Atoms, Molecules, and Radiation, in the Interstellar Medium:

Observations, Theory & Databases

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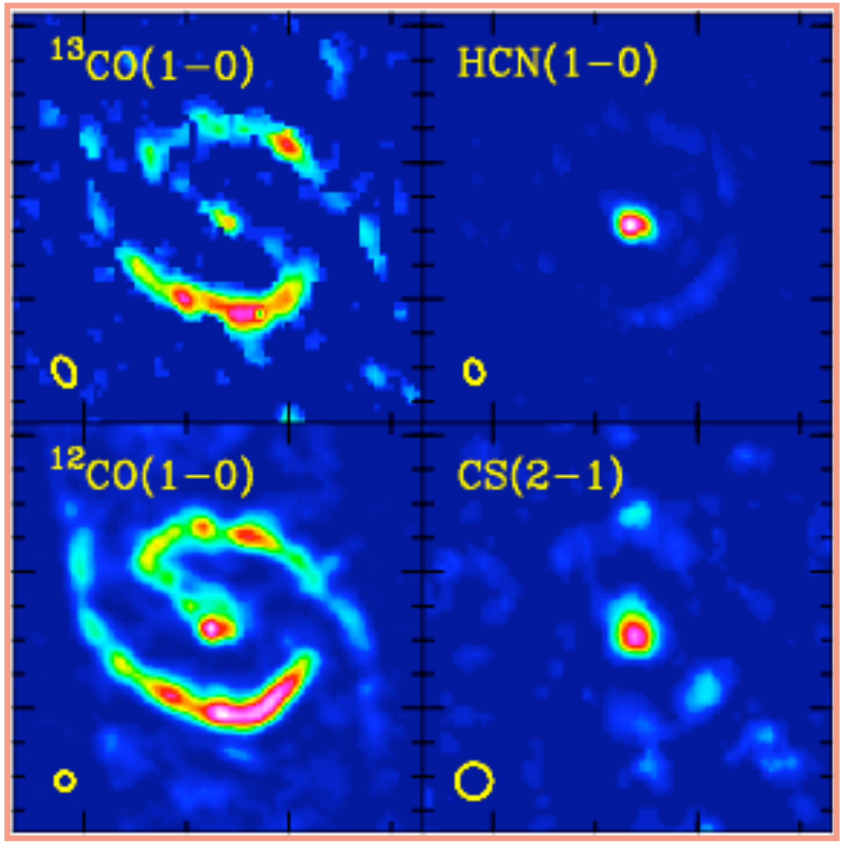
Molecules in the Seyfert Galaxy NGC 1068

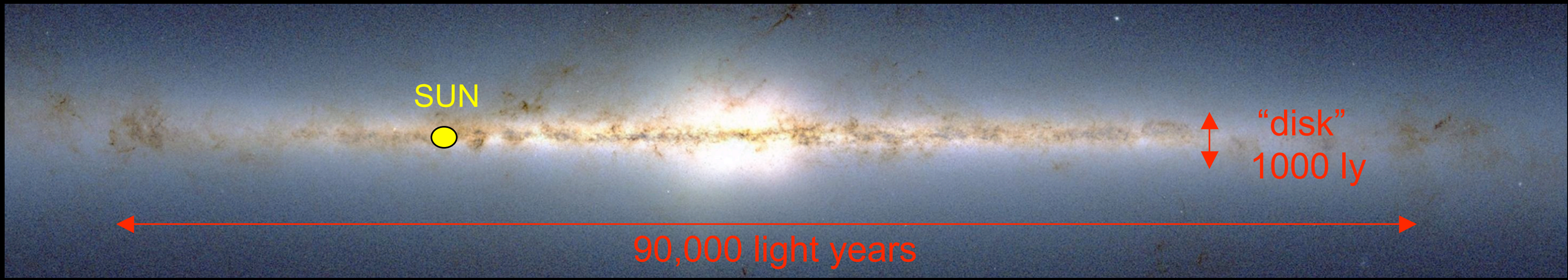


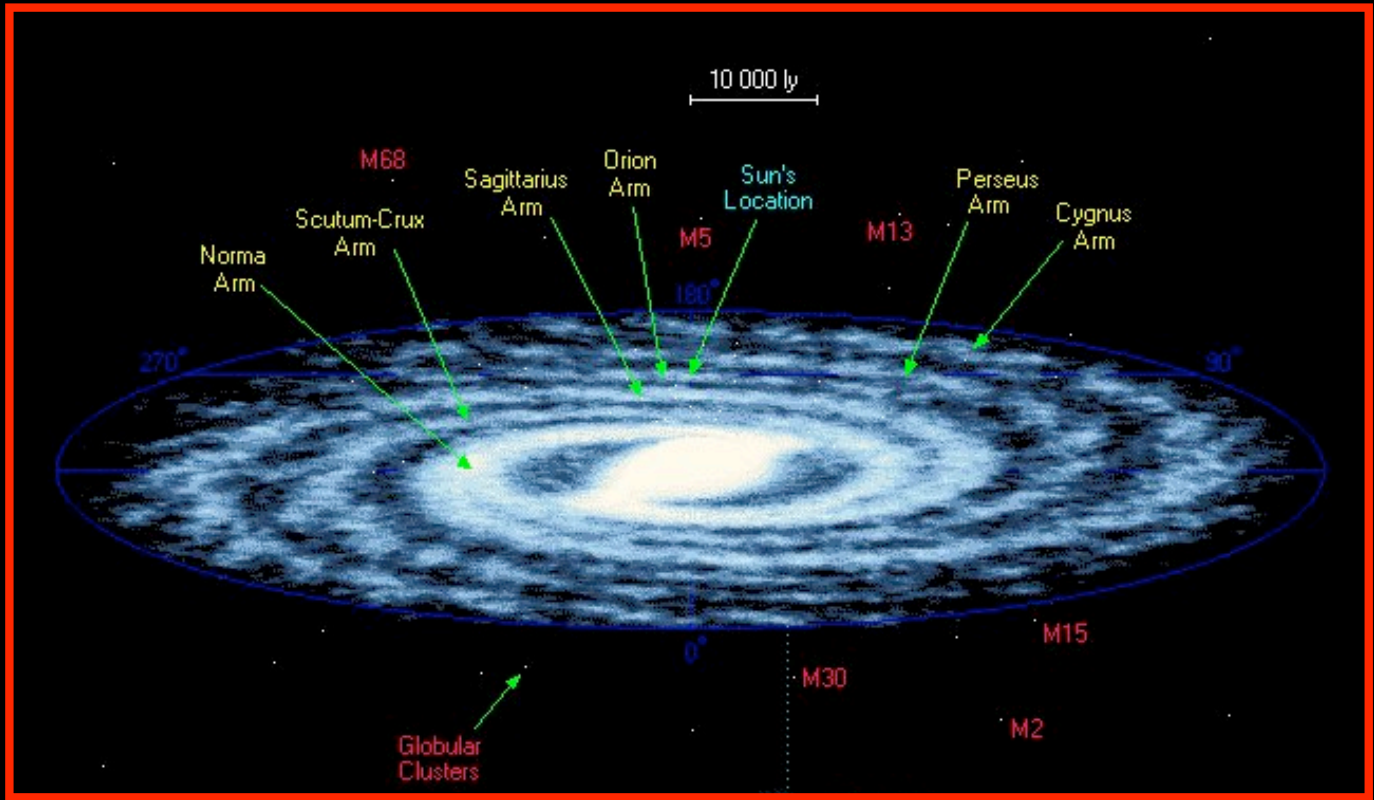
ICAMDATA 05
19 October 2006

l'Observatoire de Paris

Milky Way Galaxy: 100 Billion Stars.

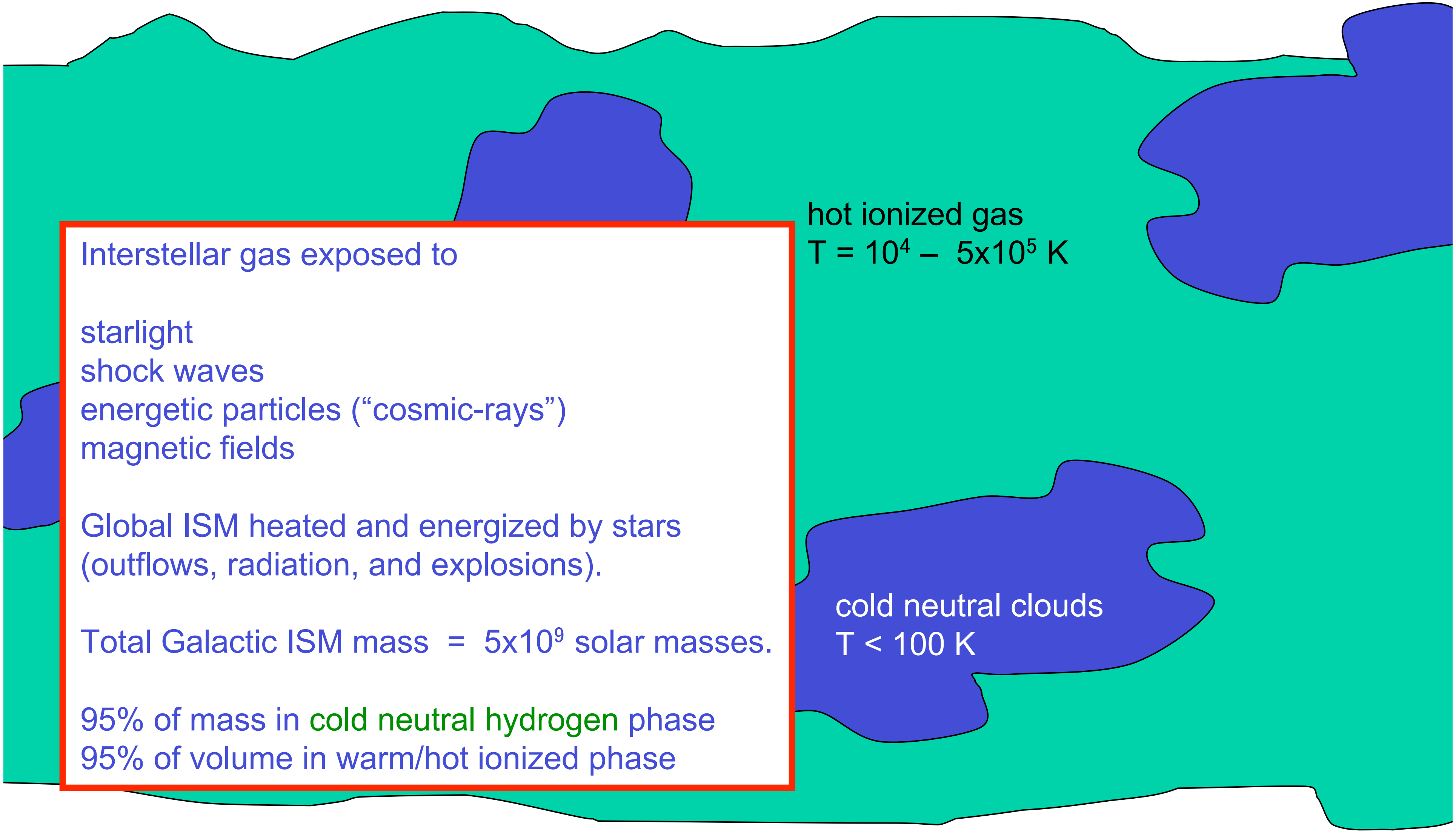
Skrutskie et al. 2001
(2MASS survey)





The Interstellar Medium (ISM):

⟨density⟩ = 1 cm^{-3}
but very inhomogeneous



Interstellar gas exposed to

starlight
shock waves
energetic particles (“cosmic-rays”)
magnetic fields

Global ISM heated and energized by stars (outflows, radiation, and explosions).

Total Galactic ISM mass = $5x10^9$ solar masses.

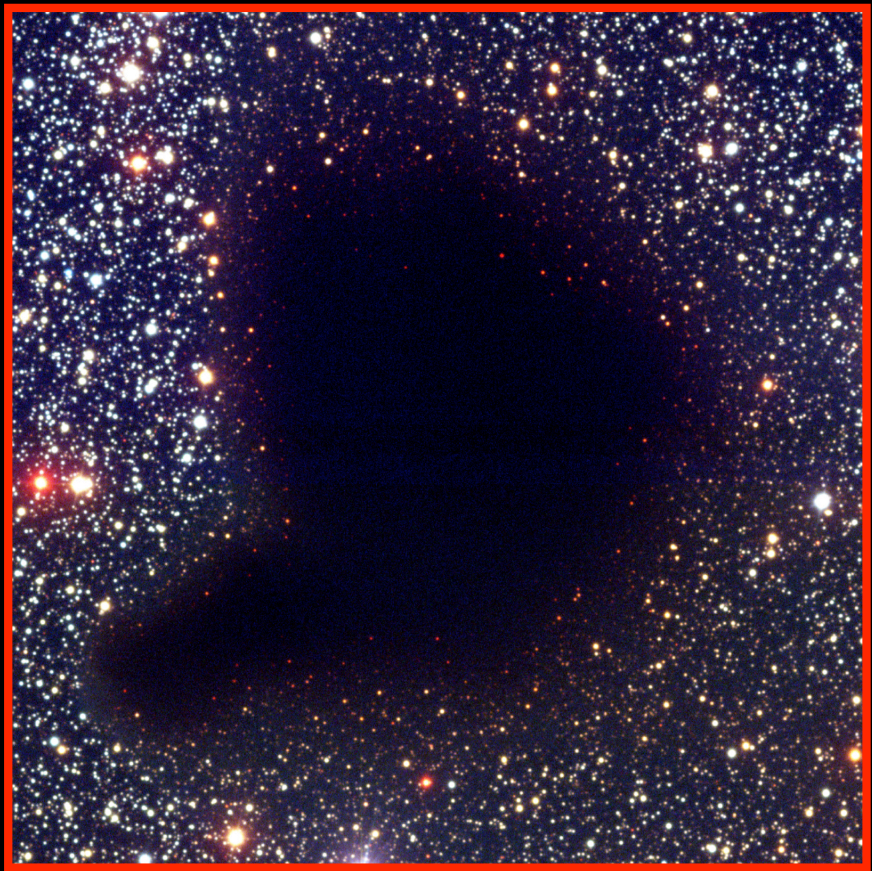
95% of mass in cold neutral hydrogen phase
95% of volume in warm/hot ionized phase

Composition by number (relative to hydrogen) of the interstellar gas:

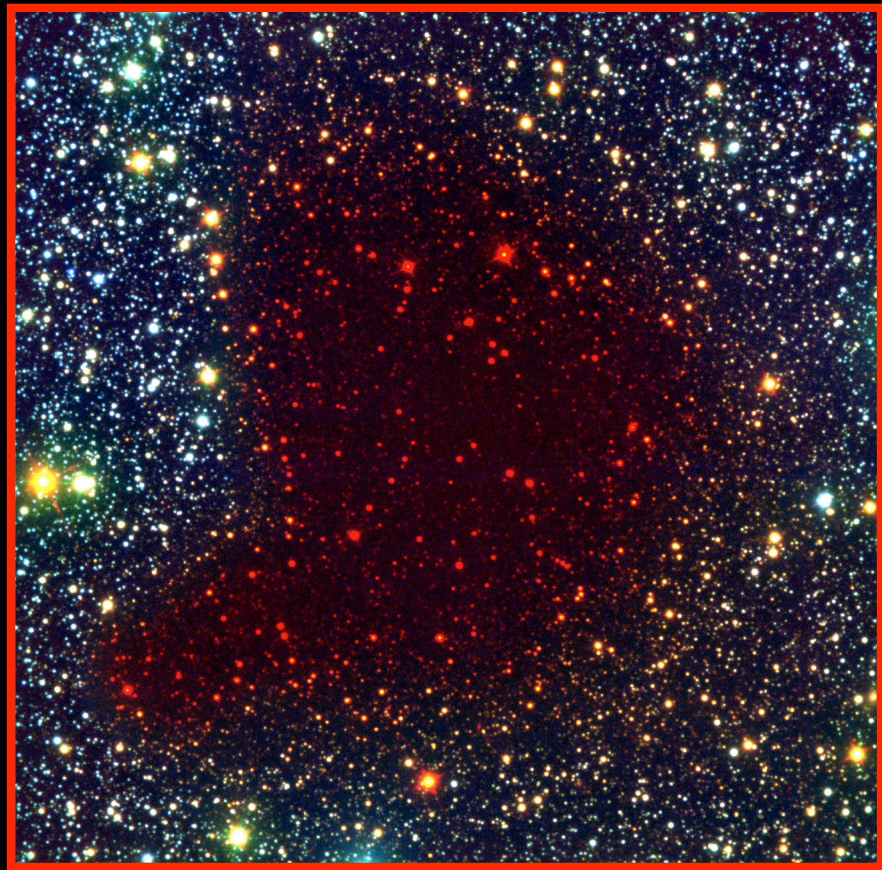
H	1.0	formed in Big-Bang
He	0.1	
C N O	10^{-3}	formed much later, in stars and stellar explosions
Si Mg Fe S ...	10^{-4}	
Varying fractions of the heavy elements are tied up in interstellar "dust grains" (< 0.1 μm).	10^{-12}	

Molecular Clouds:

"Bok Globule" Barnard 68 (optical image)



(infrared image)



Alves, Lada & Lada 2001 Nature 409 159

"reddening" of starlight due to interstellar dust particles.

