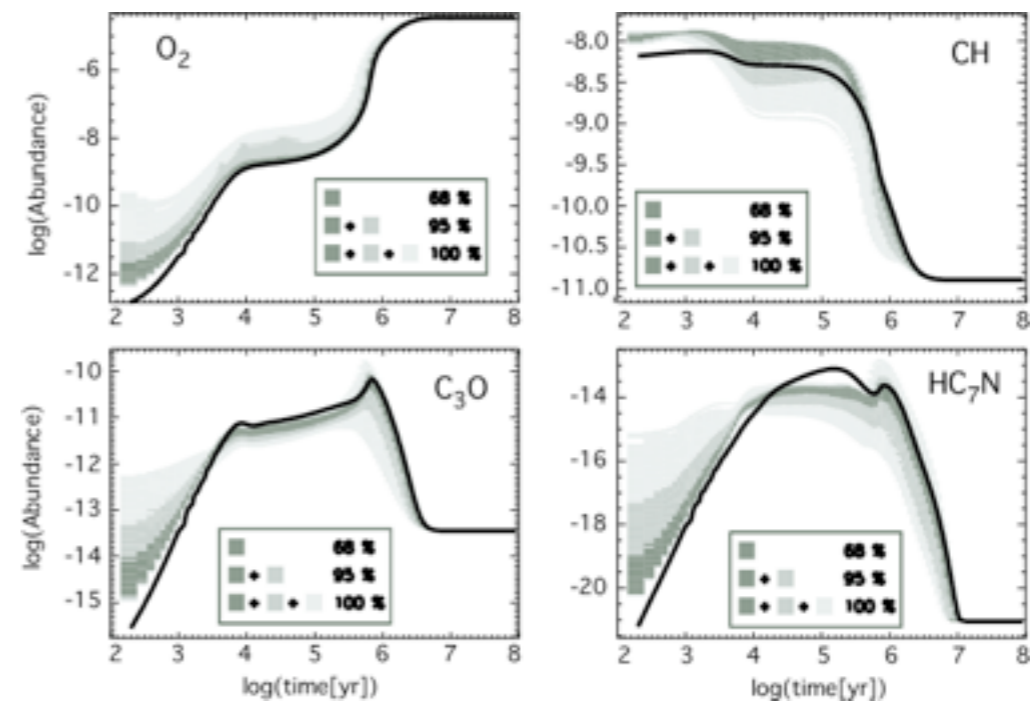
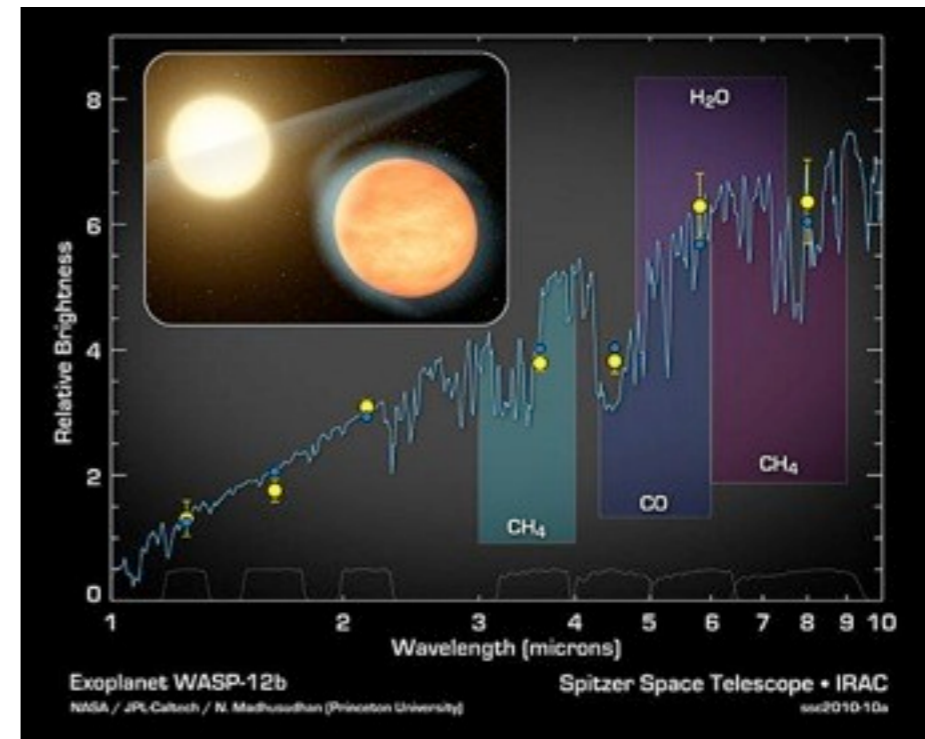
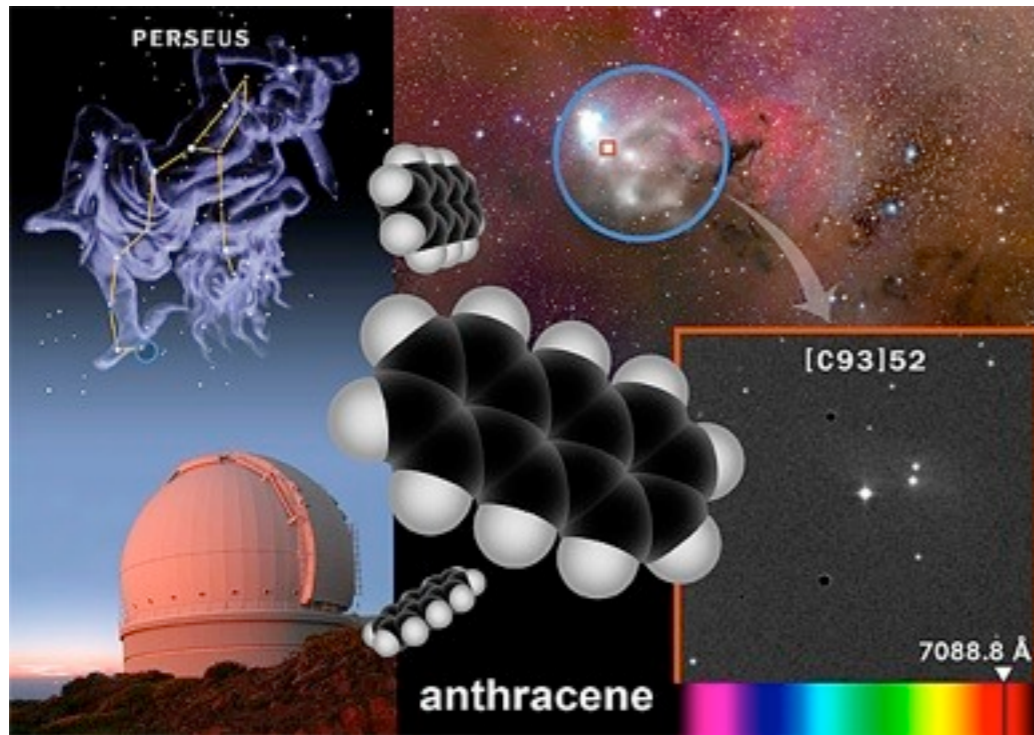


