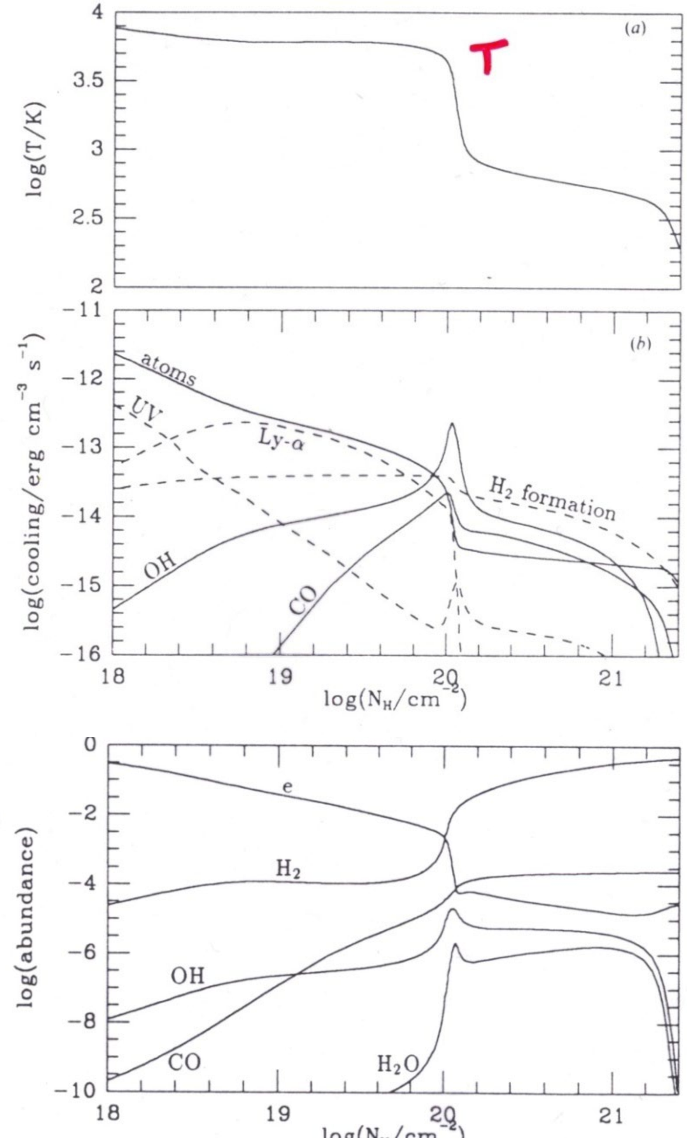
5.3 Chemistry in dissociative shocks

- Fast *J*-shocks destroy molecules, which re-form in the post shock gas
  - $v_S \geq 50$ km s^{-1} $\Rightarrow$ dissociation molecules into atoms
  - $v_S \geq 70$ km s^{-1} $\Rightarrow$ ionization atoms
  - $v_S \geq 80$ km s^{-1} $\Rightarrow$ UV radiation destroys molecules <u>ahead</u> 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 $\Rightarrow$ thermal energy
  - Radiation emitted by warm upstream gas
  - Exoergic chemical reactions
- Chemical composition determines cooling rate $\Rightarrow$ solve hydrodynamic equations together with chemistry

Dissociative shock profile



10^{13} 10^{15} cm

v_S=80 km s^{-1}

n_0=10^5 cm^{-3}

Note narrow width of shock layer: ~100 AU

Neufeld 1990

Chemistry in dissociative shocks

- $T \approx 10^5$ **K** $\Rightarrow$ collisional dissociation 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 (cont'd)

- **T<10^4 K** $\Rightarrow$ H_2 re-formation
  - Grains too hot $\Rightarrow$ gas-phase processes (as in early universe)
  - $H + e \rightarrow H^- + h\nu$ slow
  - $H^- + H \rightarrow H_2 + e$ 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** $\Rightarrow$ H_2 builds up rapidly
  - $O + H_2 \rightarrow OH + H$
  - $OH + H_2 \rightarrow H_2O + H$
  - $C^+ + OH \rightarrow CO + H^+$

Chemistry (cont'd)

- OH crucial intermediary 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 enhanced by destruction grains

Chemistry (cont'd)

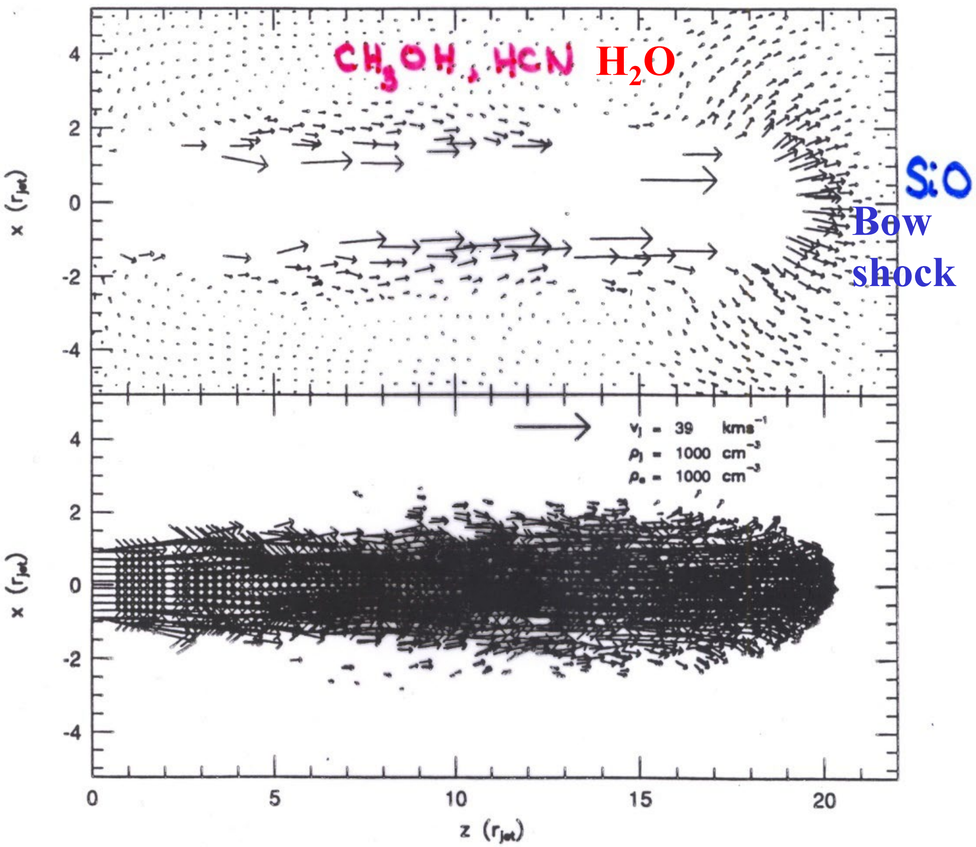
- Molecules can be destroyed by reverse reactions with H and by photodissociation. Much of shock energy emerges in Ly α 1216 Å line
  - OH, H_2O, …: can be dissociated by Ly α
  - H_2, CO, CN, …: cannot be dissociated by Ly α
  - H_2 (v=2): can be pumped by Ly α ⇒ characteristic IR + UV spectrum
  -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

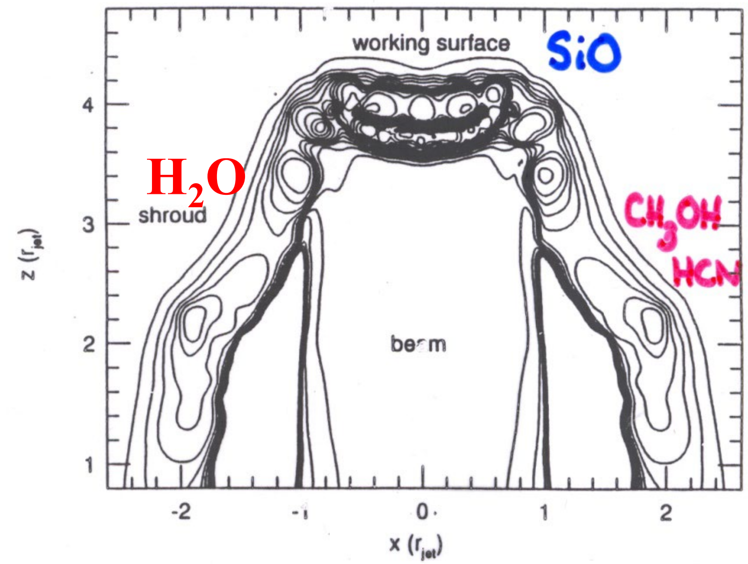
Grain destruction

- 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

Mini quiz

- Where would NH_3 be located in this picture?

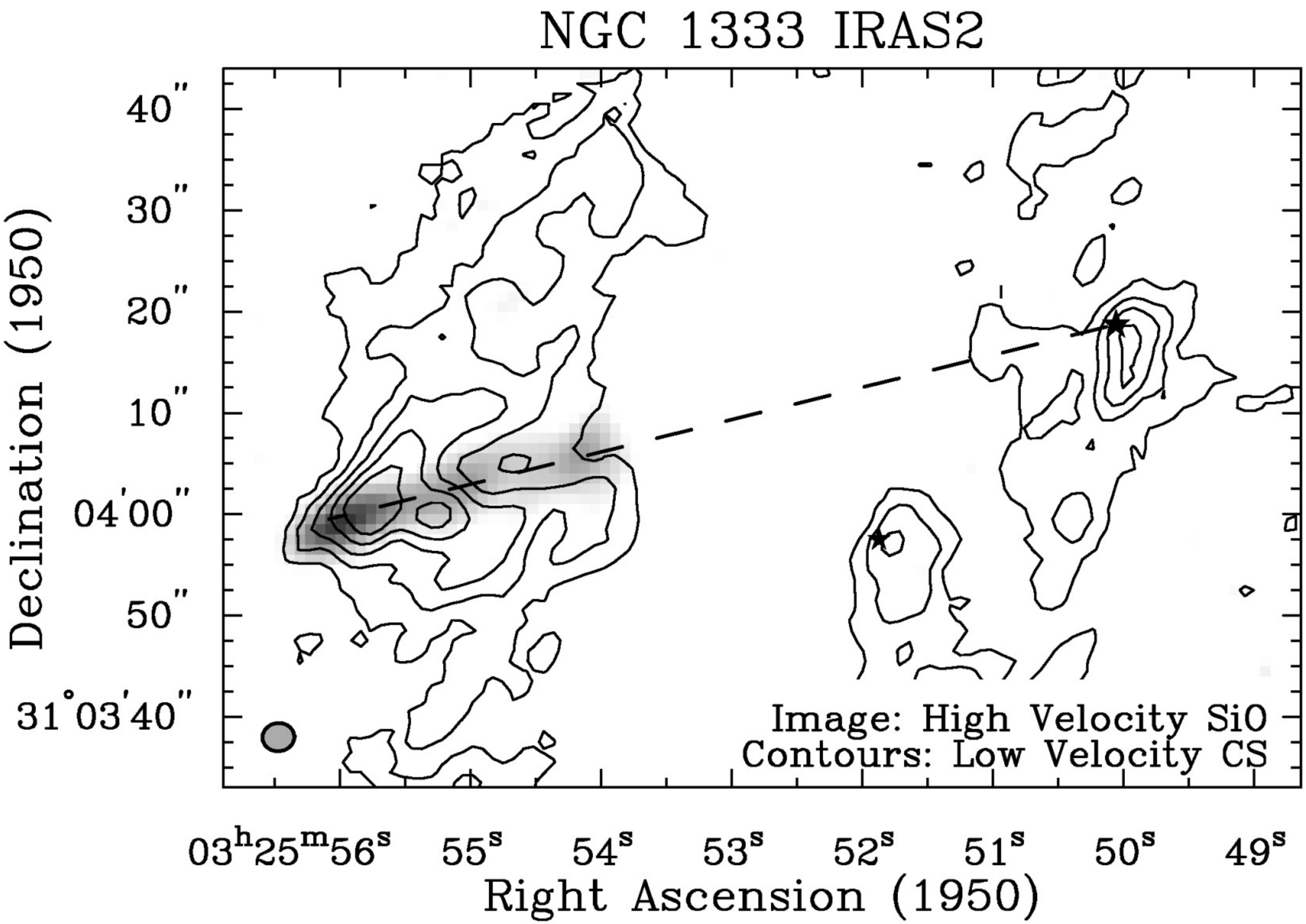
1. With SiO
2. With H_2O, CH_3OH
3. In the quiescent envelope

SiO as tracer of shocks: examples

- NGC 1333 IRAS 2
  - Extremely collimated ($<10^{16}$ cm width) SiO at tip of CO outflow $\Rightarrow$ bow shock
- L1448-mm
  - Extremely collimated SiO emission
  - Chain of high-velocity clumps up to 70 km s^{-1}
- BHR 71
  - Wide spread SiO emission $\Rightarrow$ interaction wide-angle wind with surroundings?