"Mein Gott! da ist ein Loch in Himmel!"
-Sir William Herschel (1734-1822)

Basic Fact: Stars Form in Molecular Clouds: (ongoing in the Galaxy)

A star is born in Globule GDC1 (Reipurth 2001 Nature 409 140)

Bipolar supersonic outflow.

Gas heating by shock waves and radiation.

Single-Dish Millimeter-Wave Telescopes:

IRAM 30-meter telescope (Spain)

Nobeyama 45-meter telescope (Japan)

Millimeter-Wave Interferometers:

Molecules detected in the Galactic interstellar medium (as of October 2006):

2	3	4	5	6	8
H_2	H_3^+	H_3O^+	CH_4	CH_3OH	$HCOOCH_3$
CH	NH_2	NH_3	NH_2CH	CH_3CN	CH_3COOH
CH^+	CH_2	CH_3	CH_2NH	CH_3NC	CH_2OHCHO
NH	H_2O	C_2H_2	C_3H_2	NH_2CHO	CH_2CCHCN
OH	C_2H	H_2CO	H_2CCC	CH_3SH	CH_3C_3N
HF	HCN	$HCNH^+$	CH_2CN	HC_3NH^+	C_6H_2
C_2	HNC	CH_2N	CH_2CO	HCC_2HO	C_7H
CN	HCO	C_3H	$HCOOH$	C_5H	**9**
CO^+	HCO^+	$HNCO$	C_4H	C_4H_2	CH_3CH_2OH
CO	HOC^+	HC_2N	HC_3N	C_5N	CH_3CH_2CN
NO	N_2H^+	$HOCO^+$	$HNCCC$	**7**	CH_3C_4H
HCl	HNO	H_2CS	$HCCNC$	CH_3NH_2	$(CH_3)_2O$
SiN	H_2S	C_3N	H_2COH^+	CH_3C_2H	$CH_3C(O)NH_2$
SiO	C_2O	C_3O		CH_3CHO	HC_7N
CS	C_2S	$HCNS$		CH_2CHCN	C_8H
PN	N_2O	C_3S		$(CH_3)_2O$	**10**
NS	HCS^+			C_6H	$(CH_3)_2CO$
SO^+	OCS			HC_5N	$(CH_2OH)_2$
SO	CO_2			C_2H_4O	CH_3CH_2CHO
SiS	SO_2			CH_2CHOH	CH_3C_5N
CF^+	C_3				**11**
					HC_9N
					CH_3C_6H
					12
					C_6H_6
					13
					$HC_{11}N$

Molecules detected down to abundances of

10^{-11} relative to H_2

(H_2 is the dominant component).

Many isotopes also detected.

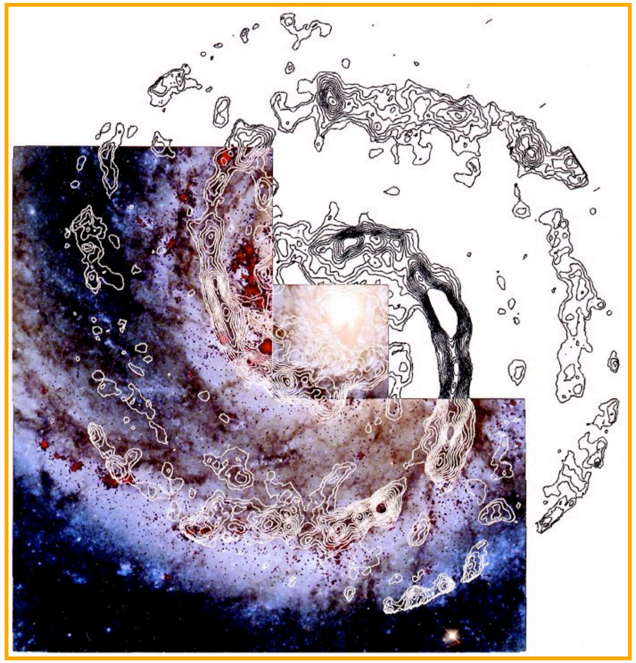
Extragalactic Molecules (as of October 2006):

2	3	4	5	6	7	8	9	10	11	12	13
H_2	H_3^+	NH_3	CH_2NH	CH_3OH	CH_3C_2H						
CH	H_2O	H_2CO	C_3H_2	CH_3CN							
CH^+	C_2H	C_3H	CH_2CN								
OH	HCN	HNCO	HC_3N								
CN	HNC	$HOCO^+$									
CO^+	HCO										
CO	HCO^+										
NO	HOC^+										
SiO	N_2H^+										
CS	H_2S										
SO	OCS										
	SO_2										

"Whirlpool" Galaxy (M51)
distance = 3.7×10^6 light-years,

as observed in the 2.6 mm rotational emission line of carbon monoxide (CO).

Rand & Kulkarni 1990 ApJ 349 L43
Scoville et al. 2001 AJ 122 3017



5×10^4 light years

Making sense of it all…

Atoms and molecules serve as “diagnostic probes” of the physical and evolutionary states of the star-forming clouds:

- Temperature
- Density
- Ionization
- Elemental Abundances
- Magnetic Field
- Dynamics
- Turbulence

Atoms and molecules also regulate the physical evolution via the coupled processes of

- Heating
- Cooling
- Chemistry
- Dynamics

Quantitative analysis requires accurate atomic and molecular data for the “microscopic processes” as determined by either theory, or laboratory experiments:

- quantum structures, energy levels, oscillator strengths, and radiative transition rates

- cross section data for inelastic collisions with e, H^+, H, H_2 and He → collisional rate coefficients
  [e.g., Close-Coupling (CC), Coupled States (CS) or Infinite Order Sudden (IOS) methods.]
  → Radiative Transfer [e.g. Large Velocity Gradient (LVG); Static Escape Probability]

- photodissociation and photoionization cross sections → photodestruction rates

- rate coefficient data for chemical kinetics

Databases for Astrophysical Molecular Spectroscopy!

http://spec.jpl.nasa.gov Pickett et al.

Leiden Atomic and Molecular Database
http://www.strw.leidenuniv.nl/~moldata/
Schöier et al. 2005 AA 432 369

Cologne Database for Molecular Spectroscopy
http://www.cdms.de
Müller et al.

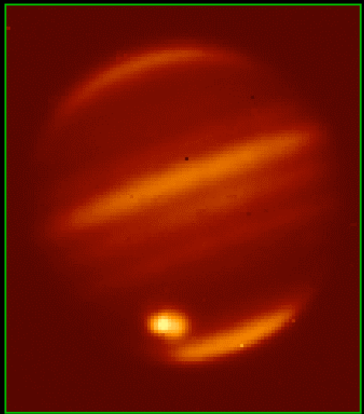
http://amdpo.obspm.fr/basecol
Dubernet et al.

http://cfa-www.harvard.edu/HITRAN
Rothman et al.

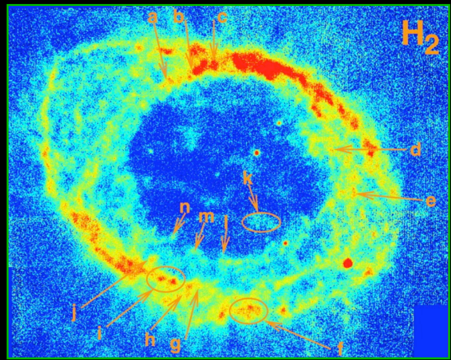
Atomic and Molecular Data
http://amrel.obspm.fr/molat/

As an example: molecular hydrogen (H_2), the most abundant molecule in the universe…

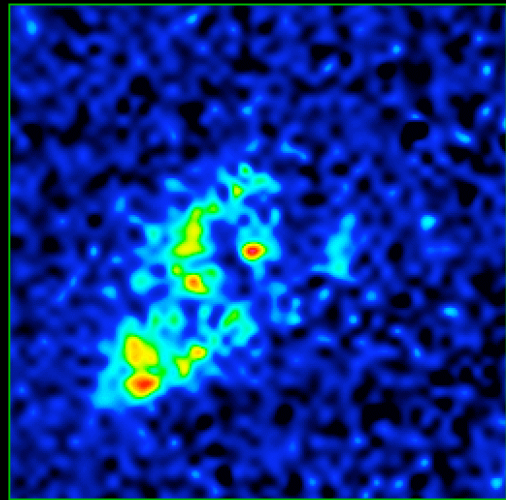
The planet Jupiter
www.as.utexas.edu/mcdonald

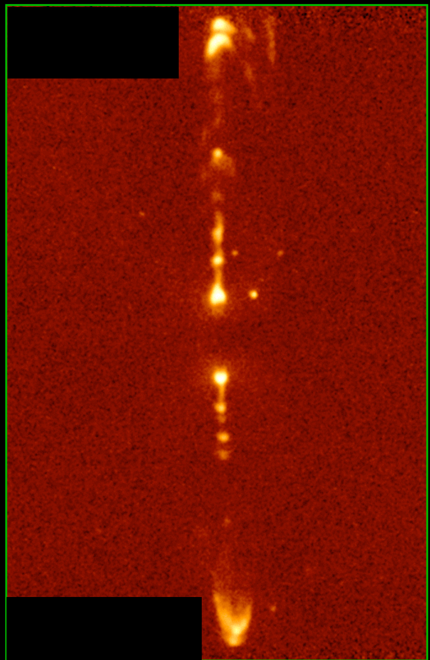


Ring Nebula:
Speck et al. 2003 PASP 115 170

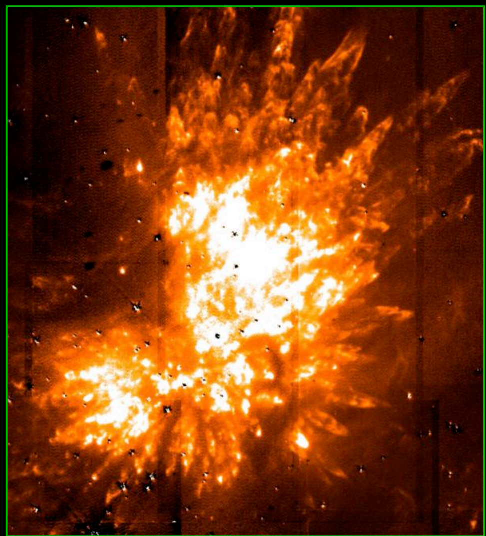


NGC 1808: A starburst galaxy.
Kotilainen et al. 1996 AA 313 771





HH224, a protostellar jet



Orion Kleinman-Low Nebula,
an embedded young stellar cluster
Subaru Telescope 1999

…as observed in the
H_2 2.12 μm 1–0 S(1)
vibrational emission line.

Starburst Galaxies:

Edwin Hubble
1889–1953

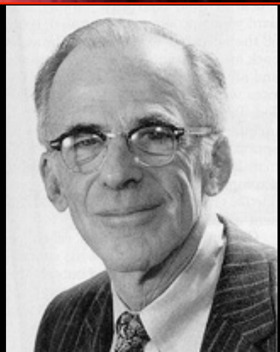
"The Antennae"
NGC 4038/4039 Colliding Galaxies

distance = 6.6 x 10^7 light years

Hubble Space Telescope (optical)
Whitmore & Schweitzer 1995

5,000 light years

Starburst Galaxies:



Lyman Spitzer, Jr.
1914–1997

"The Antennae"
NGC 4038/4039 Colliding Galaxies

distance = 6.6 x 10^7 light years

Spitzer Space Telescope (mid-infrared)
Wang et al. 2004 ApJS 154 193

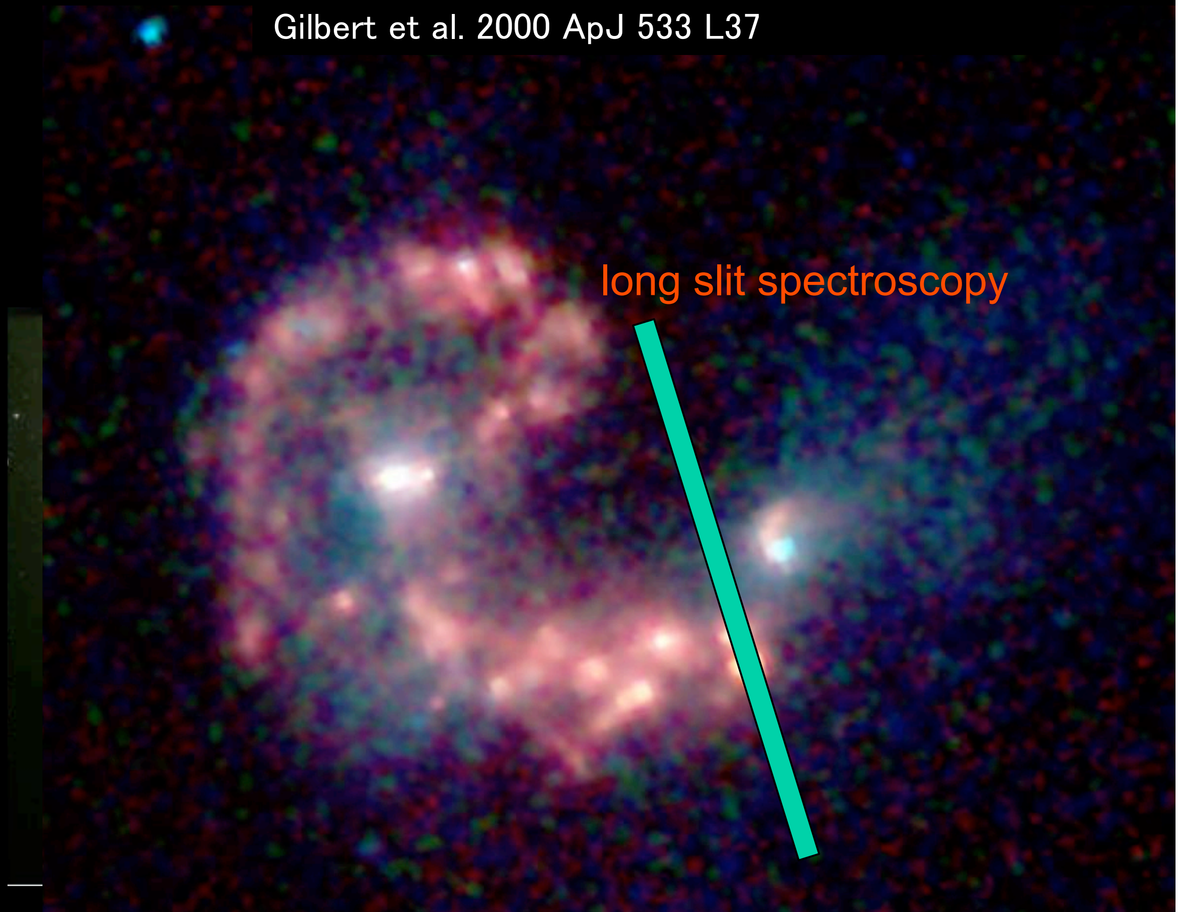
deeply embedded sites of star–formation revealed in the mid IR.