"Molecular Astrophysics: from Lab to Theory to Observations" 2012



Welcome!

- PhD and MSc students from ITA
 - ... from Max Planck Institute for Astronomy (MPIA)
 - ... from Max Planck Institute of Nuclear Physics (MPIfK)
 - ... from Astronomisches Rechen-Institut (ARI)
 - ... from HD Uni
 - others!
-
- Lectures will be accessible as PDFs online

Teachers

- Dmitry Semenov, Max Planck Institute for Astronomy (MPIA): theoretical and observational astrochemistry & astrophysics



<http://www.mpia-hd.mpg.de/homes/semenov/>

- Holger Kreckel, Max Planck Institute of Nuclear Physics (MPIfK): laboratory astrochemistry & physics



<http://www.hkreckel.de/>

Organization

- **Lectures:**

- Monday, 11:00-13:00 (10 min break?)
- April 16 till July 23
- 15–20 min for discussion of home work

- **Exam:**

- Final oral exam: Dima, Holger + 1 or 2 professors

- **Prerequisites:**

- 80% attendance
- home work
- general understanding + simple equations

Outline of the course (13 lectures)

- Molecules in space
- Molecular properties and spectroscopy
- Different ways to detect molecules
- The first 20 minutes of the Universe
- Gas-phase molecular processes and the first molecules
- Laboratory astrophysics: gas-phase experiments
- Basics of star formation and stellar nucleosynthesis
- Dust evolution and surface processes
- Laboratory astrophysics: surface and dust experiments
- Physics and chemistry of the diffuse interstellar medium
- Physics and chemistry of the dense interstellar medium
- Physics and chemistry of protoplanetary disks
- Planetary atmospheres, exoplanets, water, and life