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

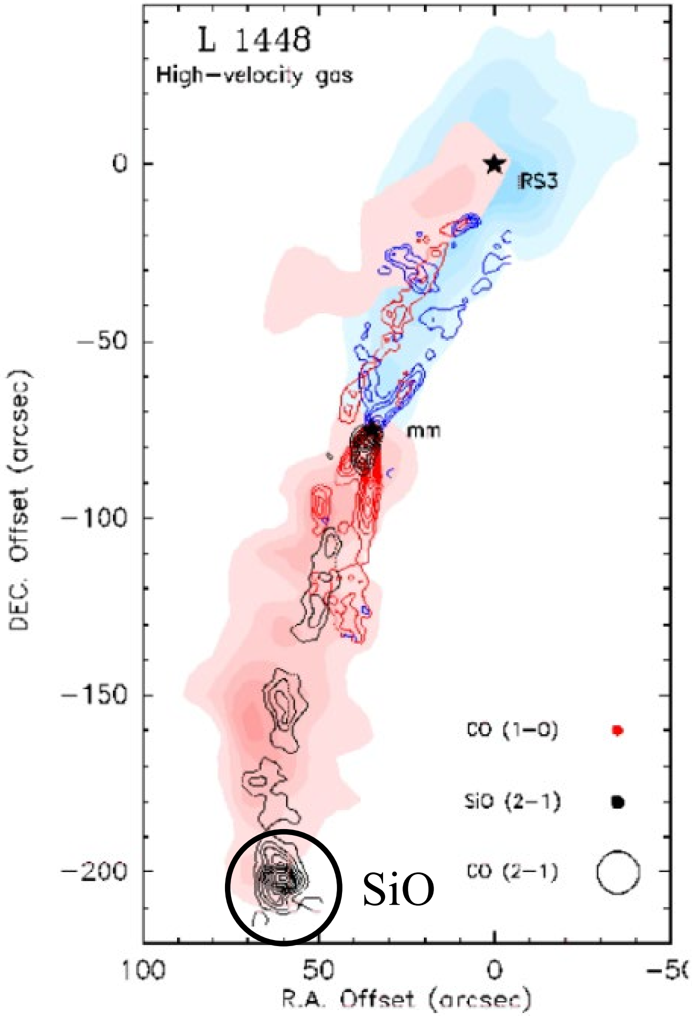
SiO at tip of jet



vD & Blake 1998
Jørgensen et al. 2005

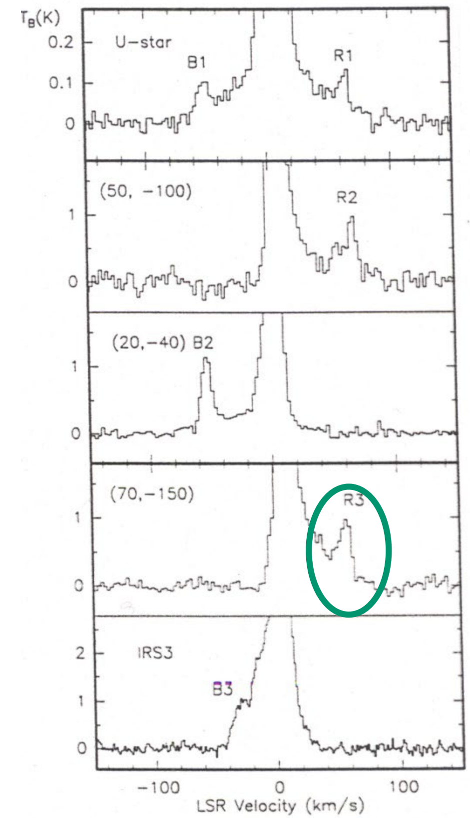
- SiO traces deeply embedded outflows

L 1448 outflow: CO vs SiO



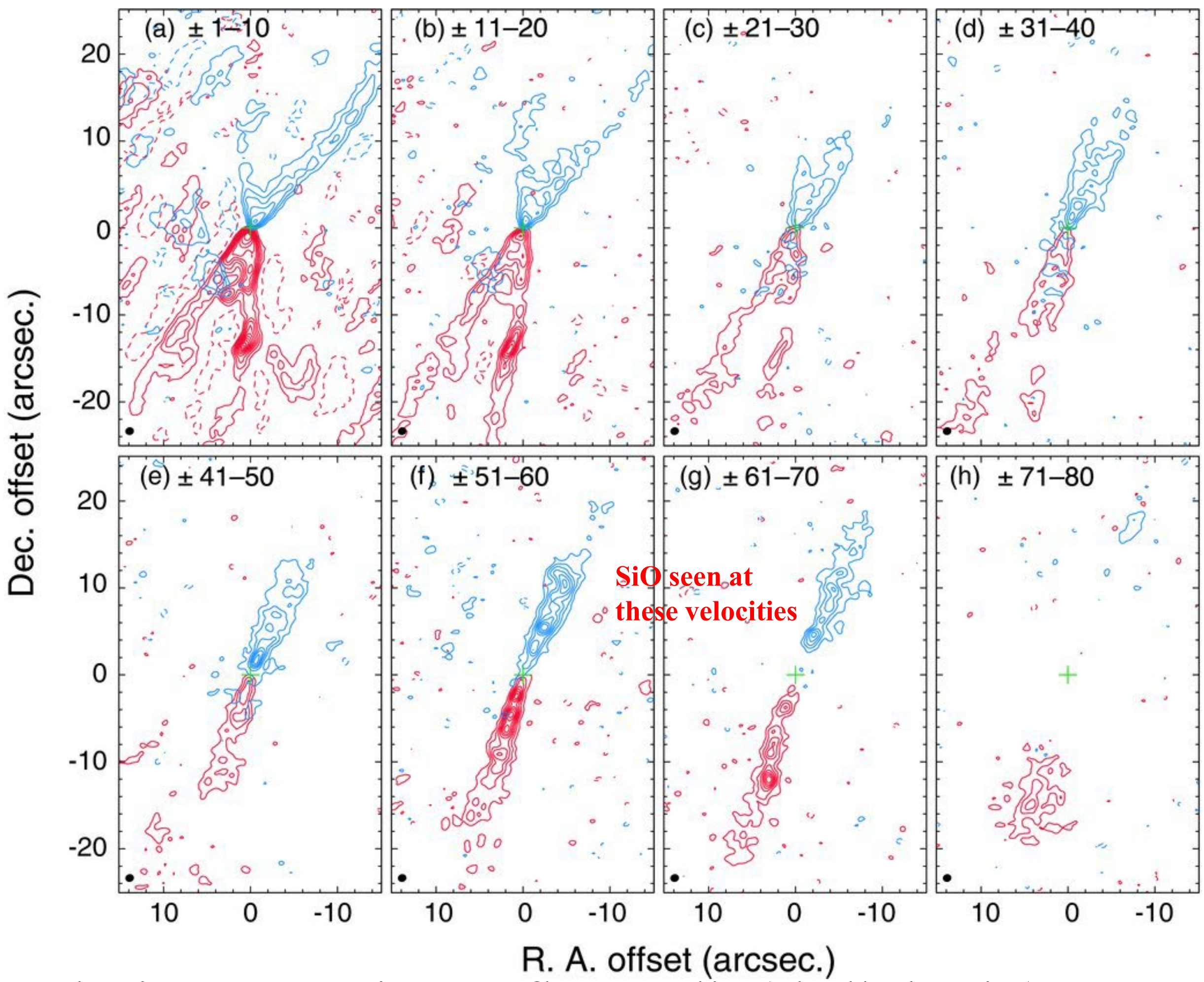
Bachiller et al. 1990, 1991
Guilloteau et al. 1992