Starburst Galaxies:

"The Antennae"
NGC 4038/4039 Colliding Galaxies

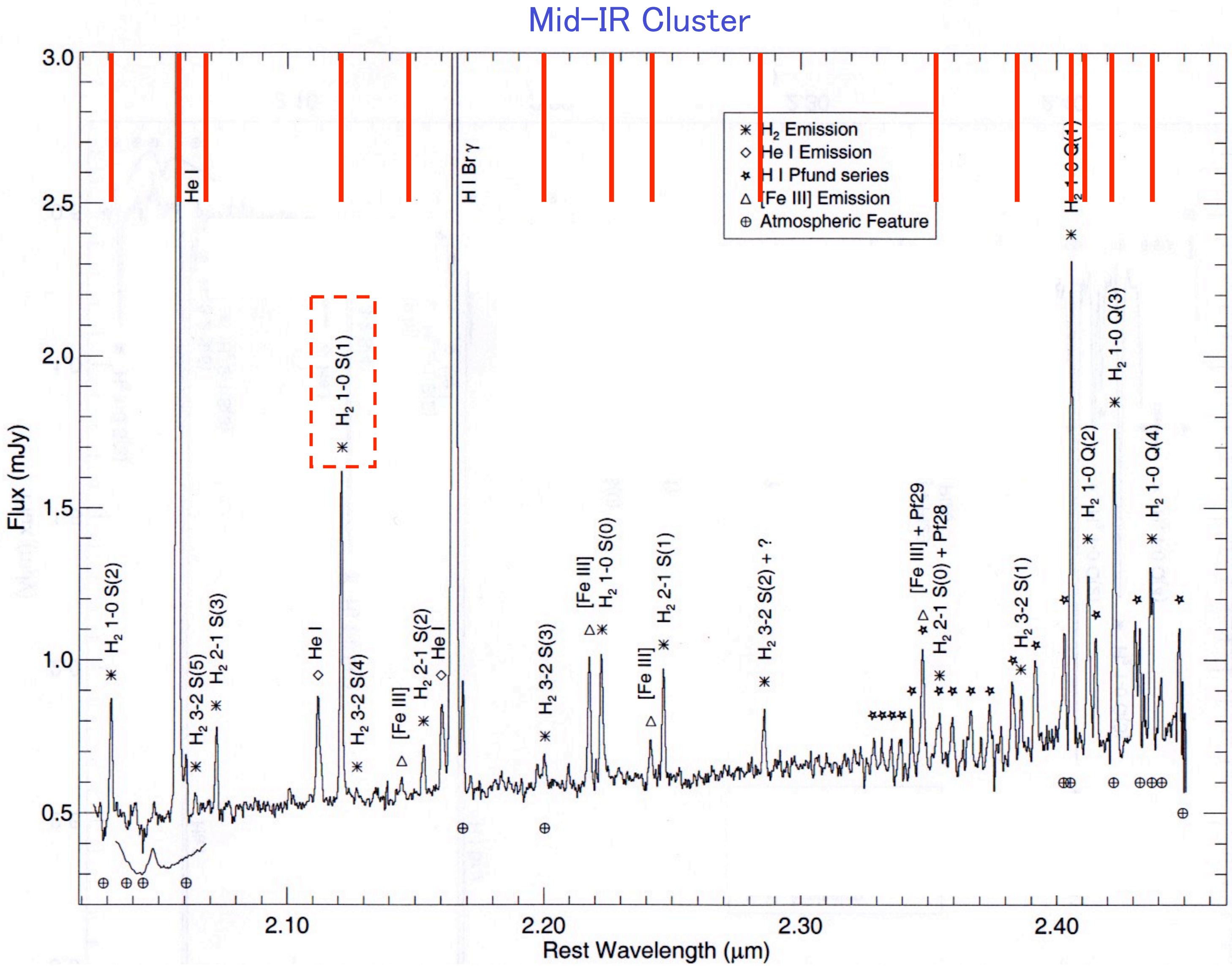
distance = 6.6 x 10^7 light years

Keck Observatory (near-infrared)
Gilbert et al. 2000 ApJ 533 L37

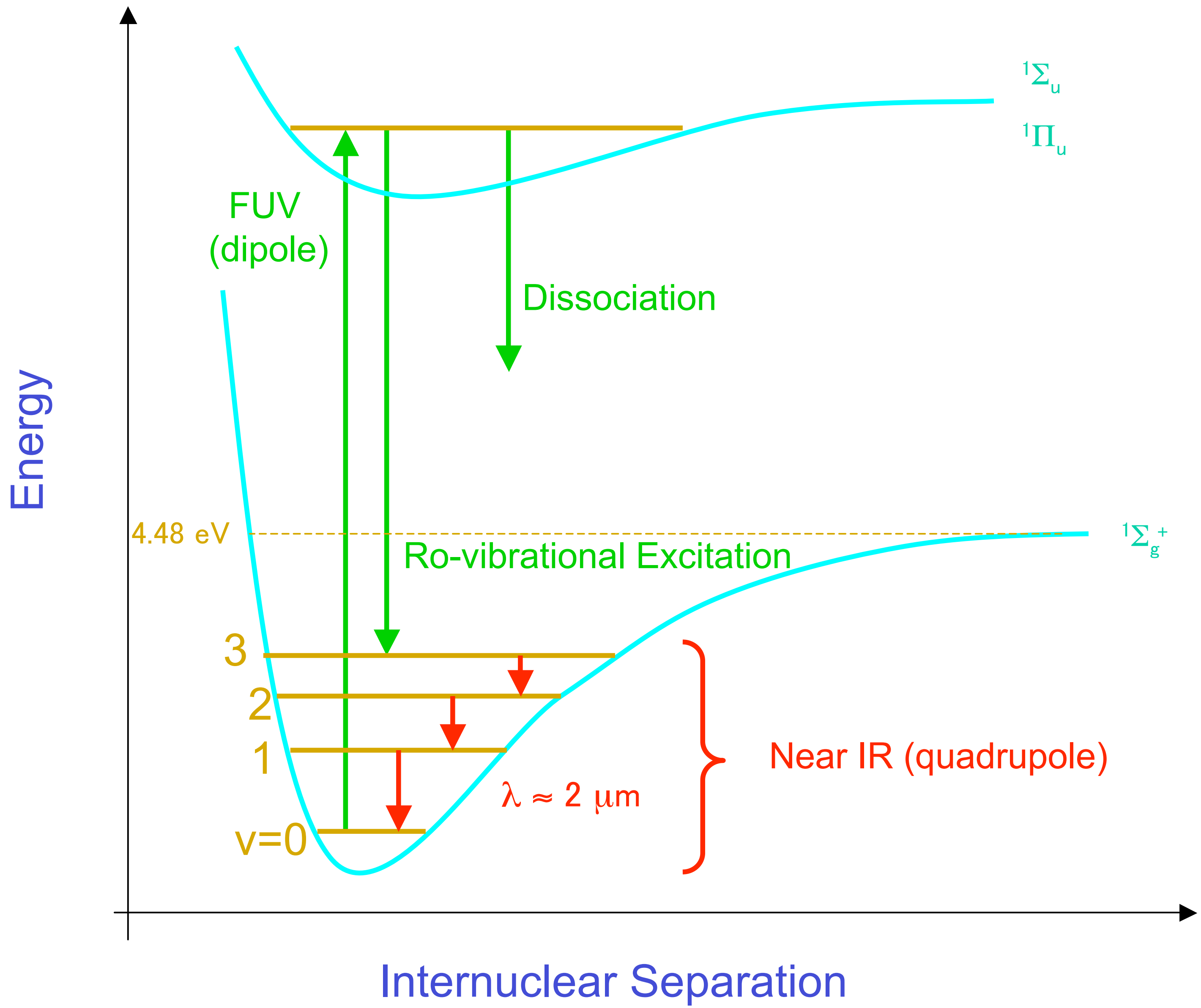


･･･Reveals Radiatively Excited Molecular Hydrogen in the Antennae:

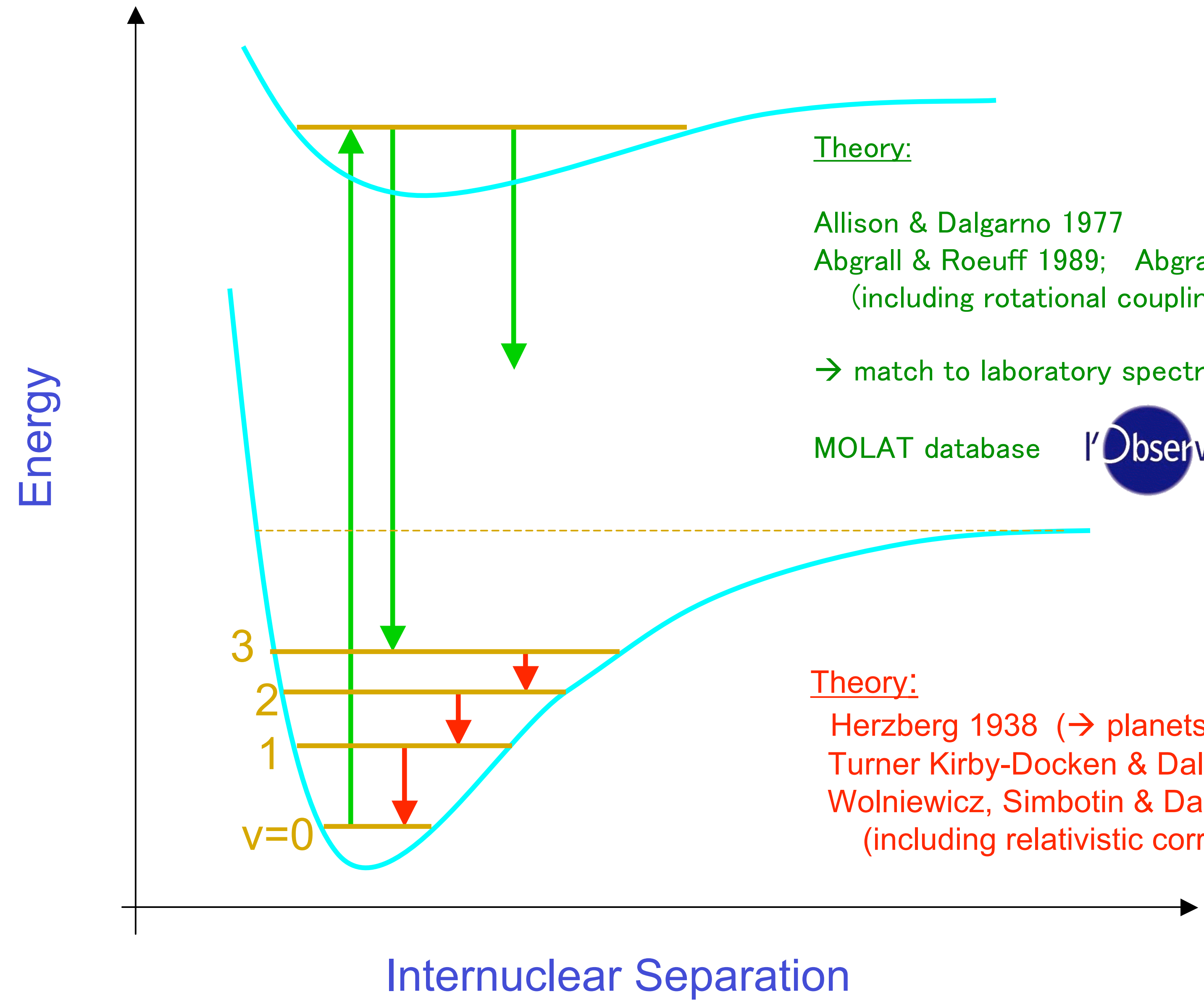
H_2 vibrational emission lines



Far-ultraviolet (FUV) Pumping and Photodissociation of Molecular Hydrogen:



Far-ultraviolet (FUV) Pumping and Photodissociation of Molecular Hydrogen:



Theory:

Allison & Dalgarno 1977
Abgrall & Roeuff 1989; Abgrall et al. 1997
(including rotational coupling)

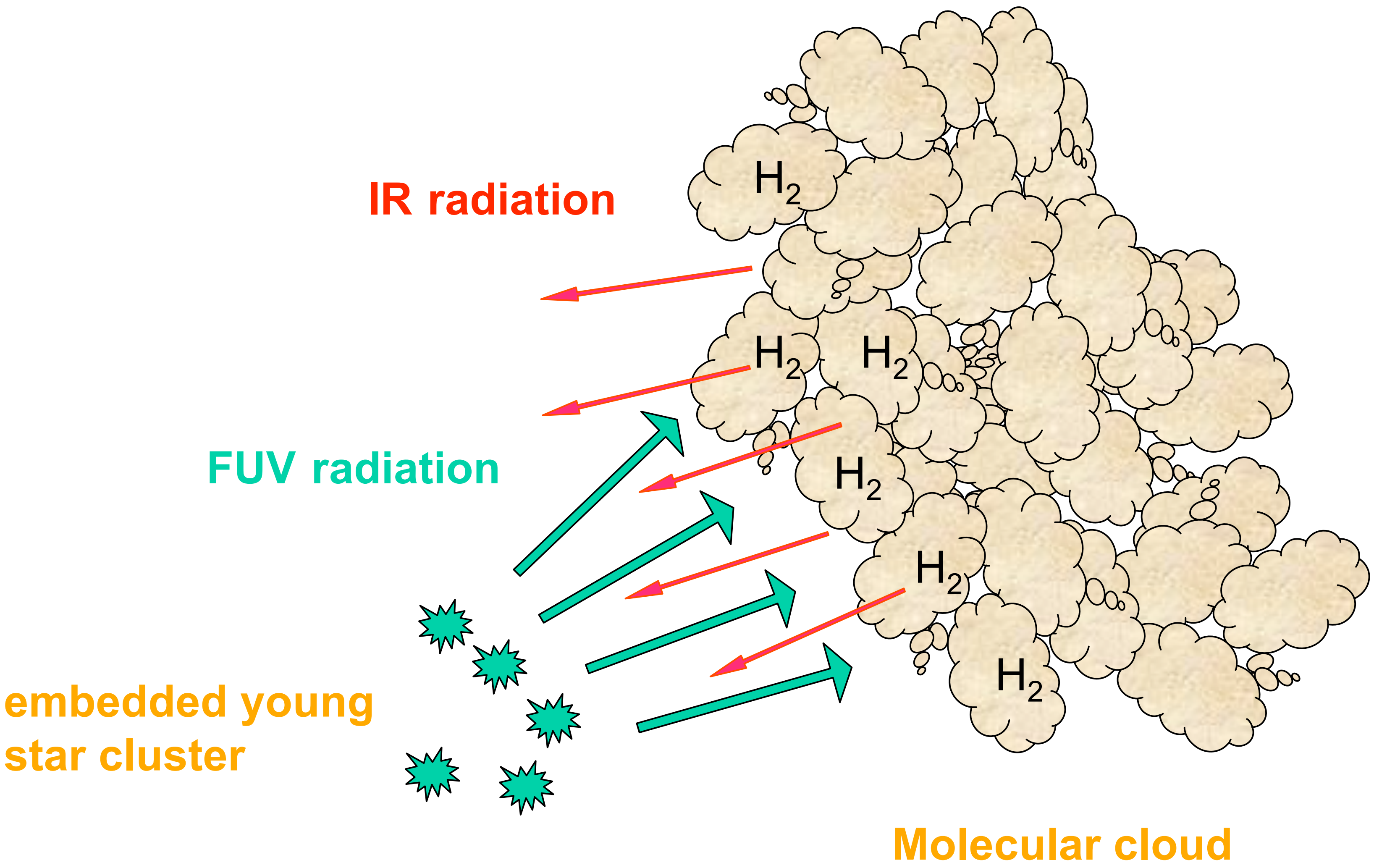
→ match to laboratory spectra.

MOLAT database l'Observatoire de Paris

Theory:

Herzberg 1938 (→ planets)
Turner Kirby-Docken & Dalgarno 1977
Wolniewicz, Simbotin & Dalgarno 1998
(including relativistic corrections)

Photon Dominated Regions (PDRs):



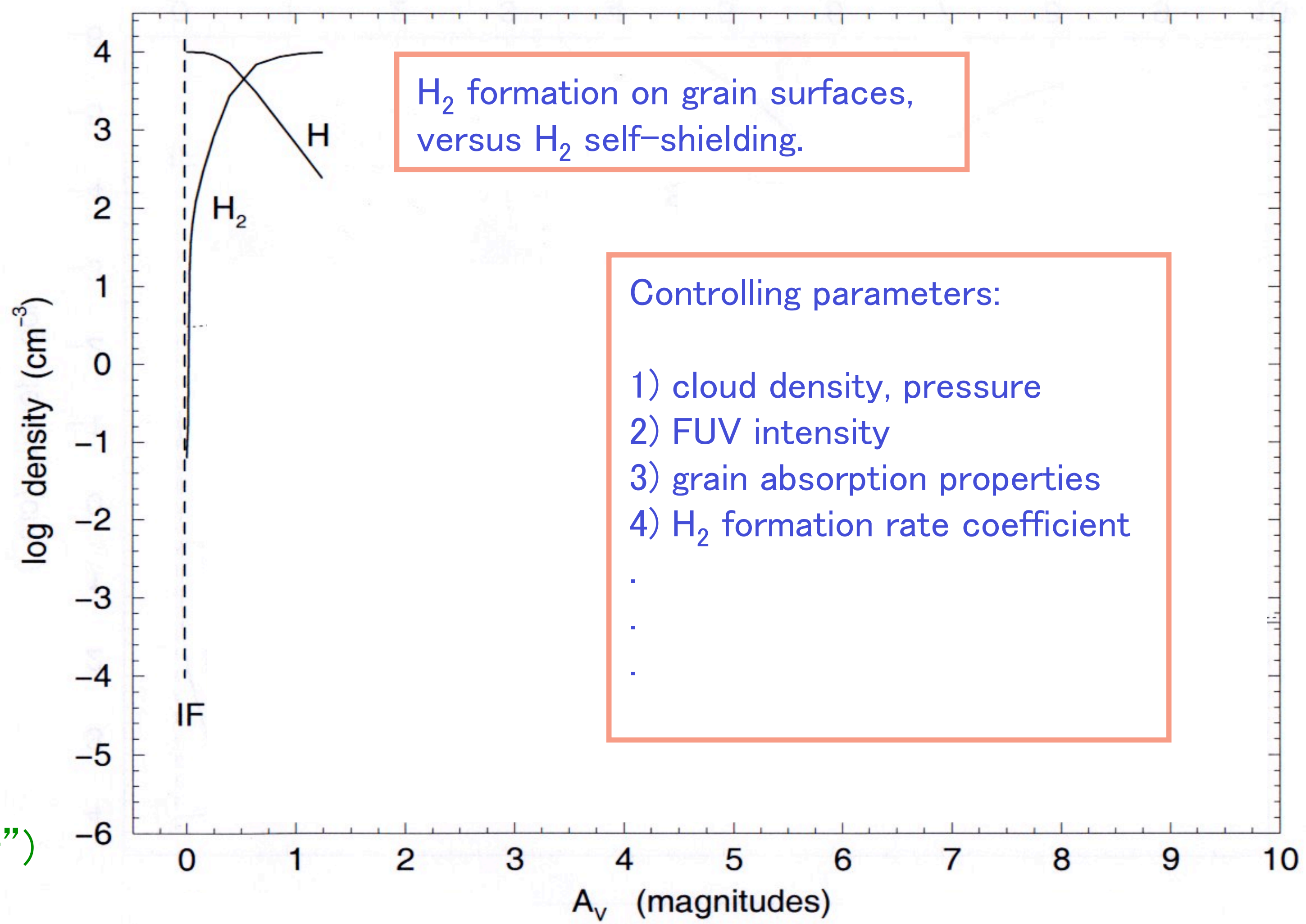
PDRs: Basic Structure: 1-D steady-state model, escape probability method.