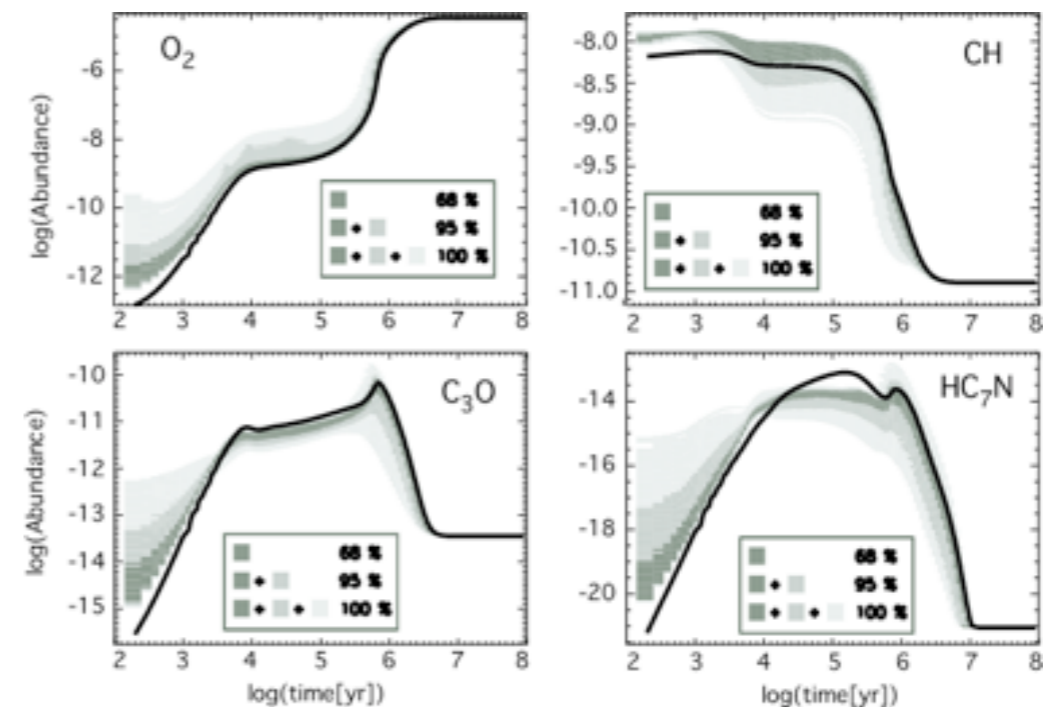
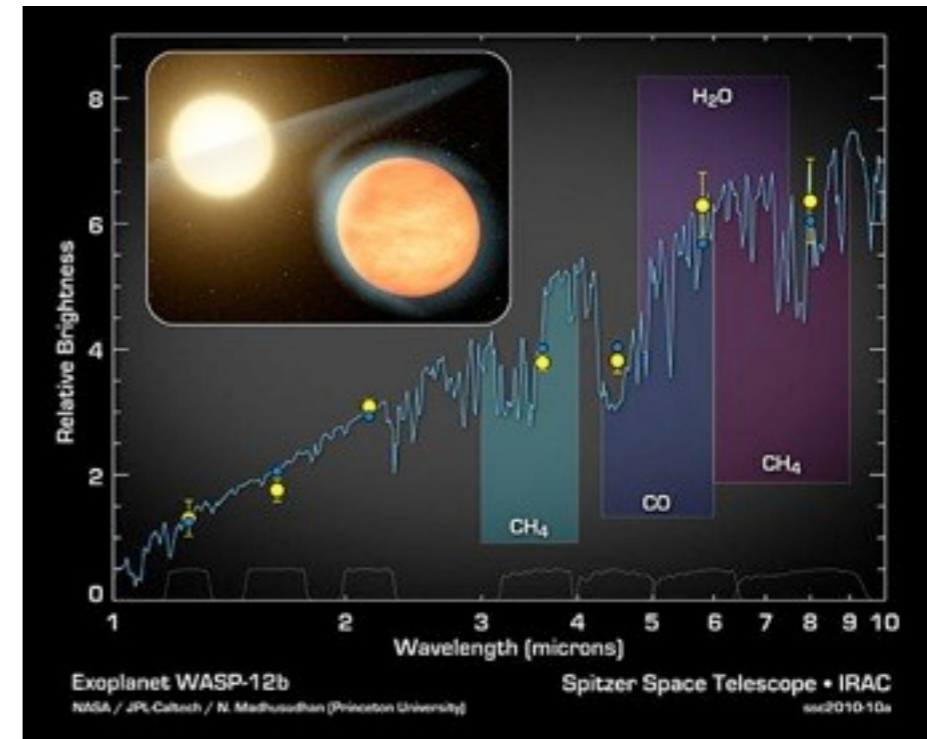
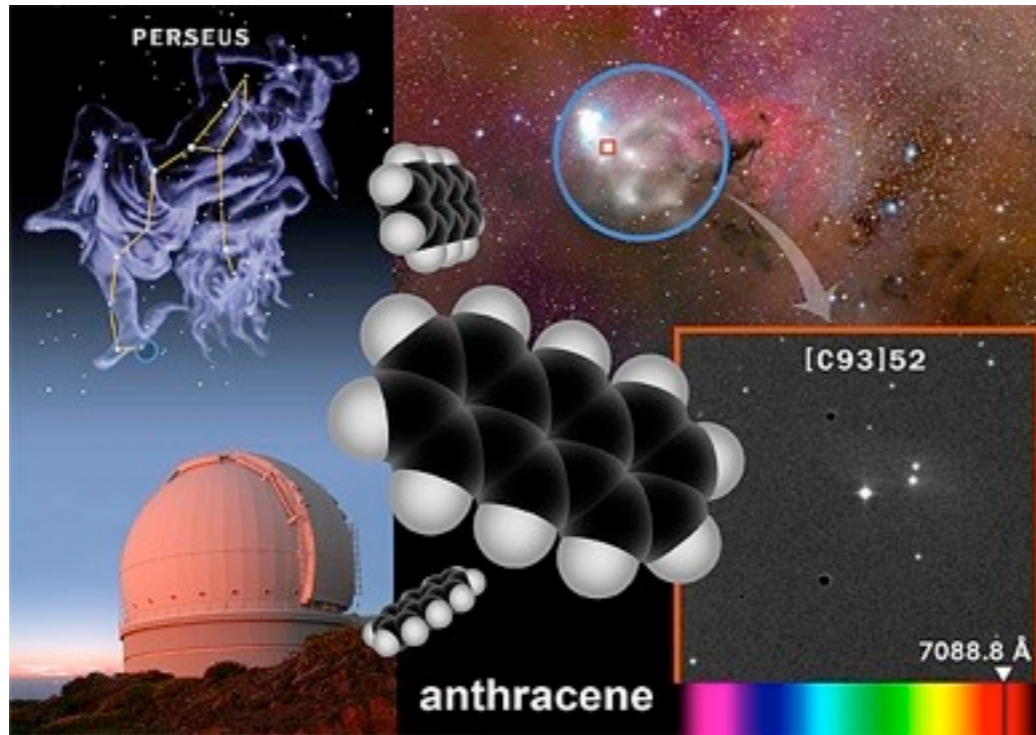
Background reading