CO



Note high-velocity ‘bullets’ a.k.a. Extremely High Velocity (EHV) gas

Extremely High Velocity gas



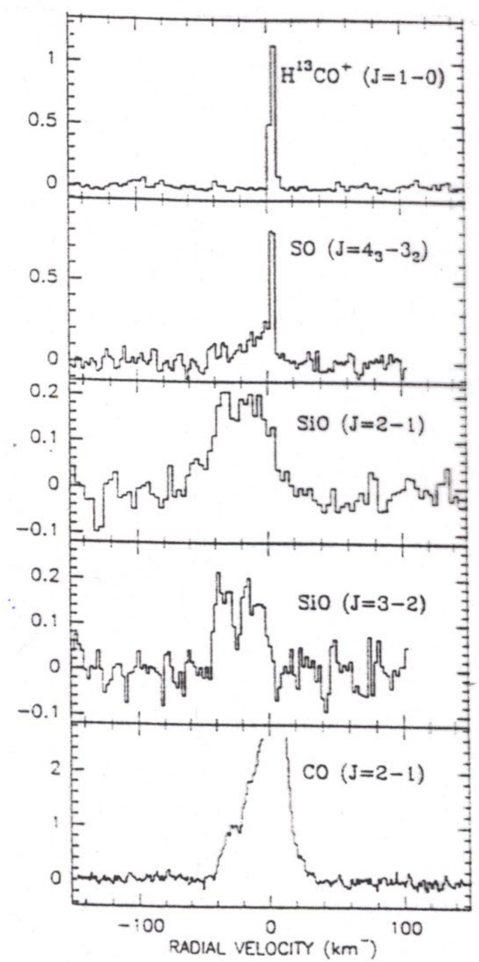
L1448mm
CO 3-2

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

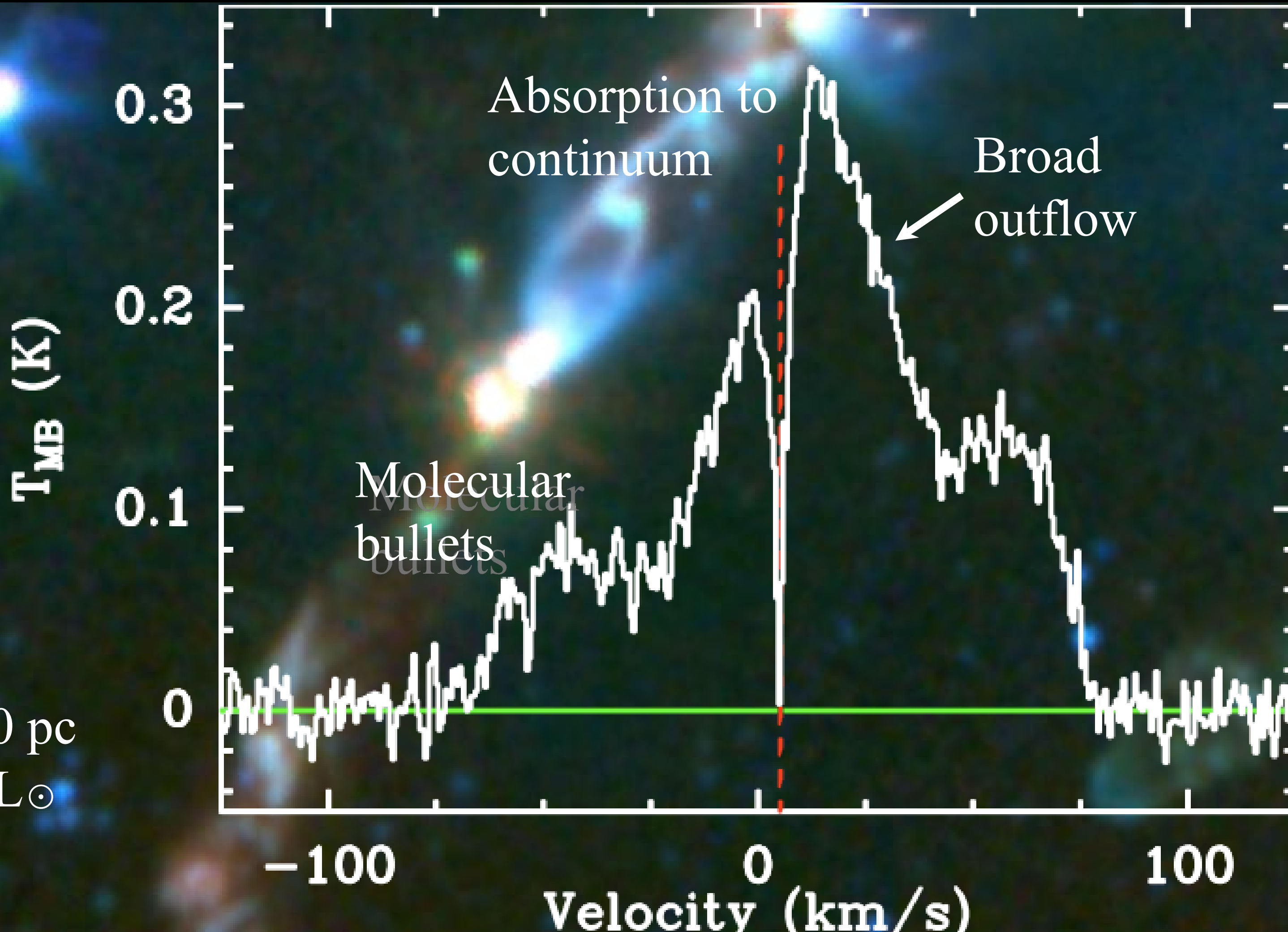
L1448



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

- Quiescent gas: Si≈10^{-6} w.r.t solar ⇒ heavily depleted
- Shocked gas: Si≈10^{-2} w.r.t solar ⇒ increase due to grain destruction