Sternberg 2006

PDR: Far-UV photon penetration limited by dust absorption.

FUV
6-13.6 eV

(“non-ionizing”)



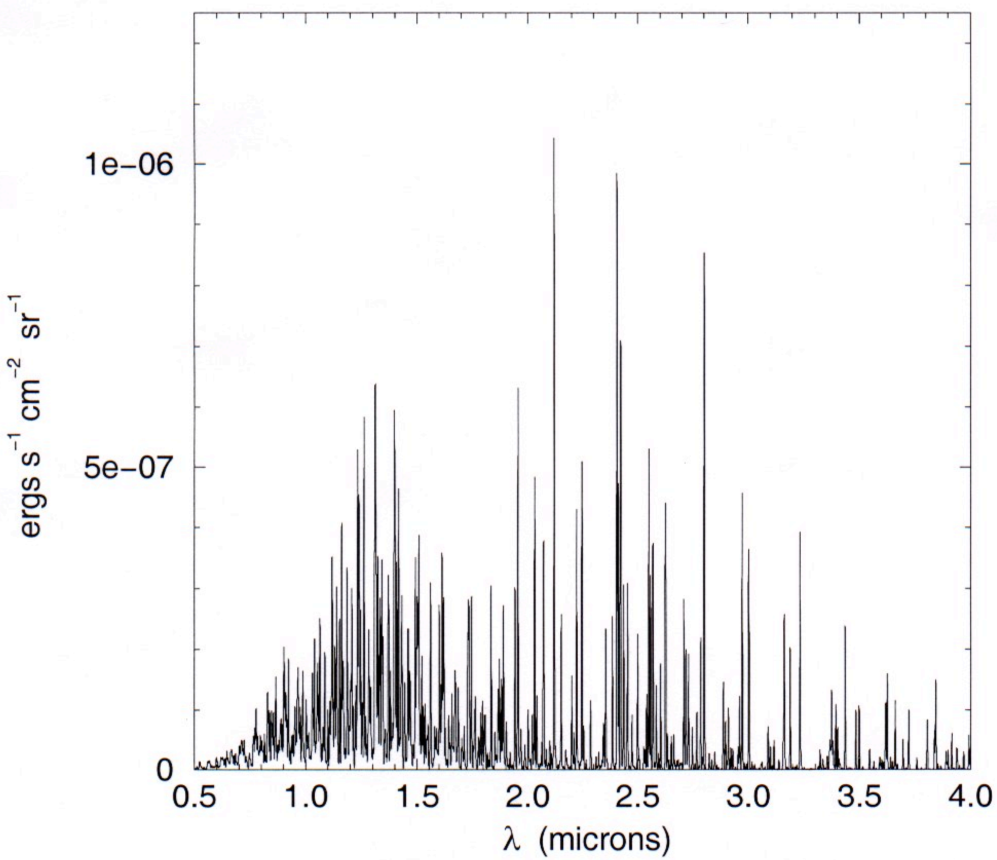
H_2 formation on grain surfaces, versus H_2 self-shielding.

Controlling parameters:

1) cloud density, pressure
2) FUV intensity
3) grain absorption properties
4) H_2 formation rate coefficient
.
.
.

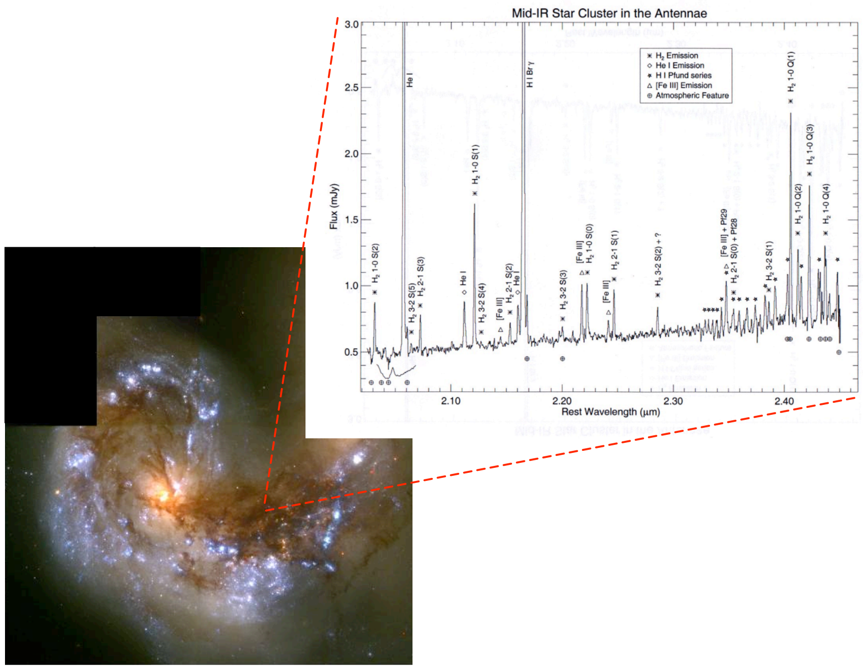
[optical depth into the cloud]

Resulting Infrared H_2 Emission Line Spectrum from the PDR:



Black & Dalgarno 1976
Black & van Dishoeck 1987
Sternberg 1988
Sternberg & Dalgarno 1989
Draine & Bertoldi 1996
Sternberg & Neufeld 1999
Shaw et al. 2005

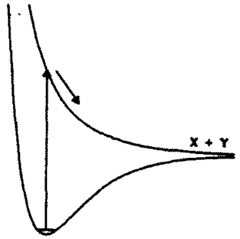
Matches the "Antennae" spectrum, and thereby constrains the H_2 gas densities, stellar radiation fields, and star-formation rates.



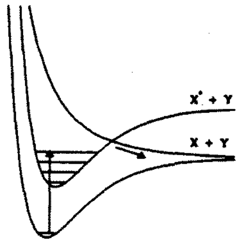
Molecular Photodissociation Processes:

potential energy curves

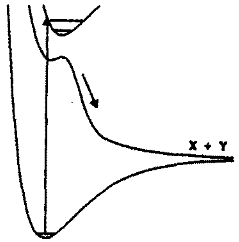
direct photodissociation



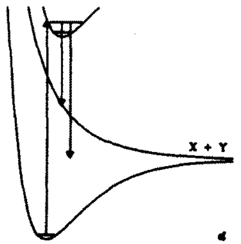
predissociation



coupled states
photodissociation



spontaneous
radiative dissociation



Molecular Photodissociation Processes:

potential energy curves

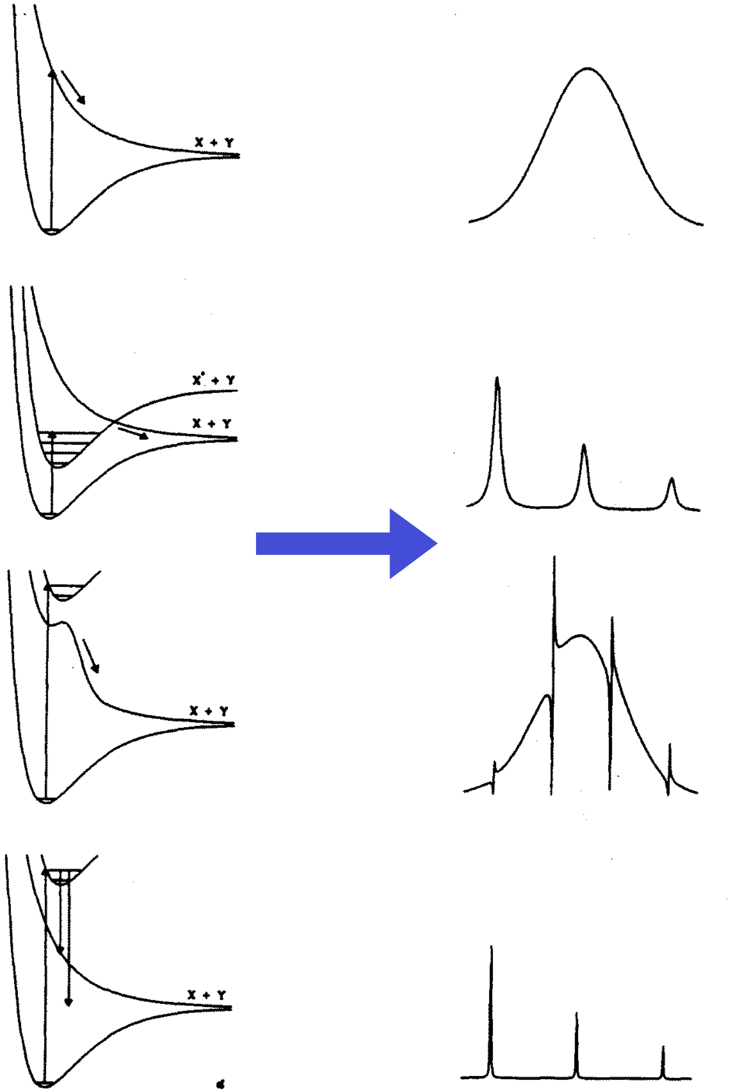
photoabsorption
cross sections

direct photodissociation

predissociation

coupled states
photodissociation

spontaneous
radiative dissociation



Molecular Photodissociation Processes:

potential energy curves

photoabsorption cross sections

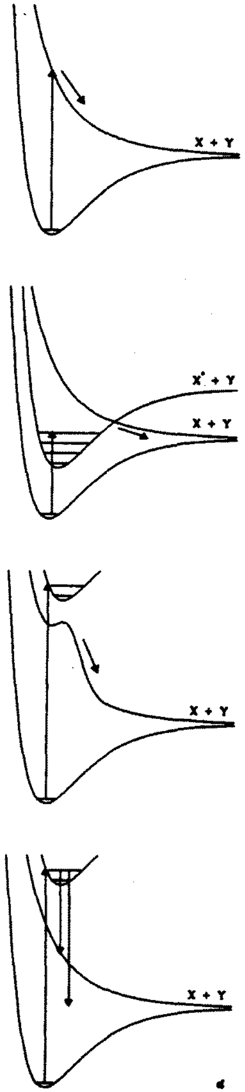
interstellar ultraviolet radiation field

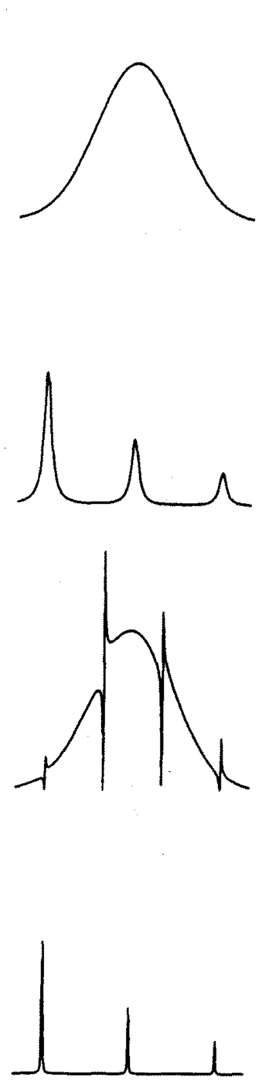
direct photodissociation

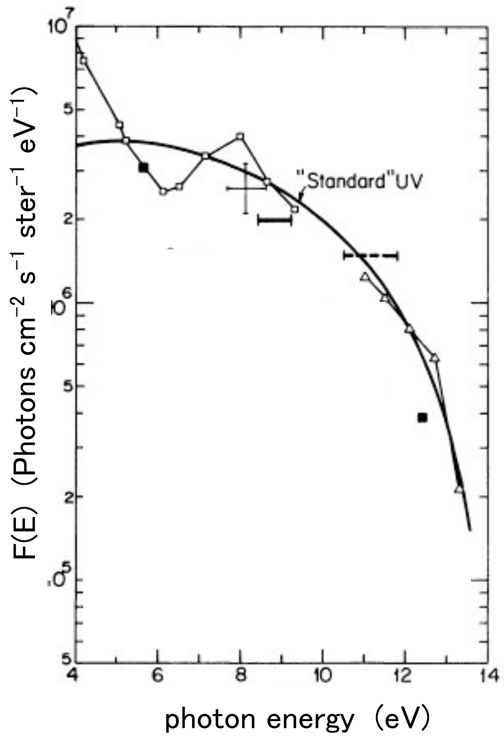
predissociation

coupled states photodissociation

spontaneous radiative dissociation







Voilà!

A database for photodissociation rates
of interstellar molecules.

Van Dishoeck 1988; 2006 Faraday Discussions 133/15

see also Bayet et al. 2006
Sternberg & Dalgarno 1995
Roberge et al. 1991

Table 2 Photodissociation rates for various radiation fields[ab]

Species	k^{o}_{pd}/s^{-1} ISRF[c]	10 000 K[d]	4000 K[d]
H_2^+	5.7(−10)	1.9(−10)	2.9(−11)
CH	9.2(−10)	2.0(−9)	1.2(−7)
CH^+	3.3(−10)	3.5(−11)	4.8(−10)
CH_2	5.8(−10)	1.2(−9)	2.1(−9)
CH_2^+	1.4(−10)	7.4(−11)	2.6(−11)
CH_3	2.7(−10)	2.5(−10)	8.2(−10)
CH_4	1.2(−9)	2.2(−10)	1.2(−12)
CH_4^+	2.8(−10)	4.2(−11)	1.3(−13)
C_2	2.4(−10)	4.1(−11)	3.2(−13)
C_2H	5.2(−10)	1.9(−10)	7.2(−12)
C_2H_2	3.3(−9)	1.2(−9)	1.3(−10)
C_2H_4	3.0(−9)	2.2(−9)	5.2(−10)
C_3	3.8(−9)	2.9(−9)	2.0(−10)
c-C_3H_2	1.9(−9)	1.7(−9)	9.2(−10)
OH	3.9(−10)	1.8(−10)	1.3(−10)
OH^+	1.1(−11)	7.8(−13)	5.8(−13)
H_2O	8.0(−10)	4.3(−10)	1.2(−10)
O_2	7.9(−10)	4.9(−10)	4.5(−11)
O_2^+	3.5(−11)	3.6(−11)	1.0(−11)
HO_2	6.7(−10)	1.9(−9)	1.2(−8)
H_2O_2	9.5(−10)	4.3(−10)	1.4(−10)
O_3	1.9(−9)	5.4(−9)	1.5(−7)
CO	2.0(−10)	1.5(−11)	1.4(−15)
CO^+	1.0(−10)	2.2(−11)	1.2(−13)
CO_2	8.9(−10)	9.0(−11)	1.2(−12)
HCO	1.1(−9)	2.5(−9)	3.5(−6)
HCO^+	5.4(−12)	4.5(−13)	7.9(−17)
H_2CO	1.0(−9)	6.7(−10)	1.8(−10)
CH_3OH	1.4(−9)	5.9(−10)	7.0(−11)
NH	5.0(−10)	1.6(−10)	3.0(−12)
NH^+	5.4(−11)	1.8(−10)	8.4(−9)
NH_2	7.5(−10)	1.0(−9)	5.7(−10)
NH_3	1.2(−9)	1.0(−9)	1.1(−9)
N_2	2.3(−10)	1.4(−11)	3.0(−16)
NO	4.7(−10)	4.3(−10)	2.9(−10)
NO_2	1.4(−9)	1.0(−9)	3.4(−10)
N_2O	1.9(−9)	4.8(−10)	2.0(−11)
CN	2.9(−10)	2.1(−11)	2.0(−15)
HCN	1.6(−9)	2.5(−10)	3.7(−12)
HC_3N	5.6(−9)	3.0(−9)	2.5(−10)
CH_3CN	2.5(−9)	4.8(−10)	8.5(−12)
SH	9.8(−10)	1.3(−9)	1.6(−8)
SH^+	2.5(−10)	3.4(−10)	4.0(−8)
H_2S	3.1(−9)	2.0(−9)	3.2(−9)
CS	9.8(−10)	2.7(−10)	3.7(−12)
CS_2	6.1(−9)	1.3(−8)	2.0(−8)
OCS	3.7(−9)	3.1(−9)	7.0(−10)
SO	4.2(−9)	4.4(−9)	9.4(−9)
SO_2	1.9(−9)	7.4(−10)	2.8(−10)
SiH	2.8(−9)	1.4(−8)	8.0(−7)
SiH^+	2.7(−9)	1.0(−8)	3.3(−6)
SiO	1.6(−9)	5.6(−10)	9.9(−12)

[a] See van Dishoeck[73] for products and references to cross section data. [b] H_3^+ radiation with $\lambda > 912$ Å, so $k^{o}_{pd} = 0$. [c] ISRF according to ref. 12 with ext radiation field with temperature T_{BB} (see text).