Also: Water ‘bullets’ in low-mass protostars L1448

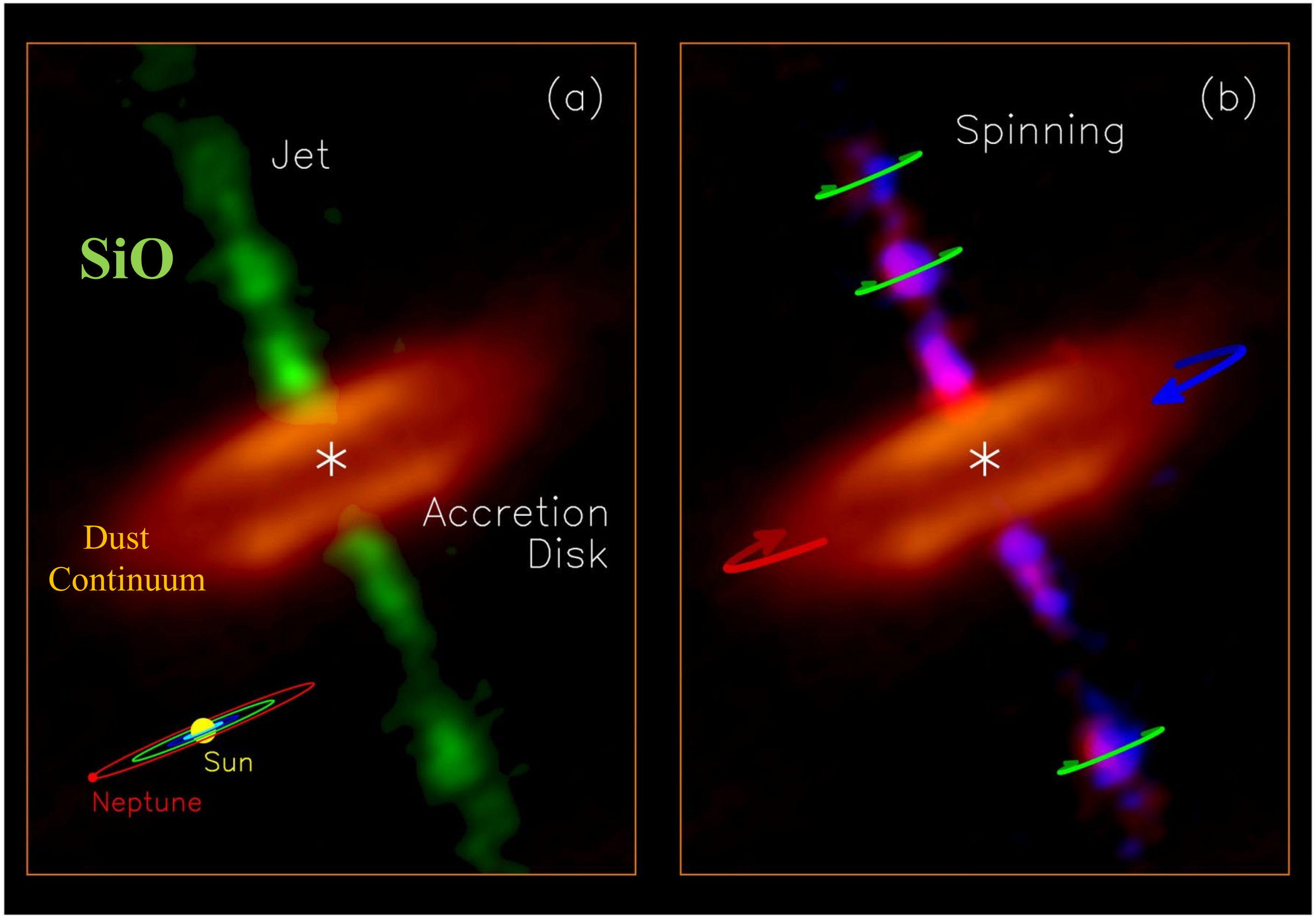


L1448:
D ~ 250 pc
L ~ 11 L$_\odot$

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

Kristensen et al. 2011

HH212: textbook example jet + disk

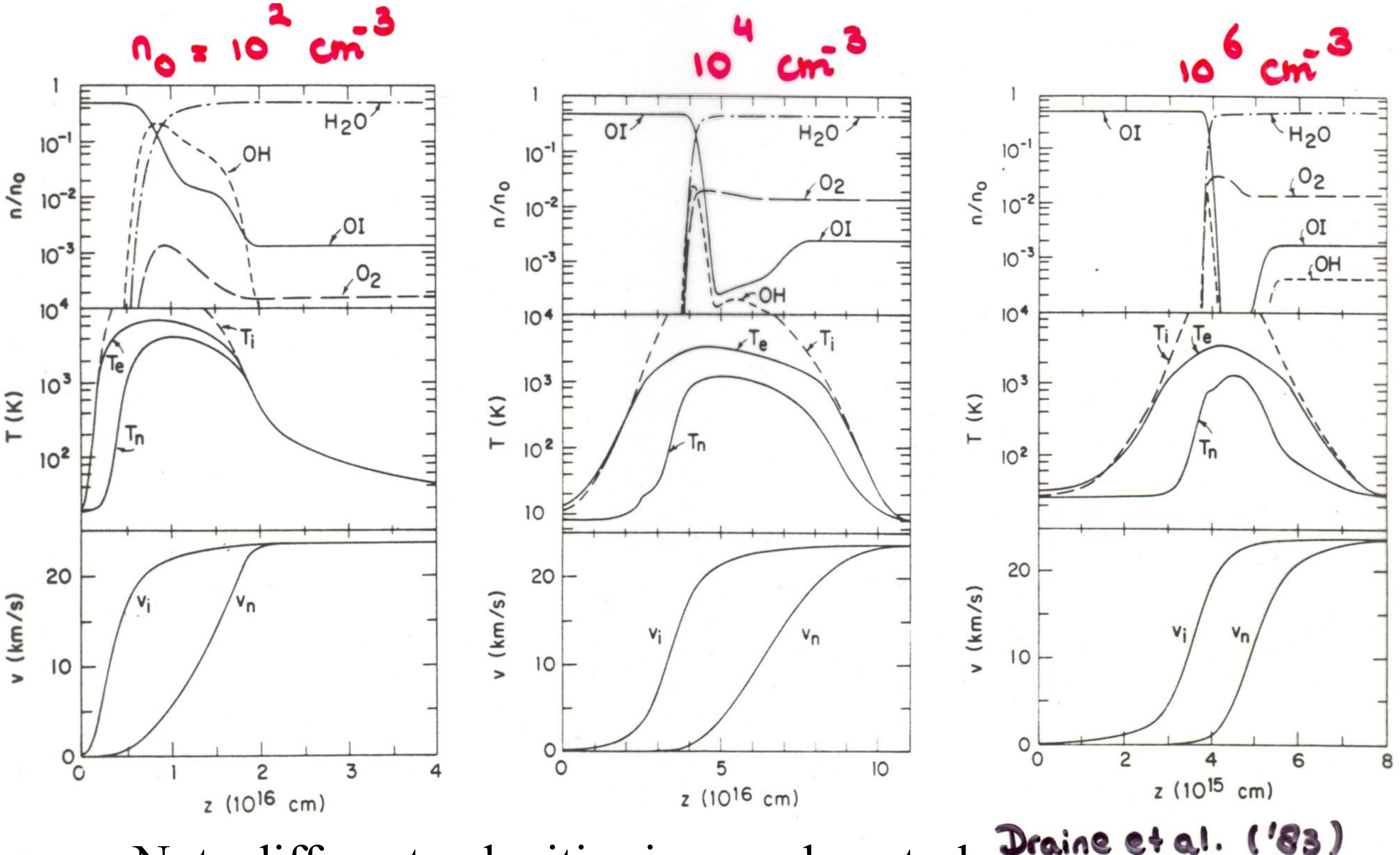


Lee et al. 2017, ALMA

5.4 Chemistry in non-dissociative shocks

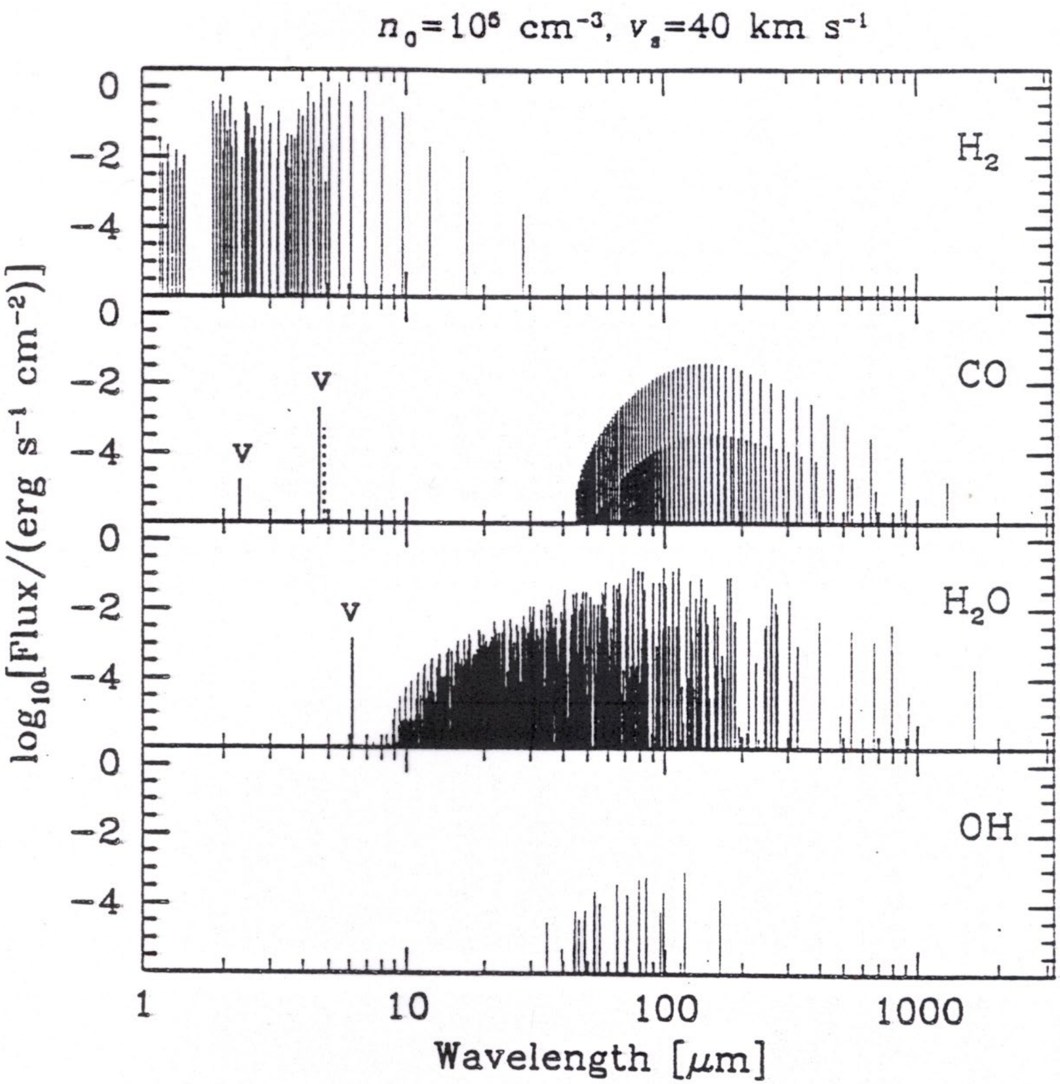
- Molecules survive shocks. Typical temperatures $T \approx 1000$-3000 K
  - $O + H_2 \rightarrow OH + H$
  - $OH + H_2 \rightarrow H_2O + H$
  - $C^+ + H_2 \rightarrow CH^+ + H$

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



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

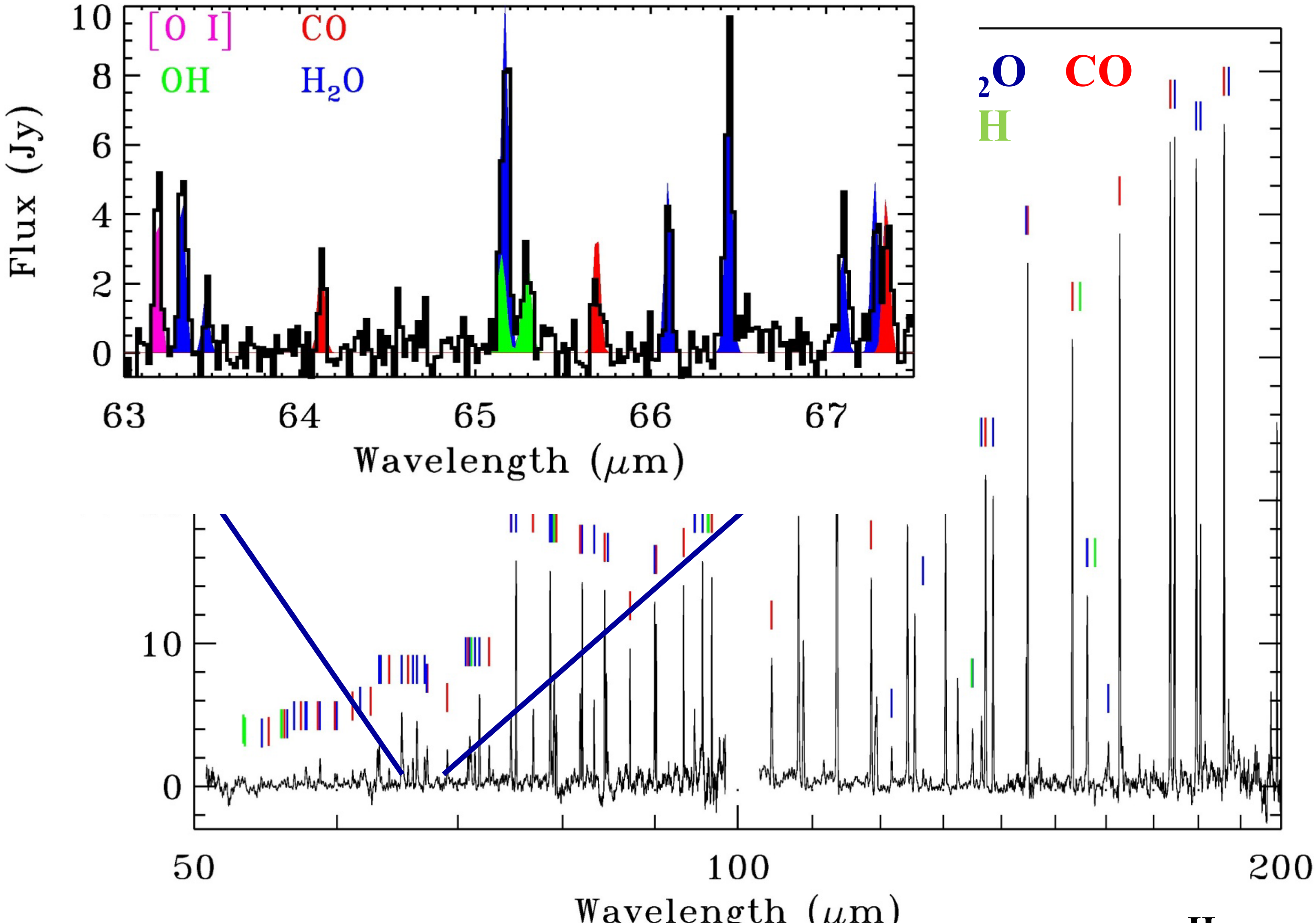
C-shock emission



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

Kaufman & Neufeld 1996

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

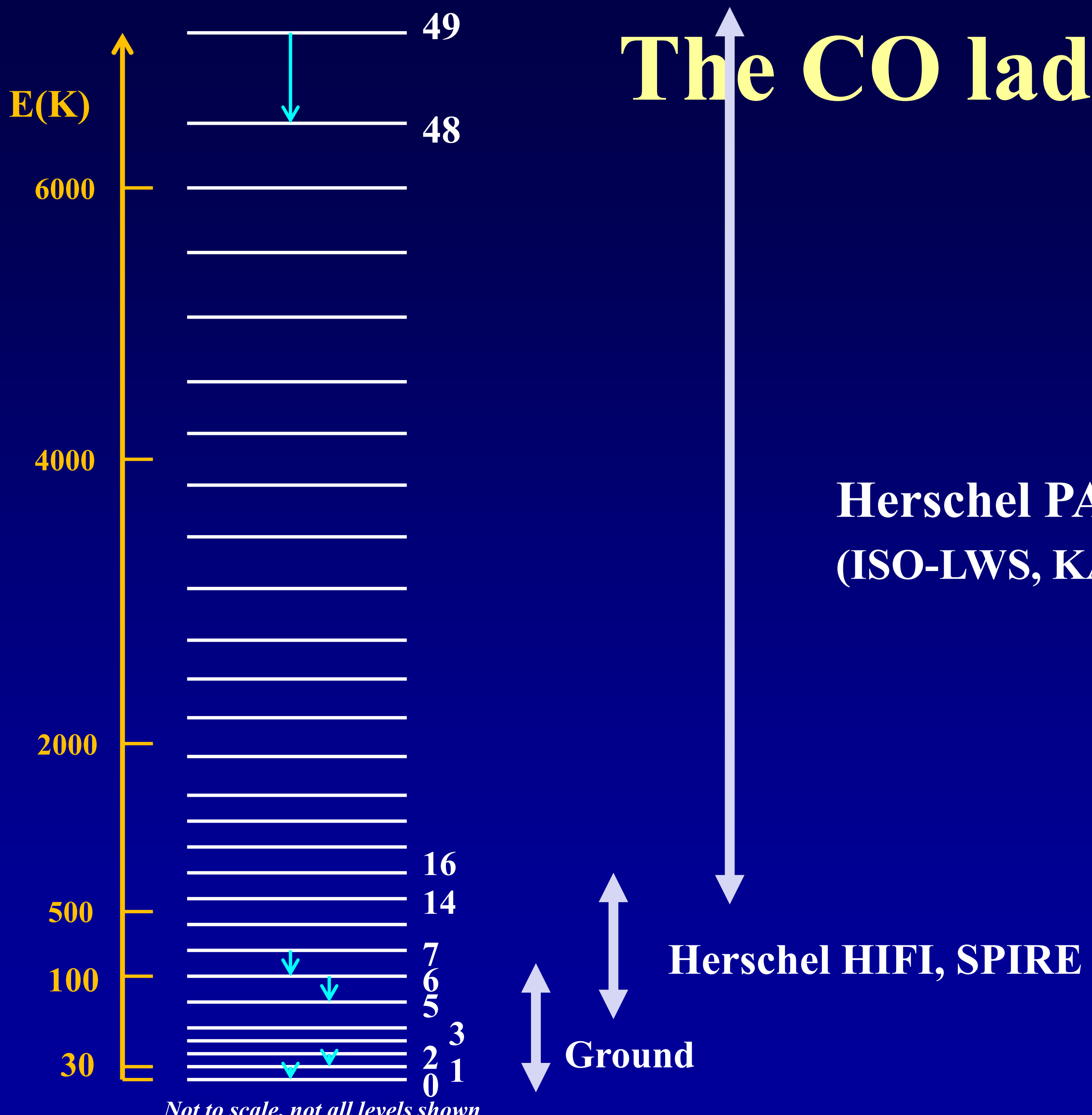


Low-mass protostar

NGC1333 IRAS4B (cont. subtr.)