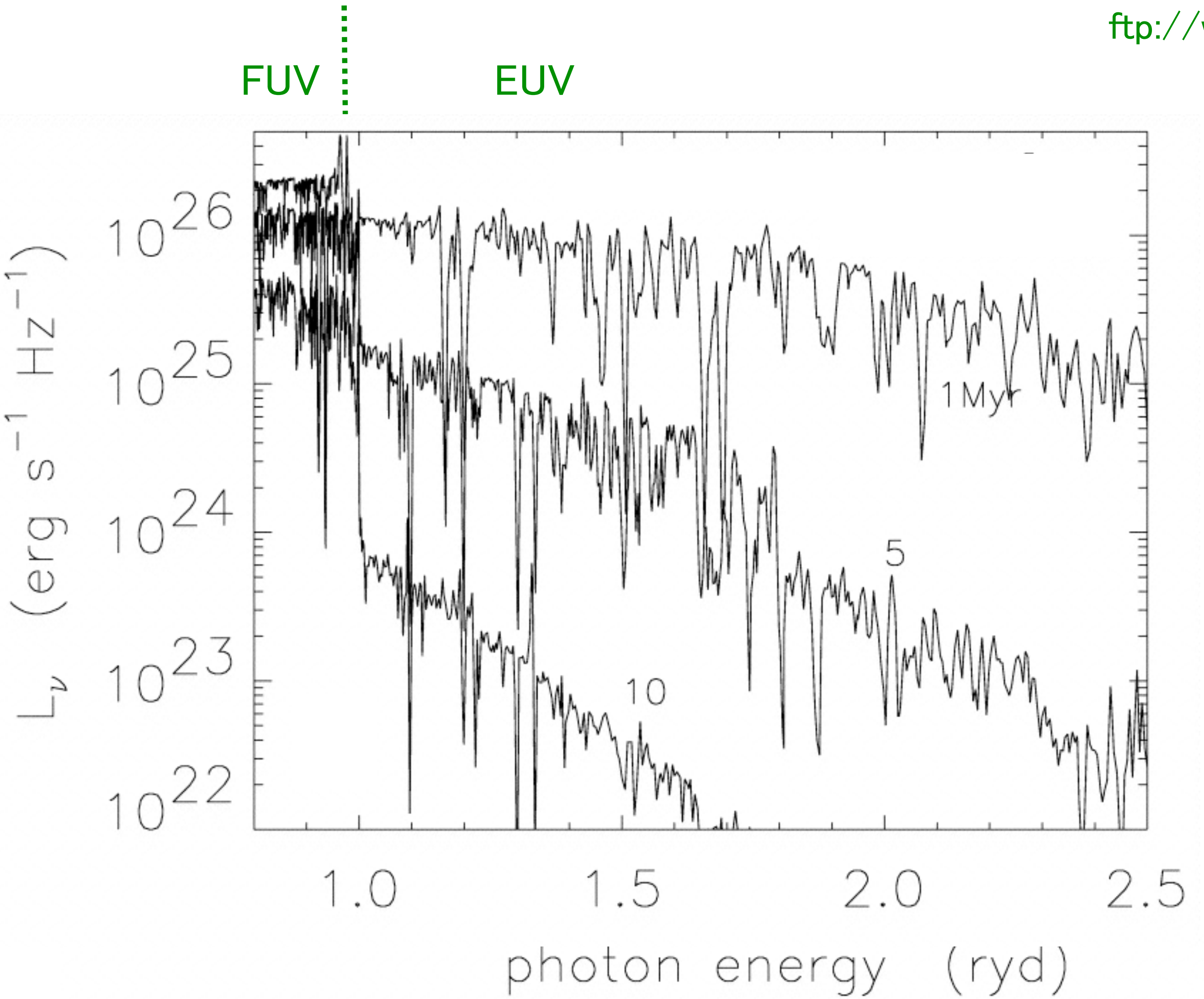
Radiation Fields of Evolving OB Clusters:

Sternberg, Hoffmann & Pauldrach 2003, ApJ, 599, 1333

[Hydrodnamics and radiative transfer in NLTE winds]

A database of
stellar atmospheres
for hot stars!

ftp://wise3.tau.ac.il/pub/stars



Intensity and
spectral shape
of FUV field
depend on cluster
mass and age

→Evolution of
photorates.

Interstellar Chemistry in a Nutshell: Basic Processes.

Bond Formation:

- radiative association $X + Y \rightarrow XY + h\nu$
- grain surface formation $X + Y{:}g \rightarrow XY + g$
- associative detachement $X^- + Y \rightarrow XY + e$

Bond Destruction:

- photodissociation $XY + h\nu \rightarrow X + Y$
- dissociative recombination $XY^+ + e \rightarrow X + Y + e$
- collisional dissociation $XY + M \rightarrow X + Y + M$

Bond Rearrangement:

- ion-molecule exchange $X^+ + YZ \rightarrow XY^+ + Z$
- charge-transfer $X^+ + YZ \rightarrow X + YZ^+$
- neutral-neutral $X + YZ \rightarrow XY + Z$

National Institute of Standards and Technology

http://www.nist.gov

udfa05

formerly UMIST99

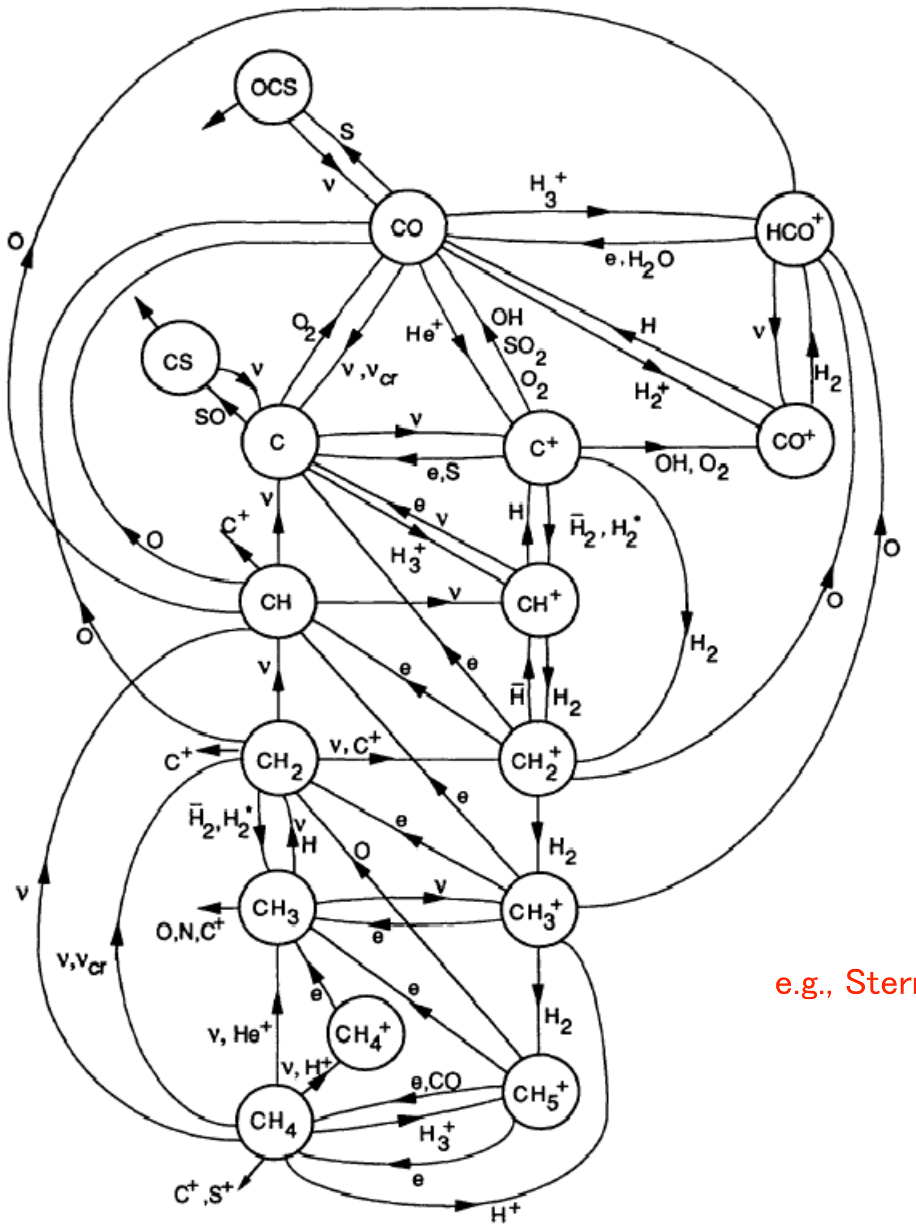
http://www.udfa.net

Le Teuff 2000 AA 146 157

http://www.physics.ohio-state.edu/~eric/

Herbst et al.

<u>Interstellar Carbon-Oxygen Chemical Network:</u>

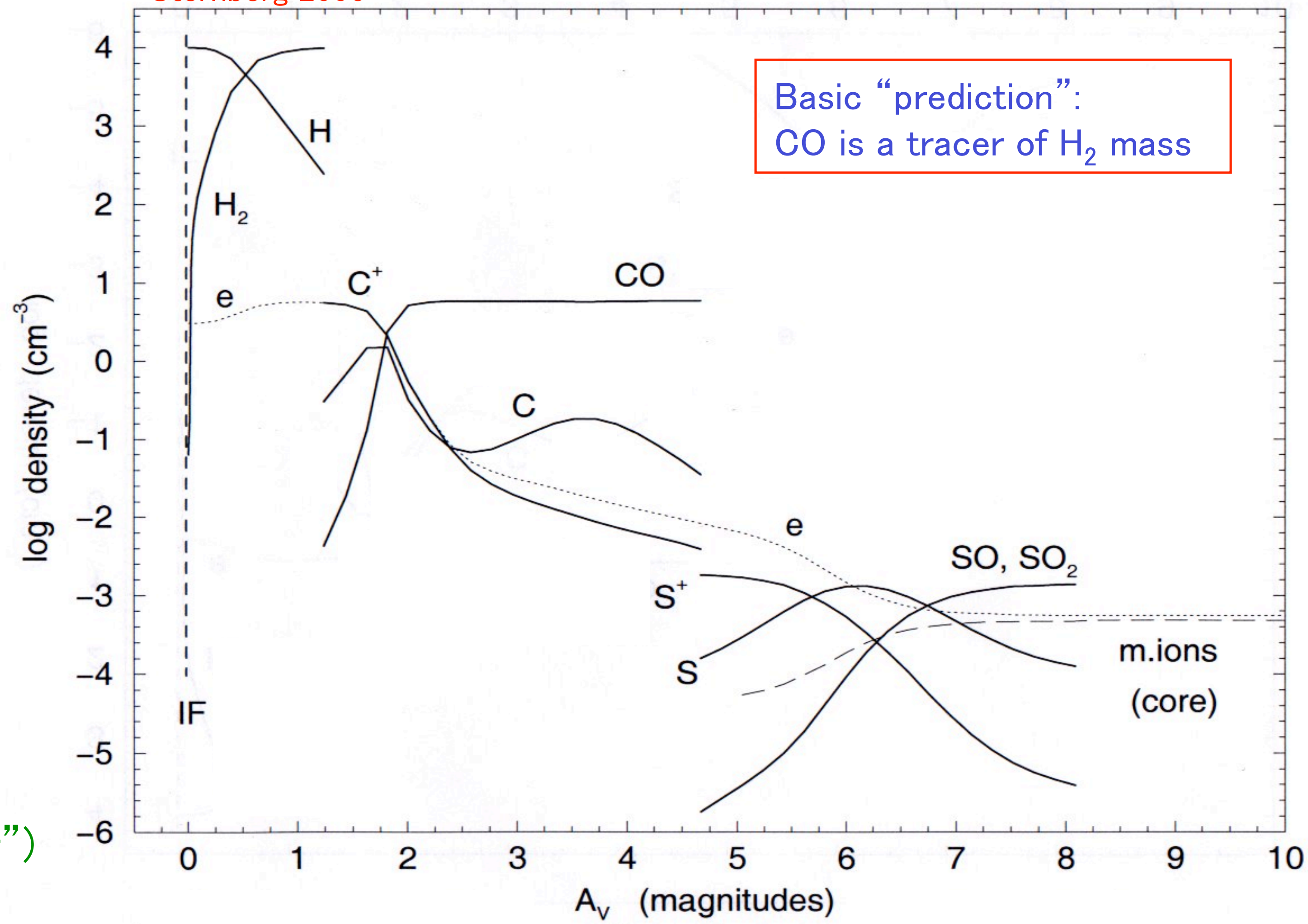


e.g., Sternberg & Dalgarno 1995 ApJS 99 565

PDR Structure:

Tielens & Hollenbach 1985
Van Dishoeck & Black 1989
Sternberg & Dalgarno 1989, 1995
Le Bourlot 1993; Le Petit et al. 2006 (Meudon PDR)
Roellig et al. 2006 (a comparison of PDR codes)

Sternberg 2006



Basic "prediction":
CO is a tracer of H_2 mass

FUV
6–13.6 eV

("non–ionizing")

Orion:

THE ASTROPHYSICAL JOURNAL, 161:L43–L44, July 1970

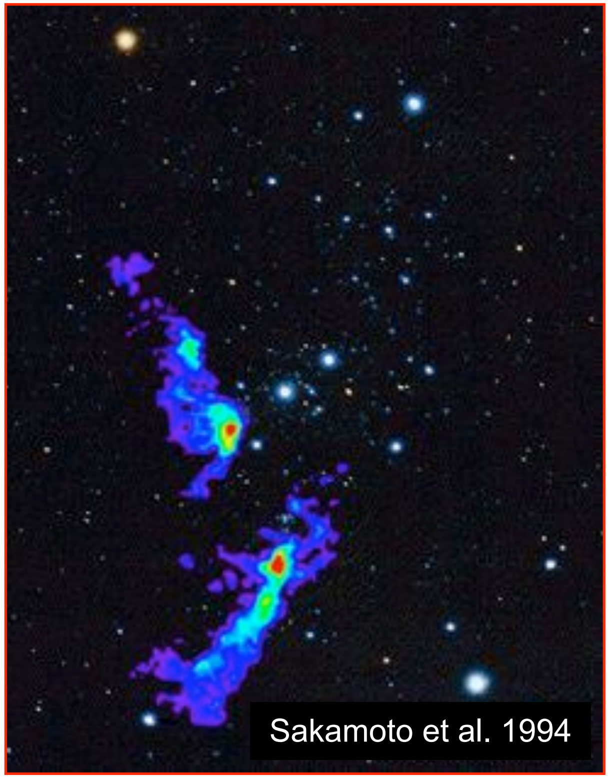
CARBON MONOXIDE IN THE ORION NEBULA

R. W. WILSON, K. B. JEFFERTS, AND A. A. PENZIAS
Bell Telephone Laboratories, Inc., Holmdel, New Jersey, and
Crawford Hill Laboratory, Murray Hill, New Jersey
Received 1970 June 5

ABSTRACT

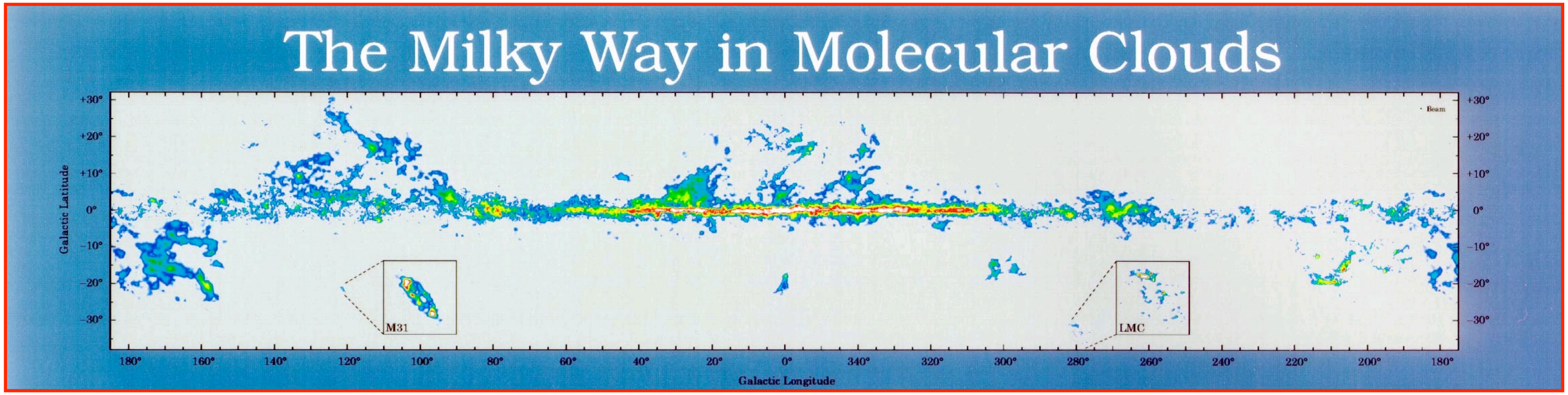
We have found intense 2.6-mm line radiation from nine galactic sources which we attribute to carbon monoxide.