Herczeg et al. 2012

The CO ladder



General trends models

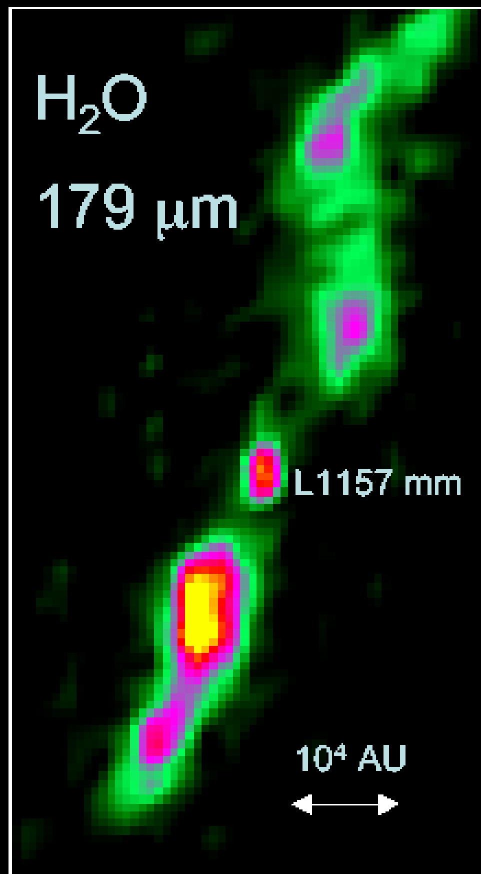
- Oxygen
  - O, OH, **H_2O** enhanced
- Carbon
  - H_2CO? (from $CH_3 + O \rightarrow H_2CO + H$)
- Sulfur
  - H_2S
  - SO, SO_2
- Silicon
  - SiO
- Nitrogen
  - NH_3, HCN?

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

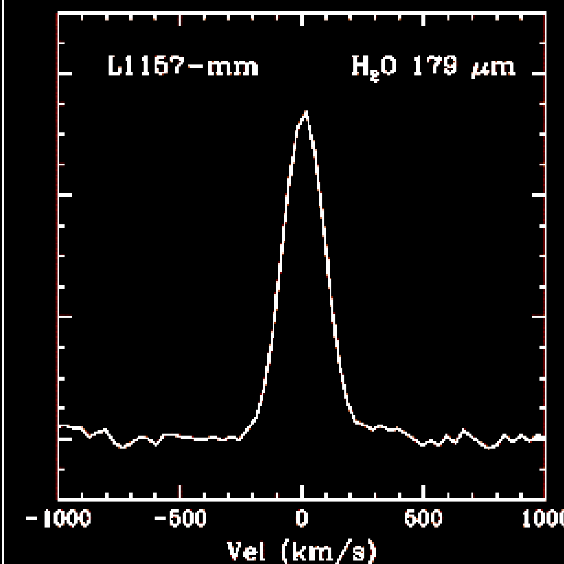
Herschel-PACS image of water in proto-stellar systems

3’



L1157-mm outflow

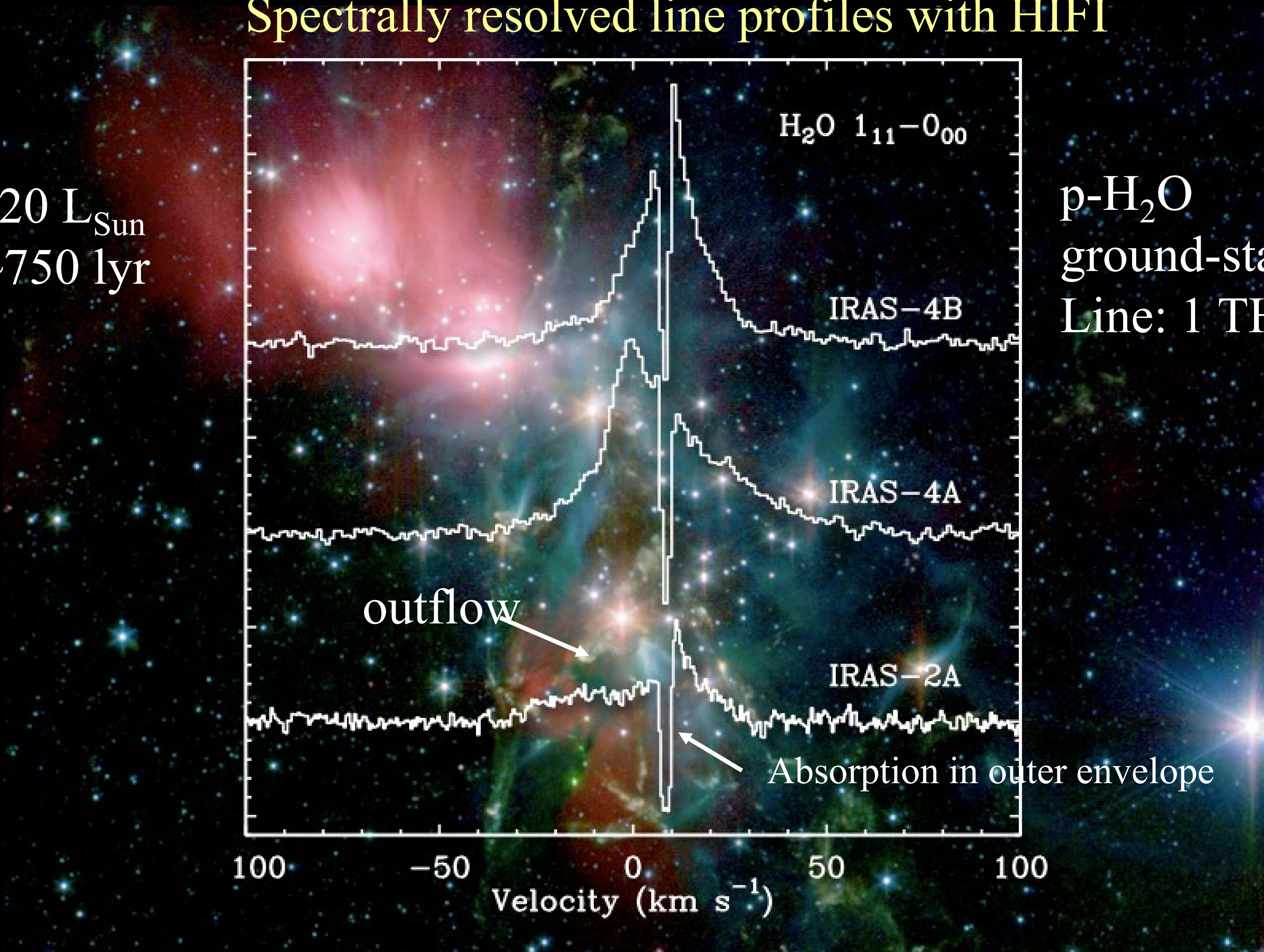
D = 440 pc, L_{bol} = 11 L_o



Nisini et al. 2010
Van Dishoeck et al. 2021

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

Low-mass protostars: NGC 1333



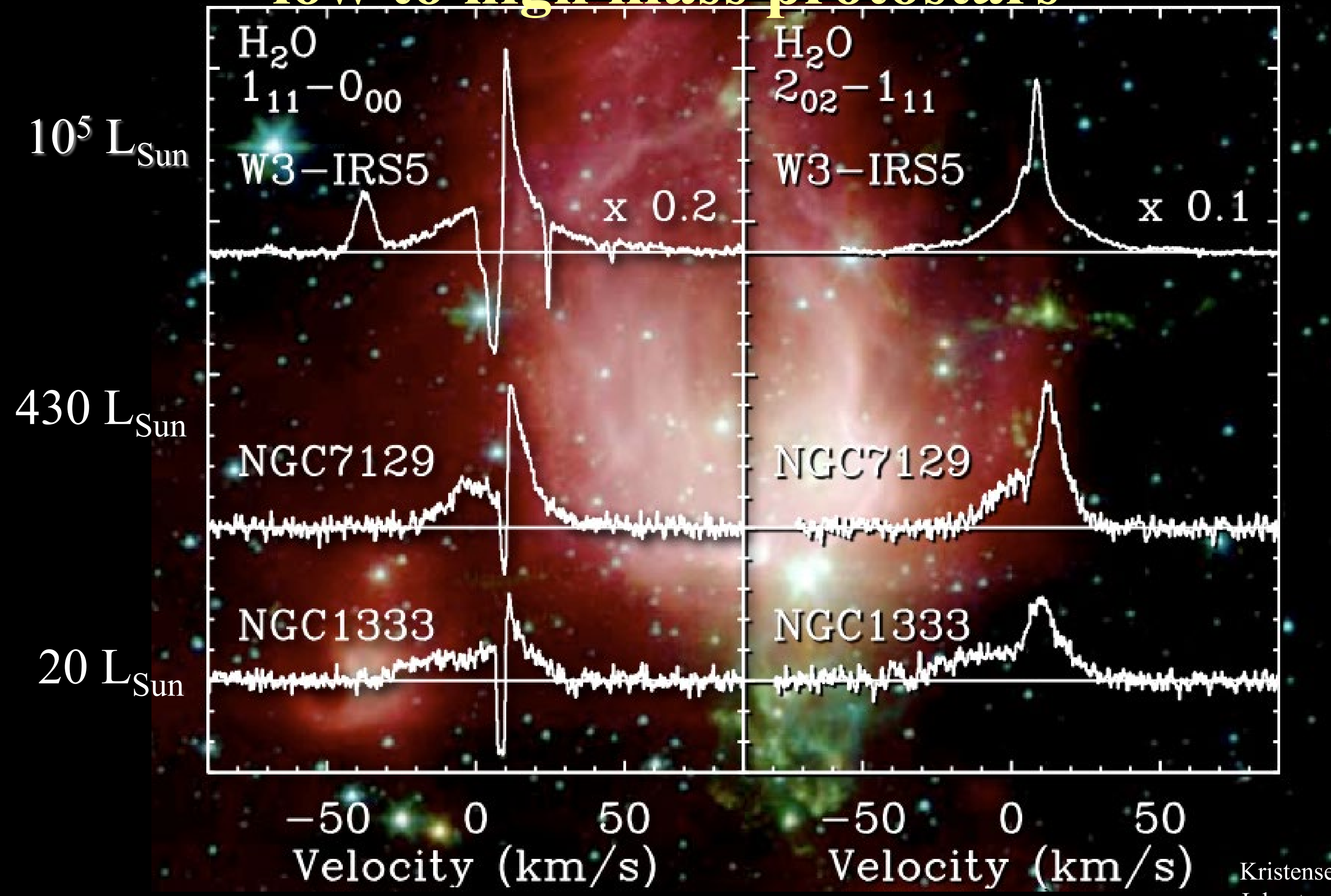
L~20 L_{Sun}
D~750 lyr

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

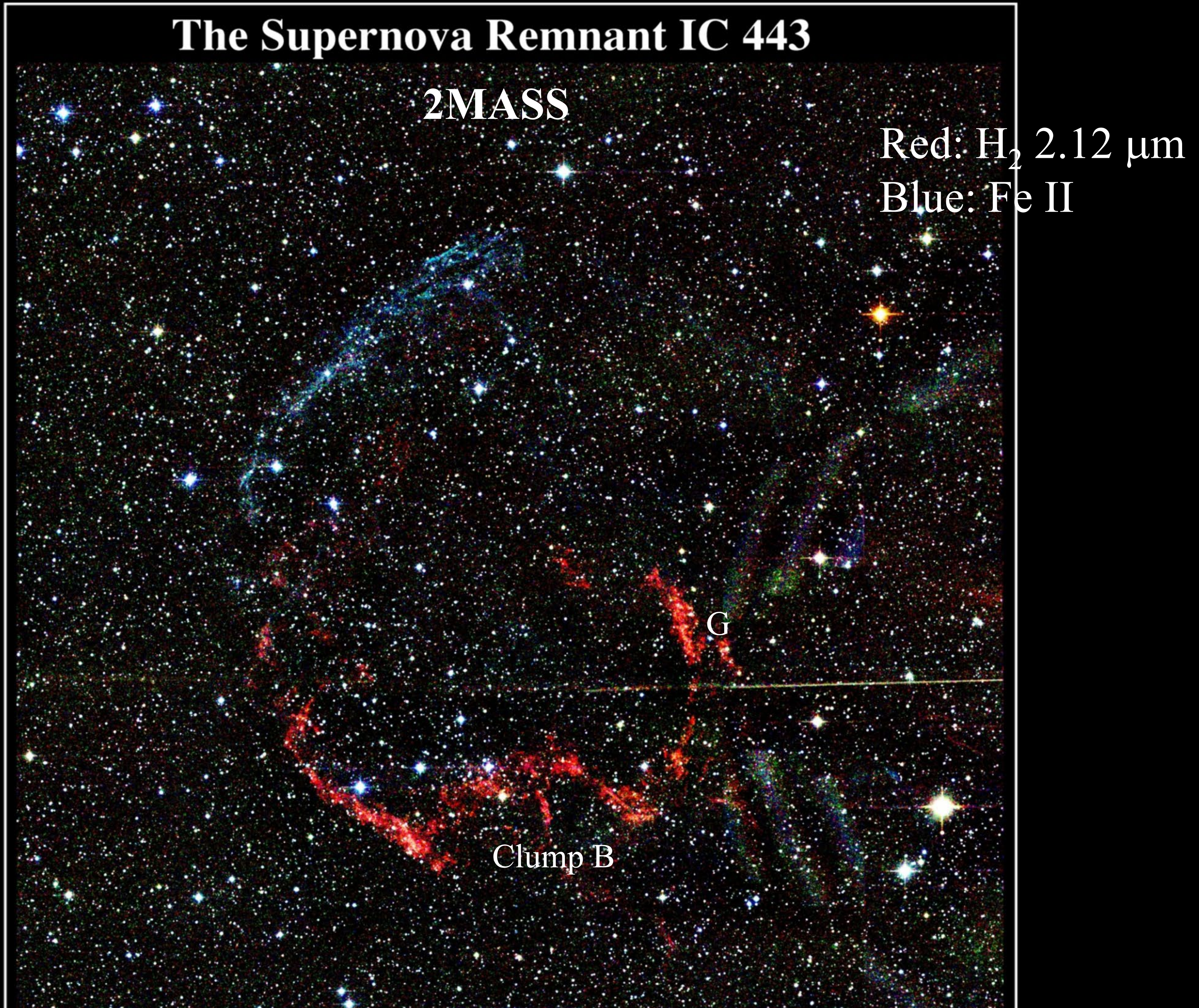
Question

- How to distinguish chemistry in shocks from that in dense PDRs?

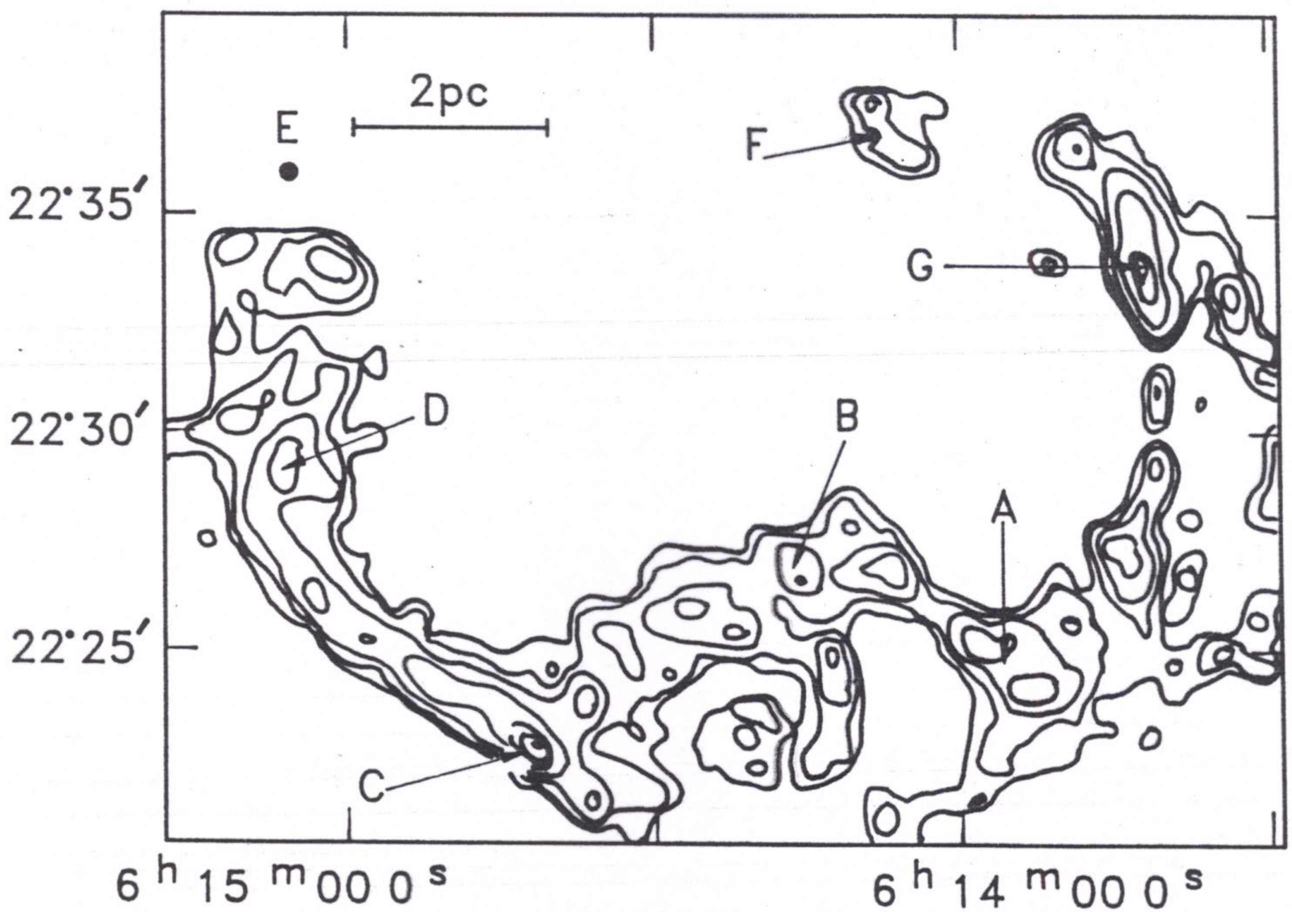
5.5 Comparison with observations

a. IC 443

- Best studied and nearest (1500 pc) example of interaction supernova remnant with molecular cloud
- Observations at optical, infrared, radio, X-ray $\Rightarrow$ 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