(Penzias and Wilson are also famous for discovering the 3° K cosmic microwave background radiation → Nobel Prize 1978)

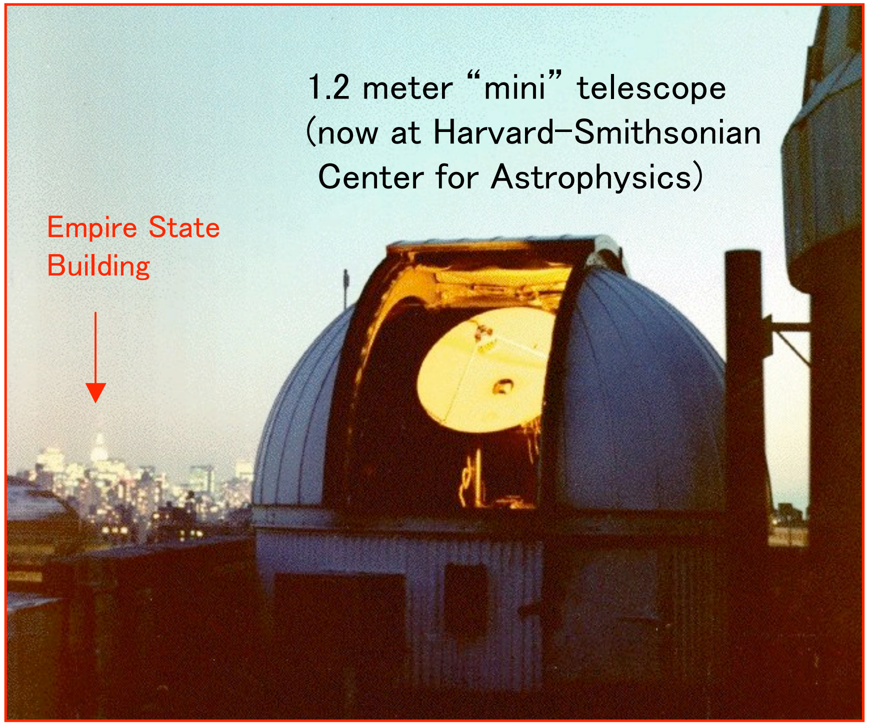


Mapping the Galaxy in Carbon Monoxide:

Dame, Hartmann & Thaddeus 2001



As observed from the other center of the universe⋯ New York City!



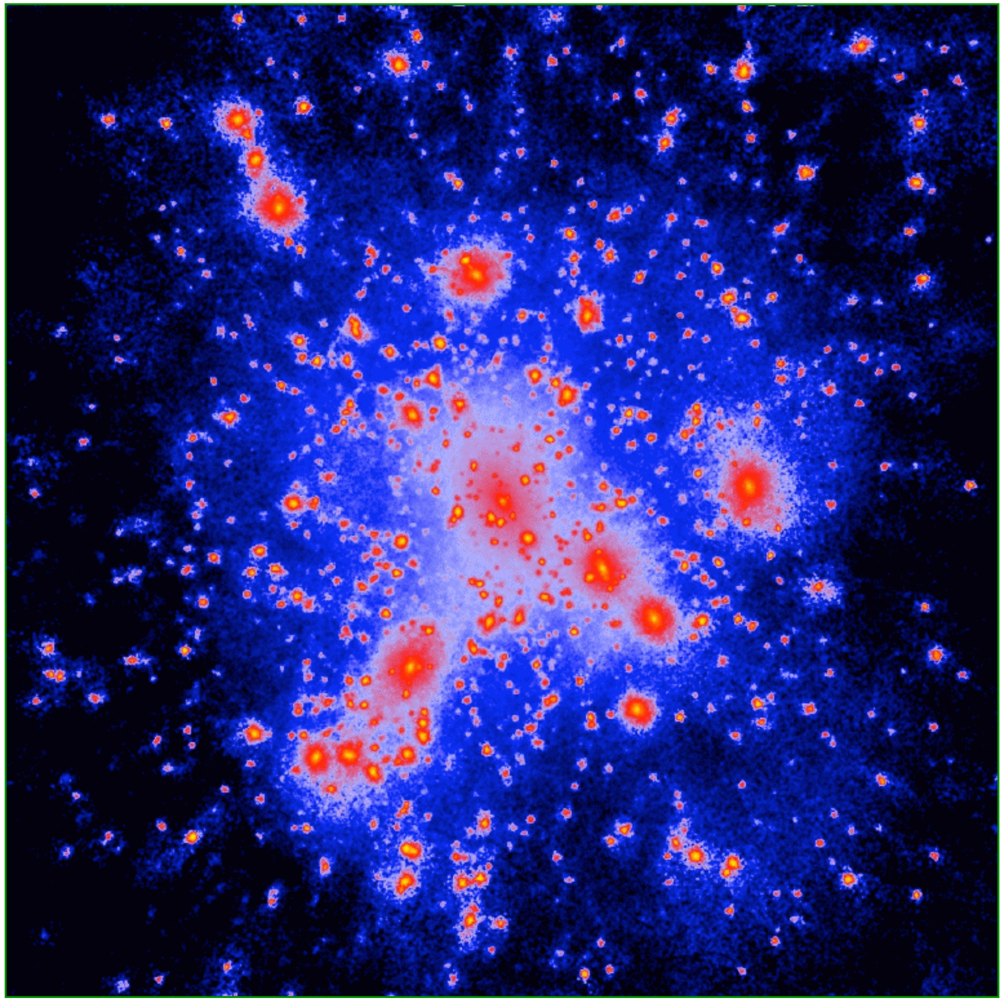
CO serves as a proxy for H_2.

Except in the vicinity of intense radiation fields and shock waves, H_2 is usually impossible to detect directly.

Galaxy Formation:

Gravitational Collapse of the "Dark Matter" Perturbations in an Expanding Universe

http://star-www.dur.ac.uk/~moore



1. Structure formation is hierarchical. Low mass objects form early. High mass objects form late.

2. Stars and galaxies form as "baryonic" gas falls into the dark-matter potential wells.

Carbon Monoxide as a Dynamical Probe at High Redshift:

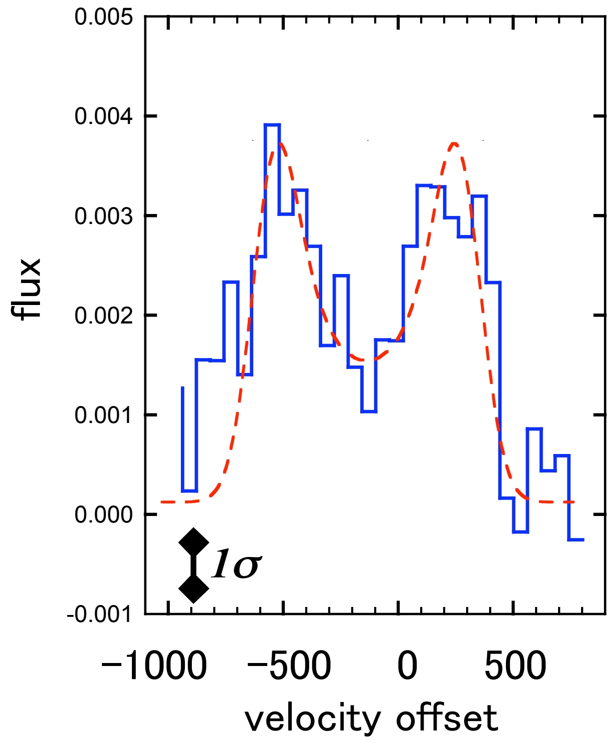
Submillimeter Galaxy J02399−0136 (at z=2.81, when Universe was ~10% its current age)

CO J=4−3 detected and resolved with PdB interferometer. Genzel et al. 2003 ApJ 584 633

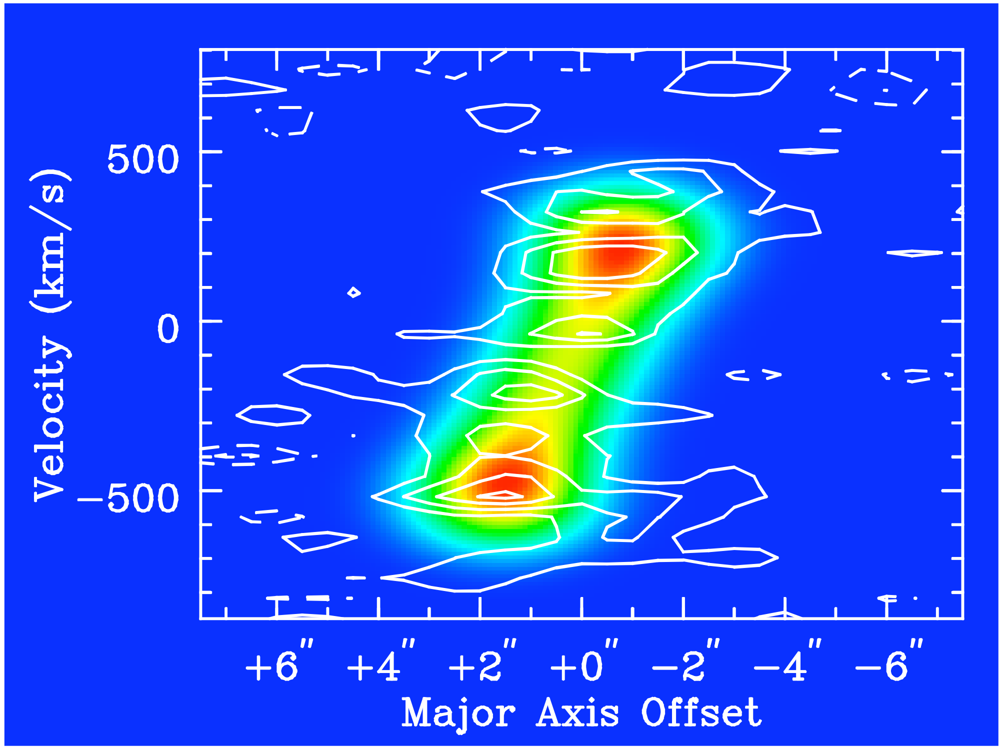
Mass = 3x10^{11} solar masses within radius = 24000 ly

Large! In conflict with "standard" structure formation theory.

CO 4−3 Line Profile

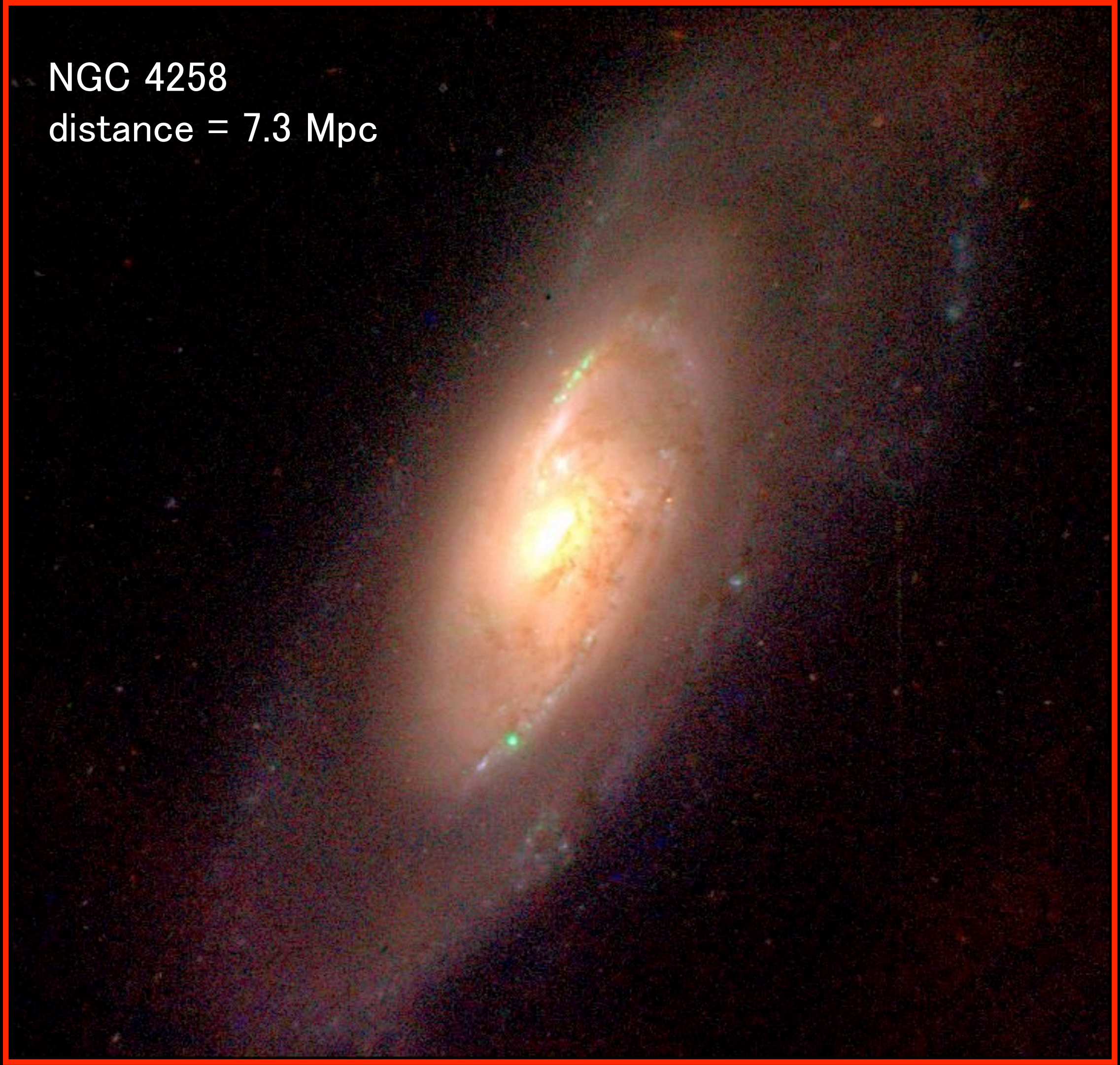


"Rotation Curve"



X-ray Dominated Regions: Active Galactic Nuclei.

optical image



Central luminosity provided by an accreting, super-massive, black hole.

X-rays.

All spiral galaxies are today thought to contain central massive black holes.

M_{BH} = 10^6 to 10^9 solar masses

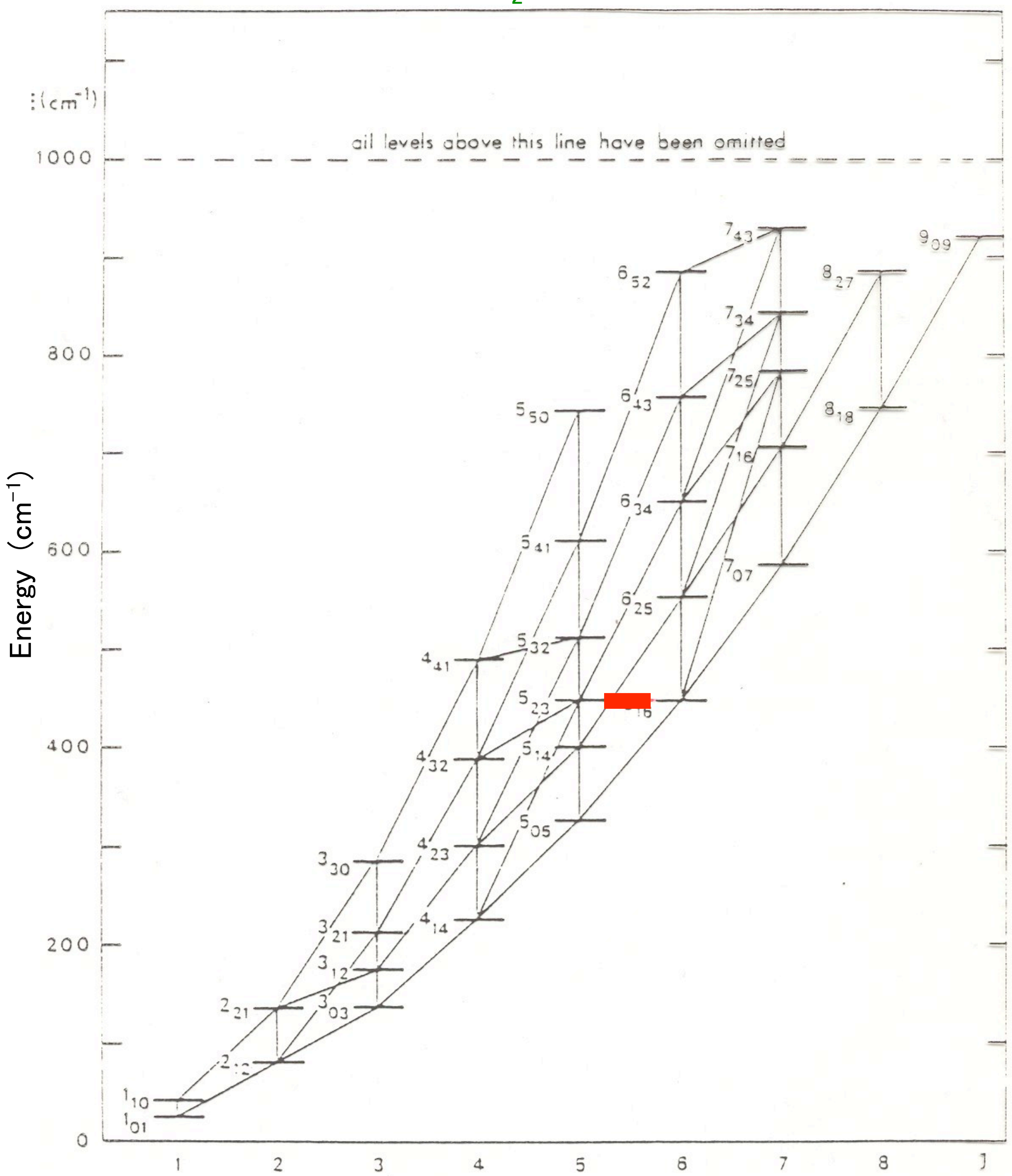
Water around the black hole…

Interstellar water (H_2O):