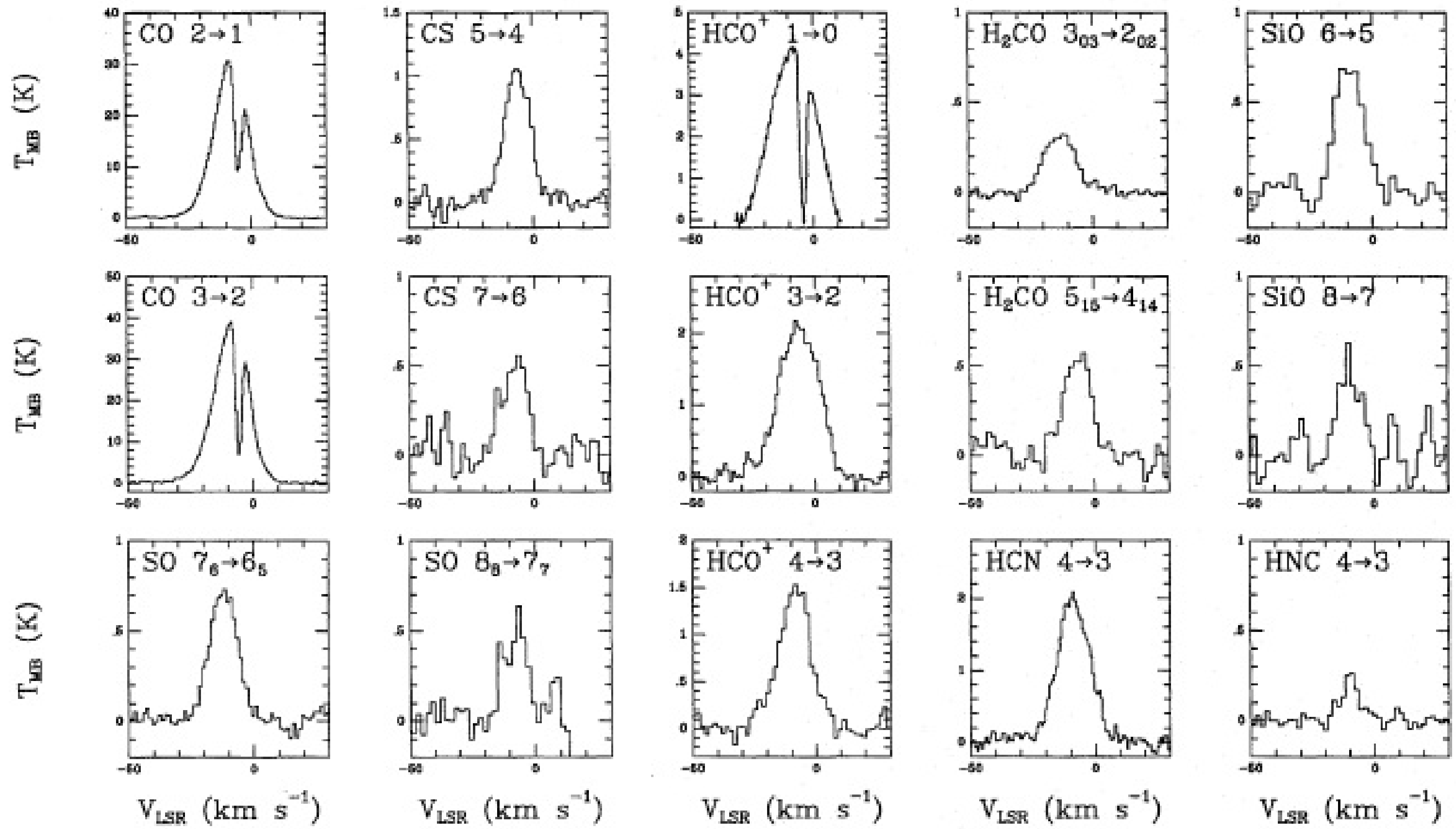

The Supernova Remnant IC 443
2MASS
Red: H2 2.12 μm
Blue: Fe II
G
Clump B

Shocked H_2 emission



Burton 1987

IC 443 clump G spectra



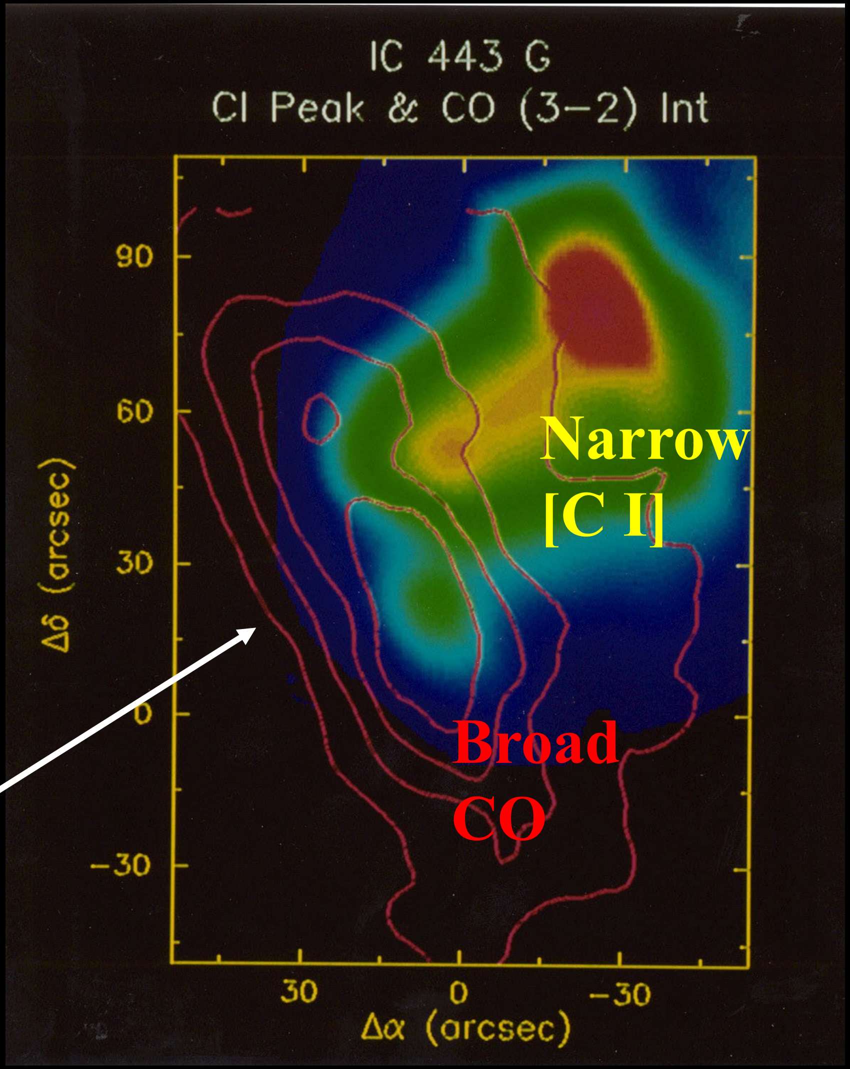
vD et al.
1993

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



Supernova
Expansion
Direction

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

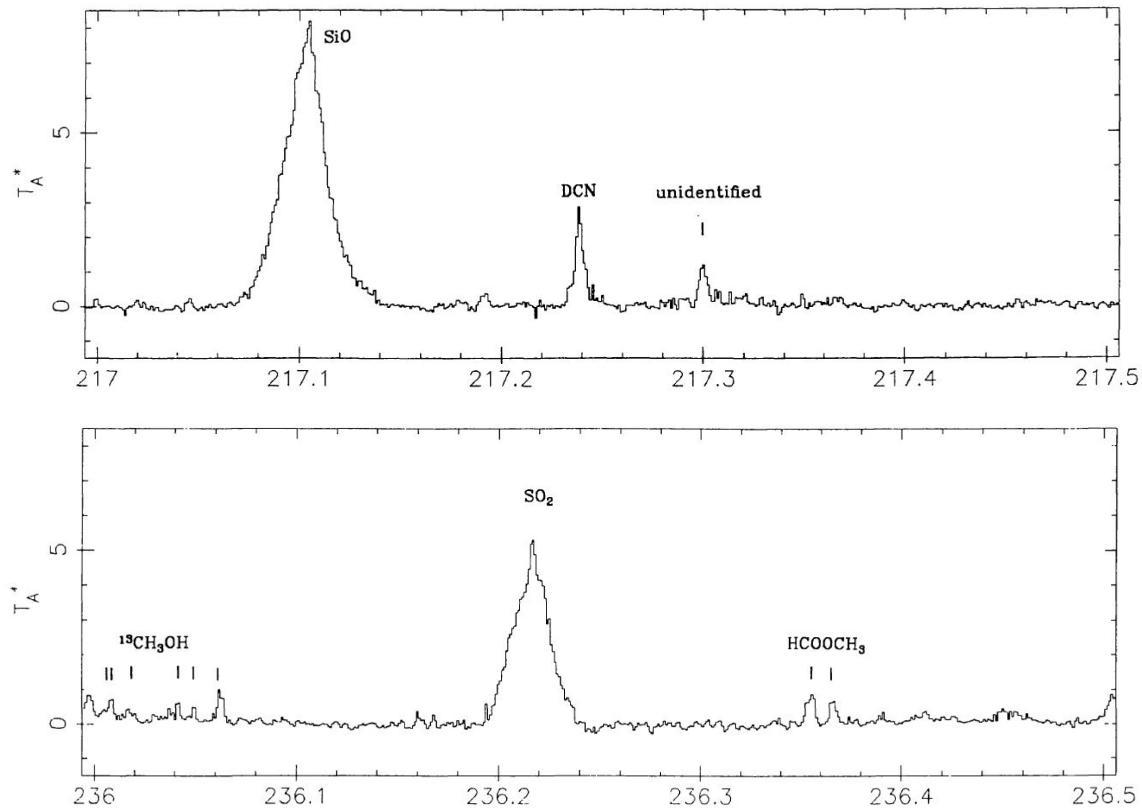
Keene et al. 1994

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 ($\Rightarrow$ back reactions important) and/or radiation field from shock
- Evidence for radiative precursor seen in strong [C I] emission <u>upstream</u> from shock

b. Orion/KL shock

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)

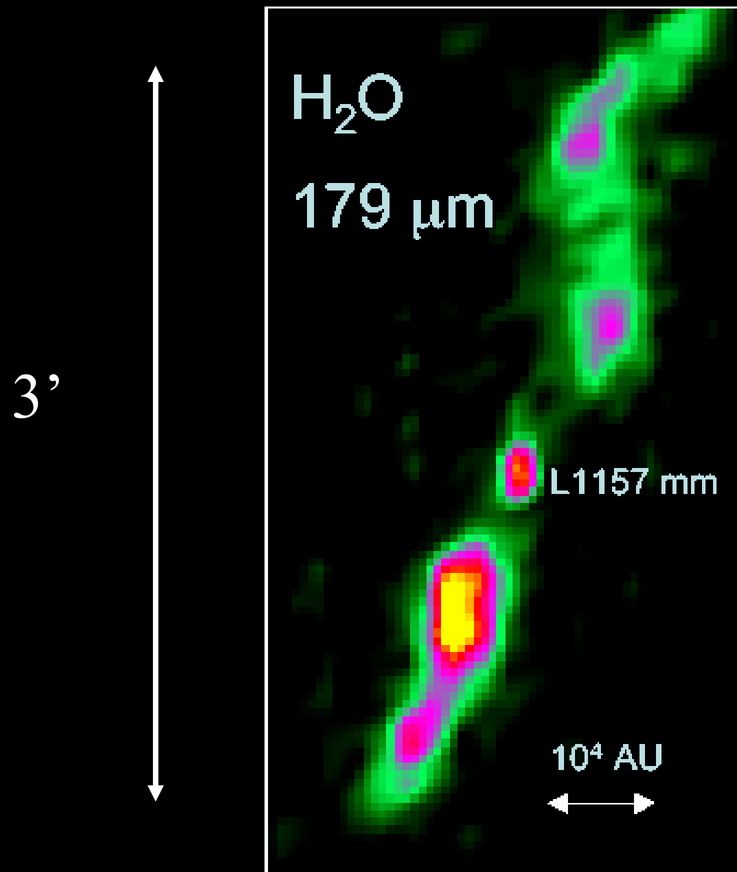
- Orion pre-shock density (~10^5 cm^{-3}) much higher than in IC 443 (~10^3 cm^{-3})
- Prominent water emission seen (Melnick et al. 2010)

c. L 1157

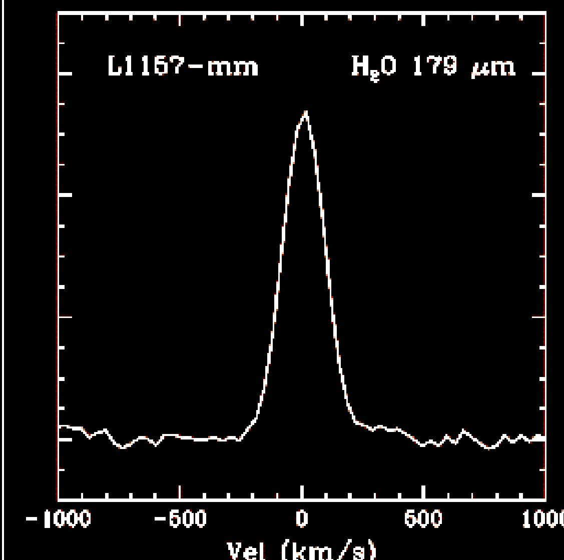
- Highly collimated outflow driven by Class 0 deeply embedded protostar, ~11 $L_{\odot}$, d=440 pc
- Shock vs. quiescent gas revealed by profiles
  - **Quiescent gas**: $C^{18}O$, N_2H^+, $H^{13}CO^+$, DCO^+
  - **Shocked gas**: SiO, CH_3OH, H_2O, CS, H_2CO, …
    - Recently: SO^+, HCS^+, $HOCO^+$, phosphor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

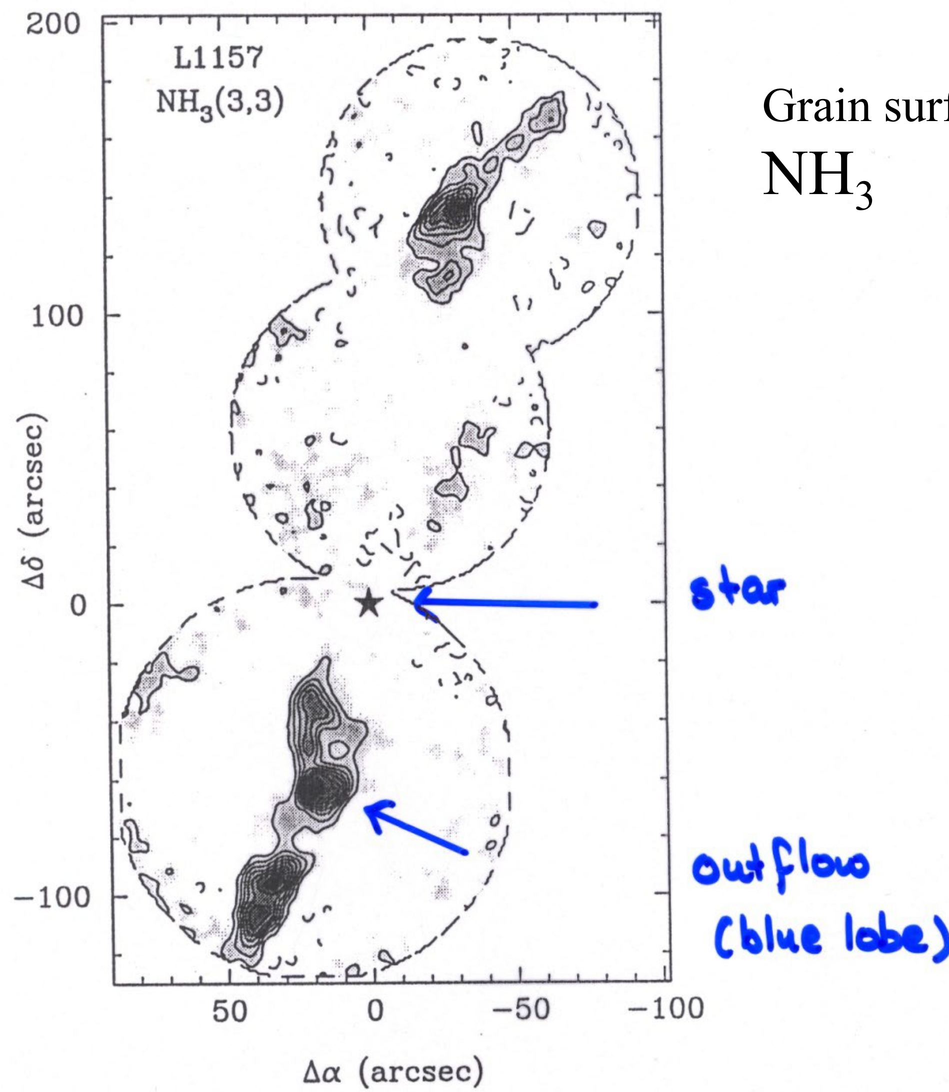


Nisini et al. 2010

H_2O abundance lower than expected (high OH/H_2O ratio) →
New class of UV irradiated shocks

Karska et al. 2018

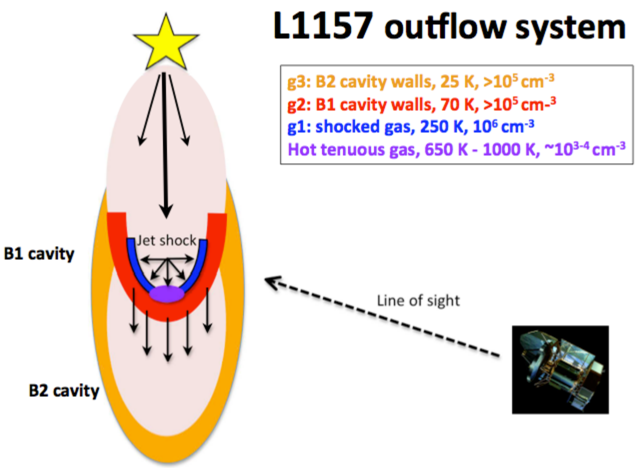
L 1157 shock



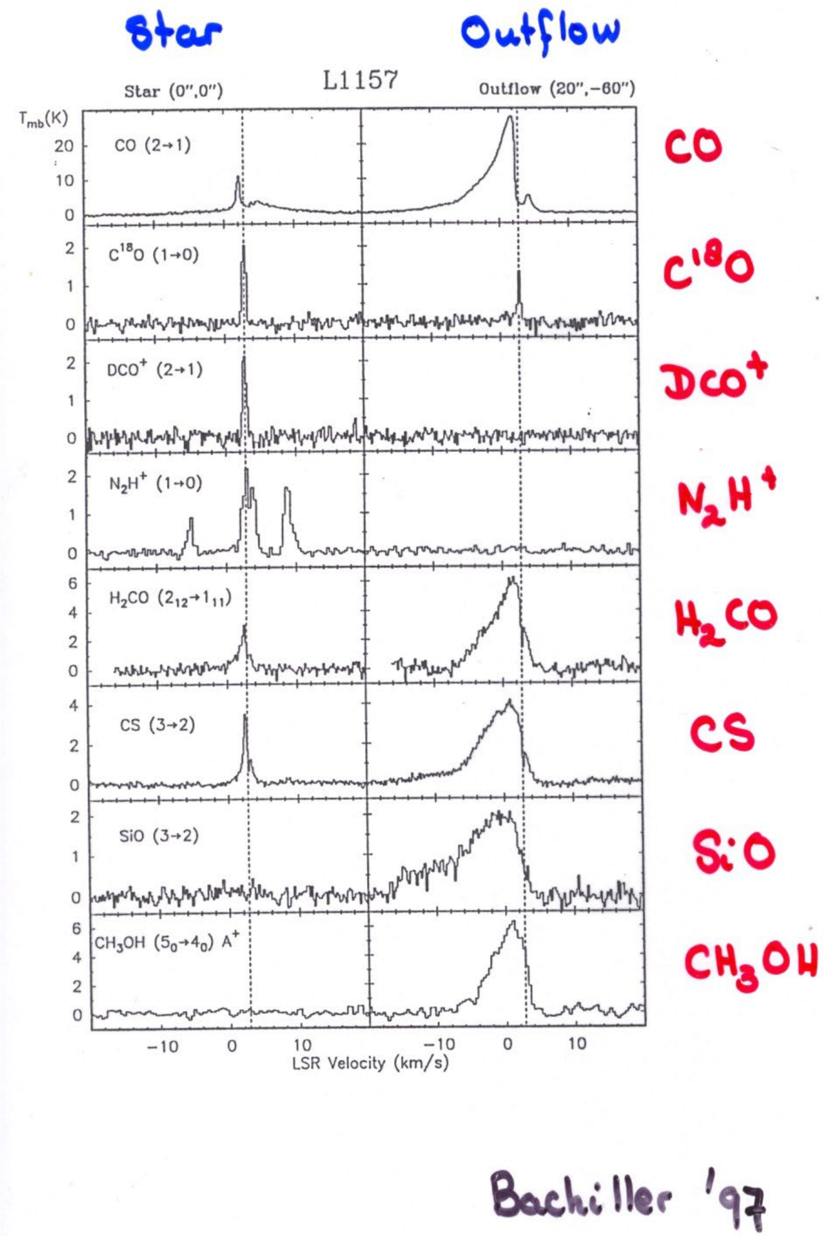
Grain surface product:
NH_3

Bachiller 1997

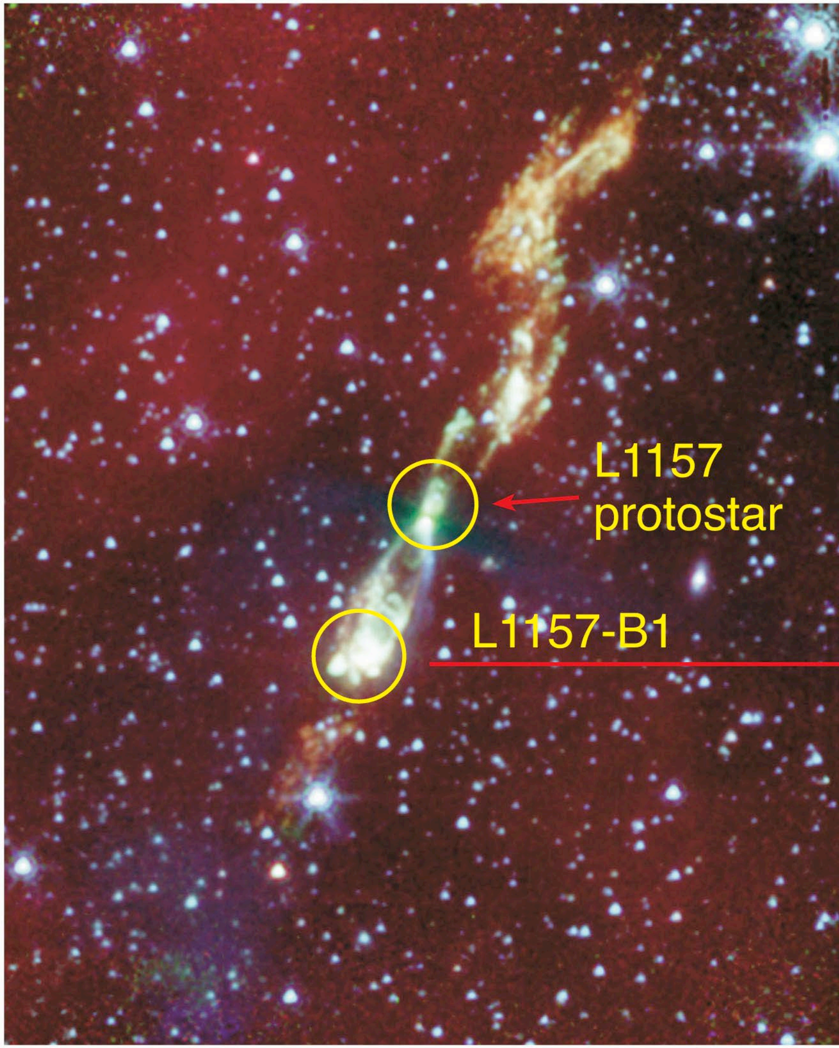
L 1157 line profiles

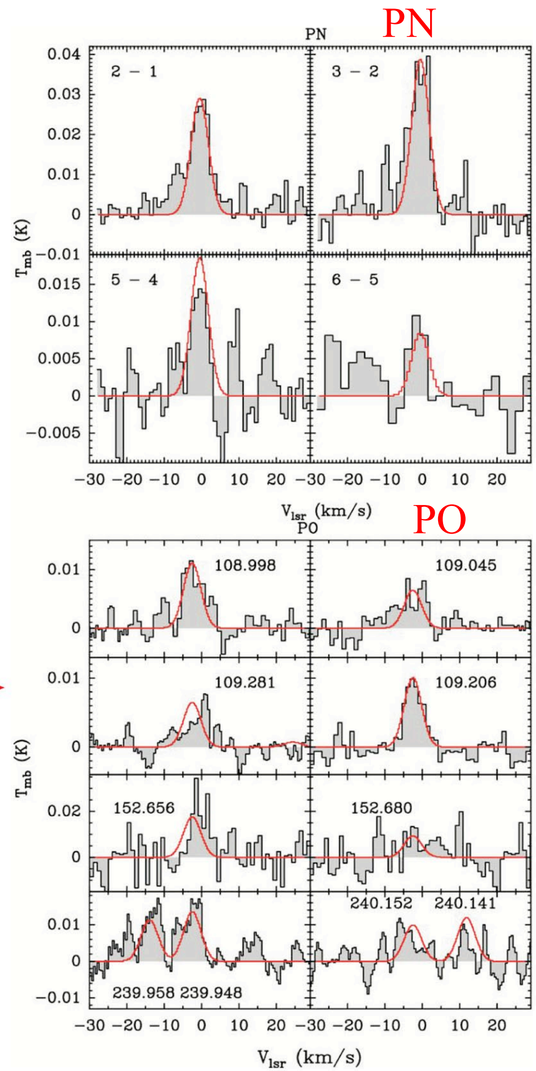


Busquet, Benedettini, LeFloch et al.
2012-2014



Rich chemistry in L1157 B1





- Complex organics, phosphorus molecules, …

Lefloch et al. 2017 + others

5.6 Summary

- Write your summary here