Interstellar water was first detected at 1.35 cm, by Cheung et al. 1969
22 GHz

But something unusual is happening...

ortho – H_2O (asymmetric top)



Interstellar water masers:

Interstellar water was actually first detected at 1.35 cm, by Cheung et al. 1969
22 GHz

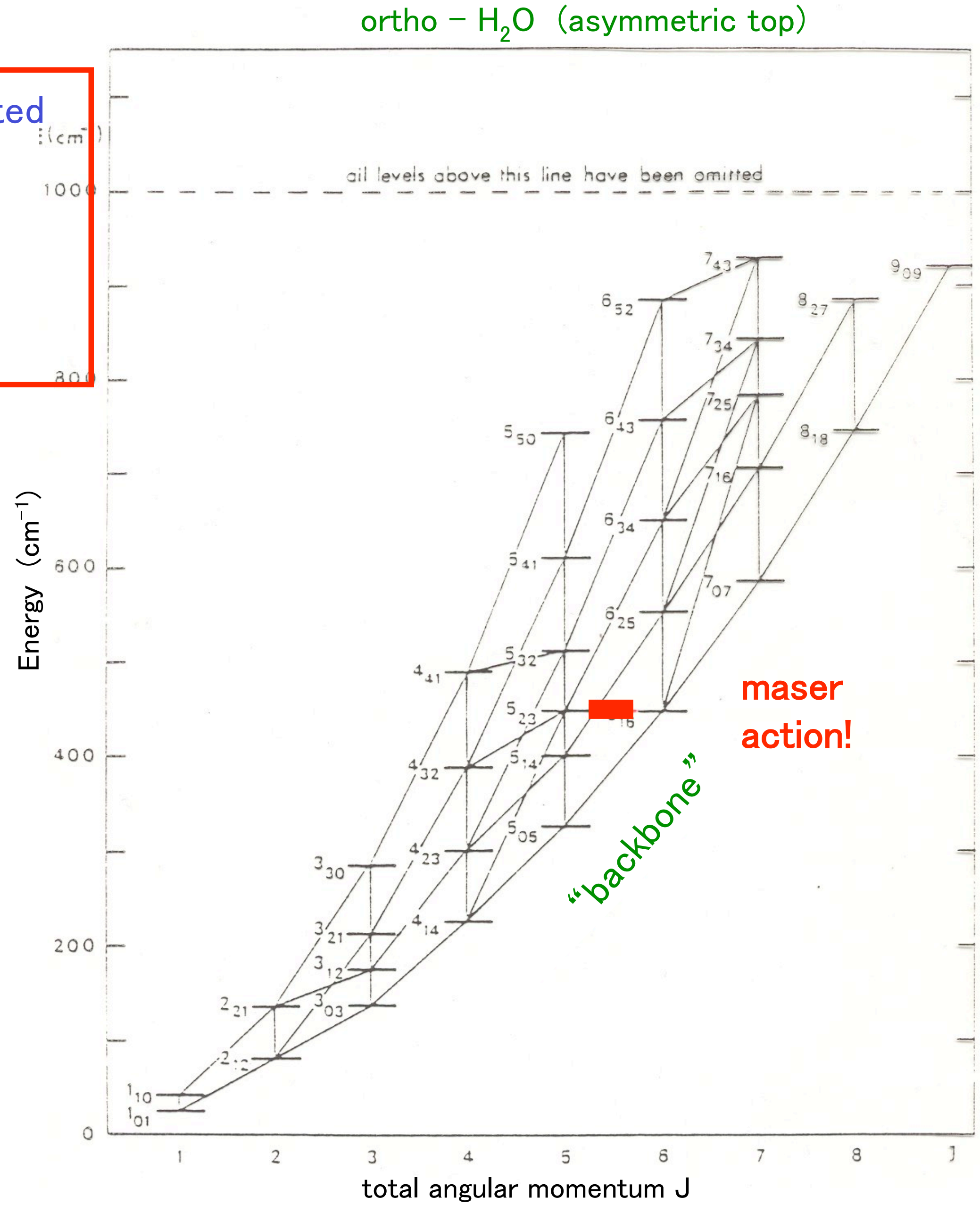
But something unusual is happening...

Equivalent blackbody intensities can exceed 10^{15} K !

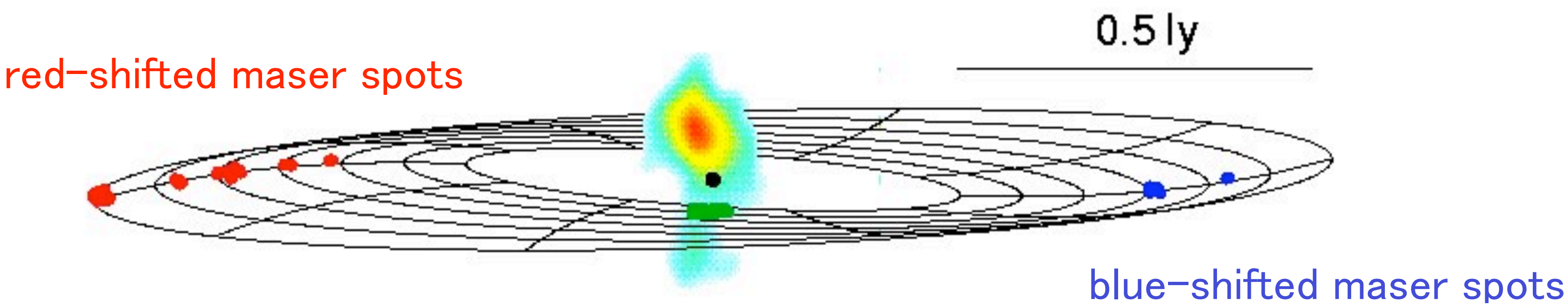
Luminosities as high as 500 times solar in this single spectral line!

Explanation: The line intensity is exponentially amplified by stimulated emission, due to naturally occurring energy-level population inversions.
Natural lasers in the sky!!!

Very useful as dynamical probes...



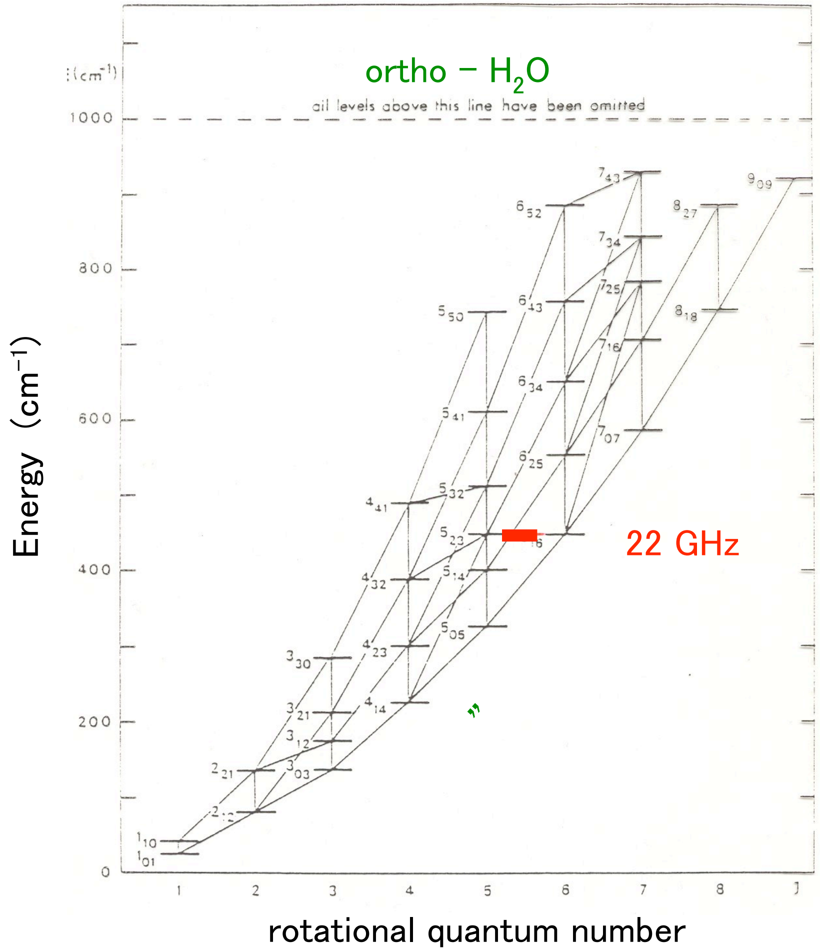
Water Masers Around the Supermassive Black Hole in NGC 4258:



In the center of NGC 4258:
A resolved Keplerian disk
with orbiting water maser spots.

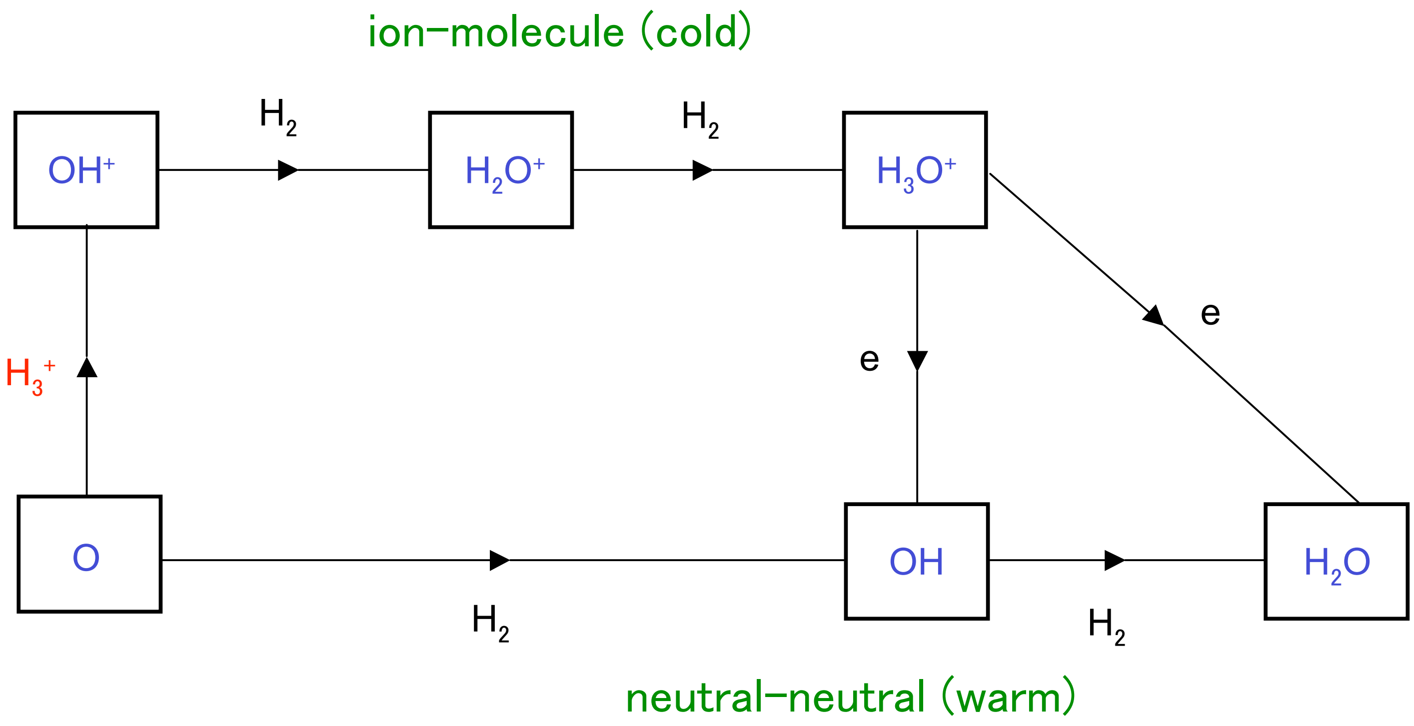
$v^2 = GM / R$

$M = 3 \times 10^7 M_\odot$



Moran et al. 1995 PNAS 9211427
Herrnstein et al. 2005 ApJ 629 719

H_2O Formation:



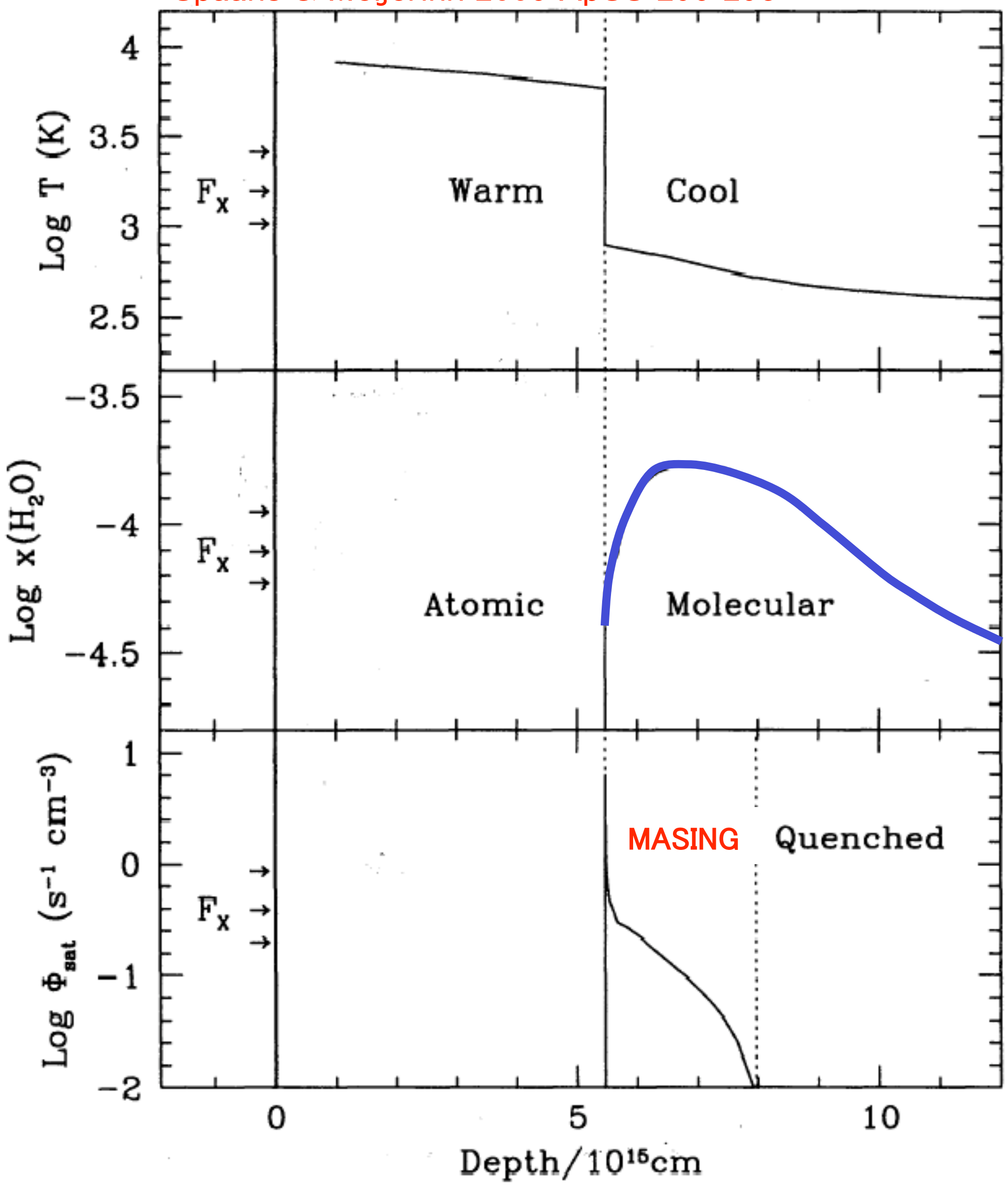
Neufeld & Dalgarno 1989 ApJ 340 869 (J-shocks)

Sternberg & Dalgarno 1995 ApJS 99 565 (PDRs)
Boger & Sternberg 2005 ApJ 632 302

Maloney, Hollenbach & Tielens 1996 ApJ 466 571 (XDRs)

Production of H_2O in X-ray Dominated Regions:

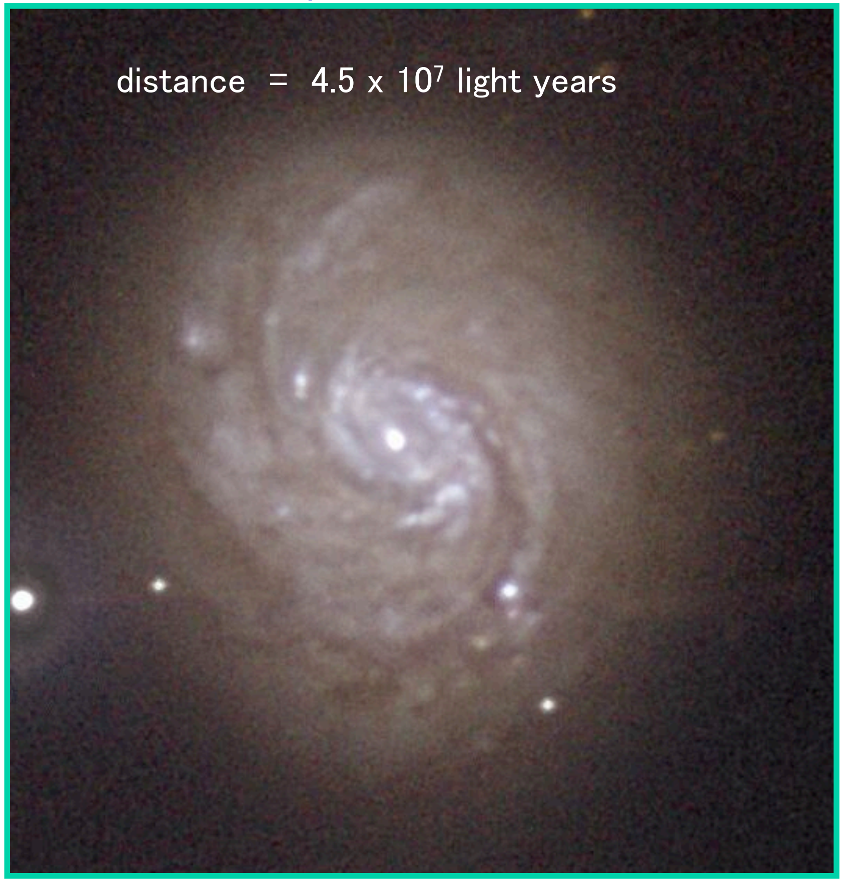
Neufeld, Maloney & Conger 1994 ApJ 436, L127
Spaans & Meijerink 2005 ApSS 295 293



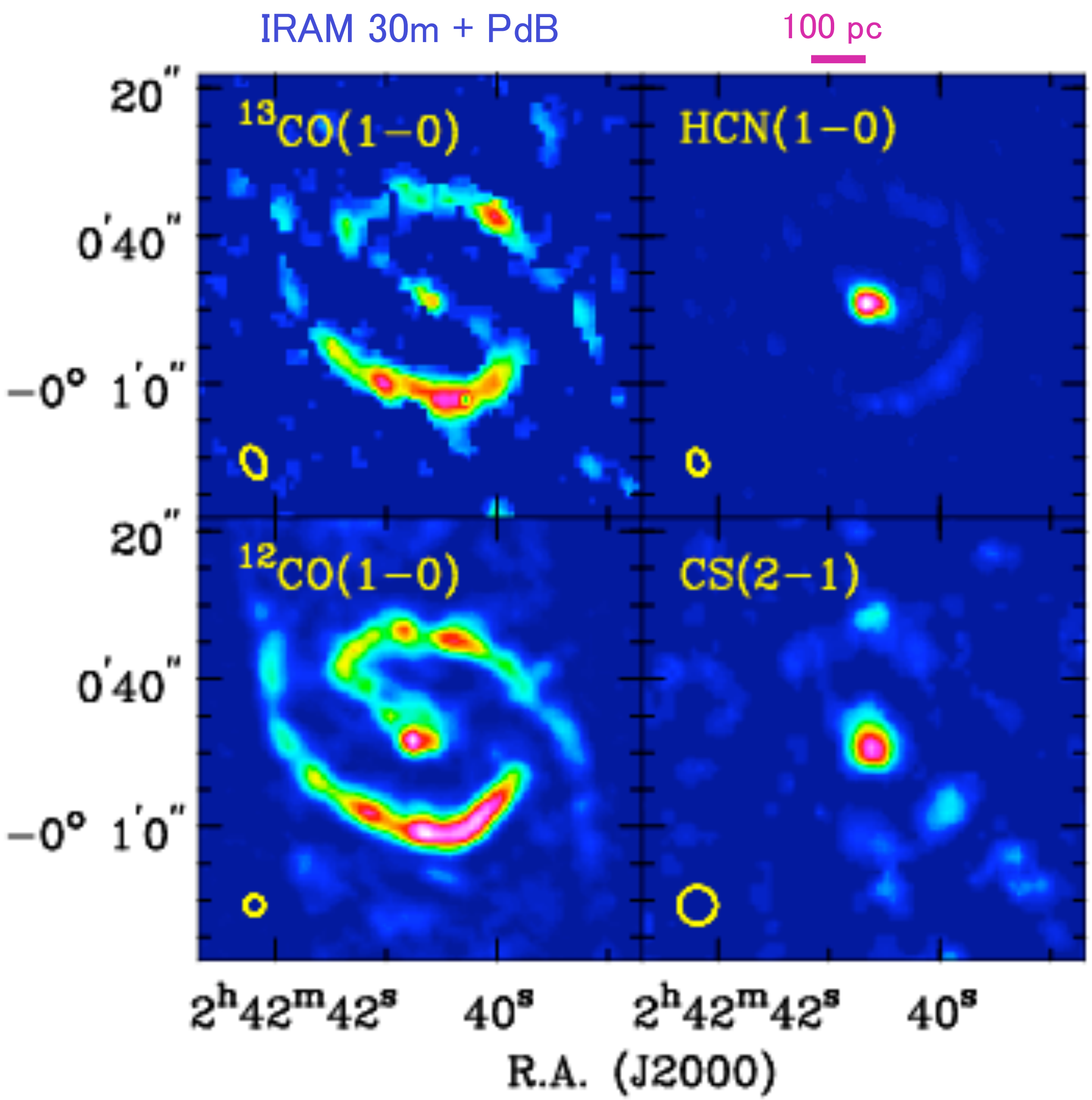
However, because the maser emission is exponentially amplified cannot easily extract water abundances from the observations.

Molecules in the Seyfert-2 Galaxy NGC 1068 (M77):

NGC 1068 (optical)



Molecules in the Seyfert-2 Galaxy NGC 1068:



Tacconi et al. 1994 ApJ 426 L77

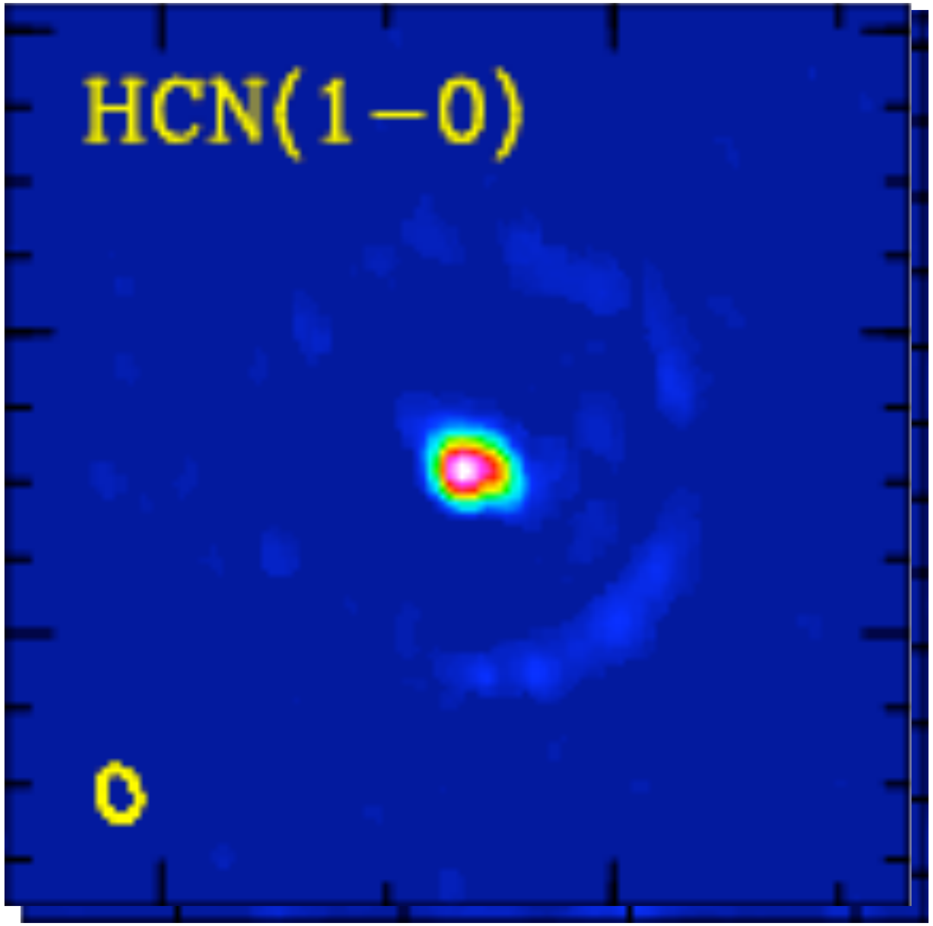
Sternberg, Genzel & Tacconi 1994 ApJ 436 L131

Helfer & Blitz 1995 ApJ 450 90

Usero et al. 2004 AA 419 897

X–ray Dominated Regions in NGC 1068 ?

In the nucleus, HCN/CO ≈ 10^{-3} (large!)･･･



･･･possible signature of enhanced ionization rate in molecular gas exposed to X–rays.

Lepp & Dalgarno 1996 AA 306 L21

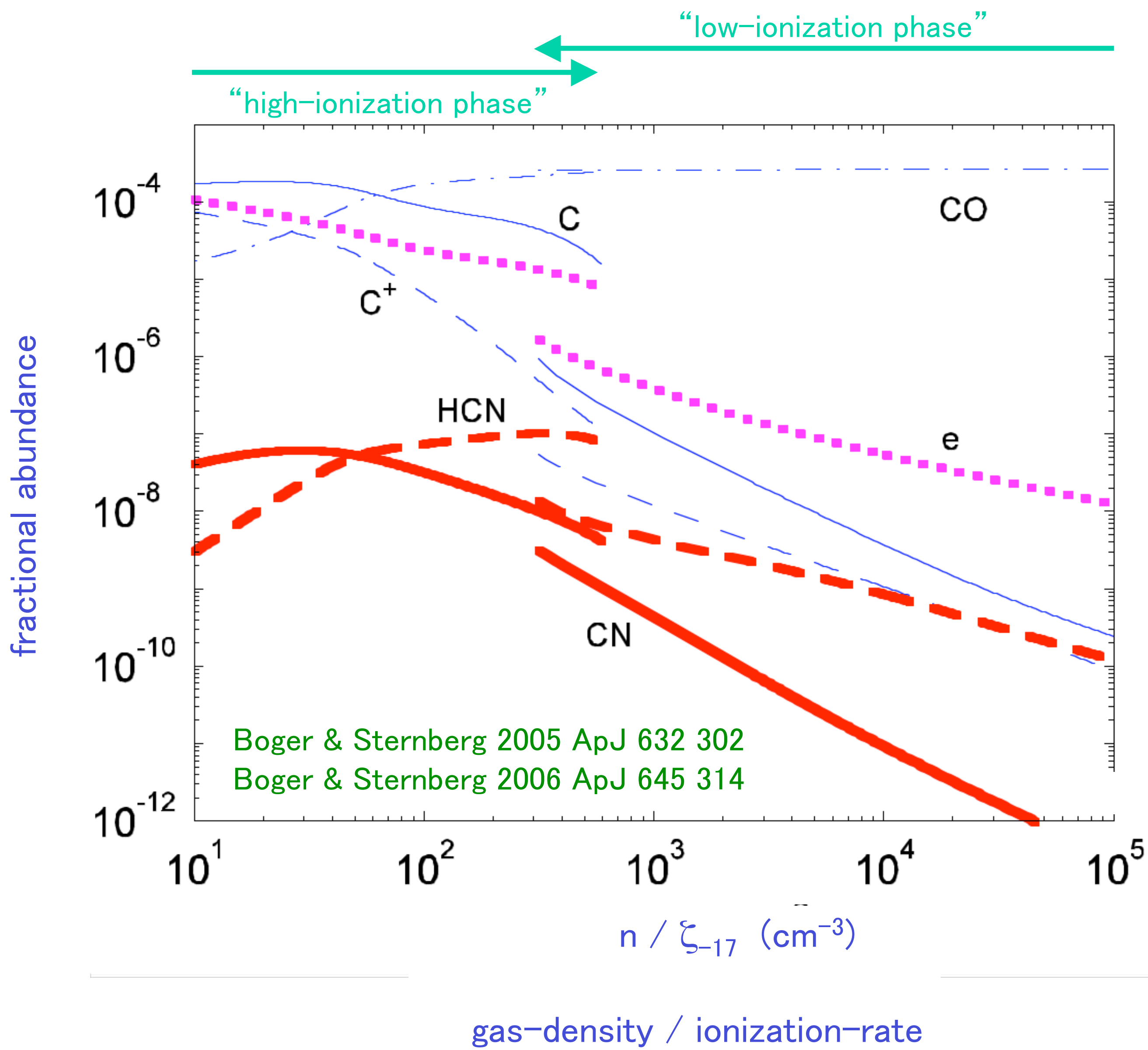
Usero et al. 2004 AA 419 897

Boger & Sternbeg 2005 ApJ 632 302

$M_{gas} \approx 5 \times 10^{7}\ M_{\odot}$

$L_{Xray} \approx 2 \times 10^{11}\ L_{\odot}$

Chemistry Near Black Holes:



High-ionization rate gives large

HCN / CO

as observed in NGC 1068.

Also predicts large

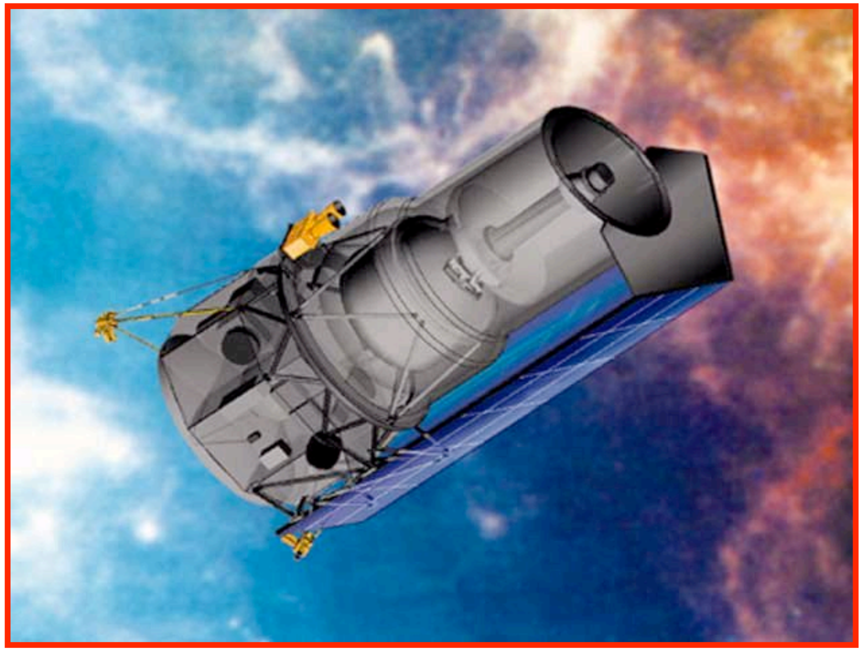
CN / HCN

consistent with recent observations by Usero et al. 2004

A Golden Age!

Cost: ~10 cents per star in the Galaxy!

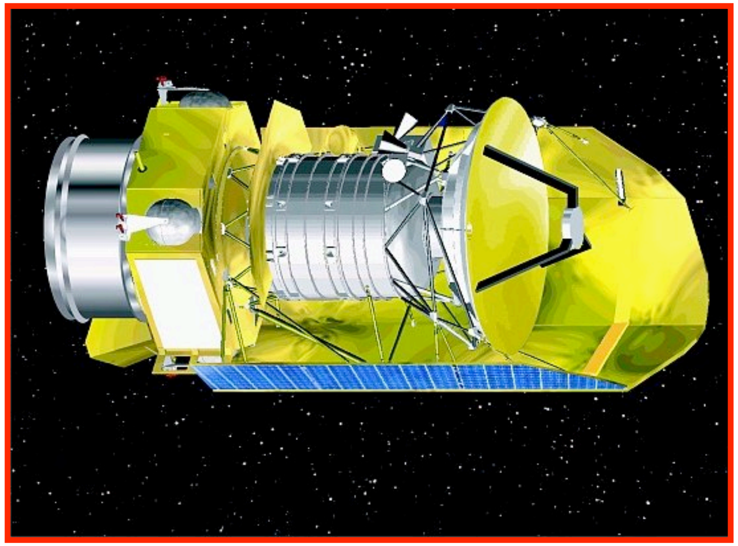
Spitzer Space Telescope (now operational)



Stratospheric Observatory for Infrared Astronomy

Atacama Large Millimeter Array (ALMA)

Herschel Space Observatory (submillimeter)



Laboratory Astrophysics & Theory →The Databases: Maintain with Tender Loving Care!

http://spec.jpl.nasa.gov

Molecular Spectroscopy
Jet Propulsion Laboratory
California Institute of Technology

udfa05

formerly UMIST99

http://www.udfa.net

Leiden Atomic and Molecular Database

http://www.strw.leidenuniv.nl/~moldata/

Leiden Observatory
Universiteit Leiden

Cologne Database for Molecular Spectroscopy

http://www.cdms.de

National Institute of Standards and Technology

http://www.nist.gov

HITRAN

The Ohio State University

Herbst et al.

l'Observatoire de Paris

Atomic and Molecular Data

http://amrel.obspm.fr/molat/

http://cfa-www.harvard.edu/HITRAN