- Relevant reviews for each lecture
- S. Kwok, "Physics and Chemistry of the Interstellar Medium" (2006)
- A. G.G.M.Tielens, "The Physics and Chemistry of the ISM" (2007)
- Master course in Astrochemistry, Ewine van Dishoeck (2011)
<http://www.strw.leidenuniv.nl/~sanjose/astrochem>
- E. Herbst & E. van Dishoeck, "Complex Organic Interstellar Molecules" (2009), Annual Rev. in Astron. & Astrophys., 47, 427
- "Protostars & Planets V" (2007), Part VI, eds. B. Reipurth et al., Univ. Arizona P.
- T. Wilson et al., "Tools of Radioastronomy" (2009), Springer

Astronomical units

- 1 pc = parsec = 206,265 AU = 3.086×10^{18} cm
- 1 M_{sun} = solar mass = 1.99×10^{33} g
- 1 L_{sun} = solar luminosity = 3.90×10^{33} erg s⁻¹
- 1 eV = 1.602×10^{-12} erg
- 1 Å = 10^{-8} cm
- 1 Jansky = 10^{-23} erg s⁻¹ cm⁻² Hz⁻¹
- 1 Debye = 10^{-18} esu cm
- 1 Kcal/mol = 6.947×10^{-14} erg atom⁻¹
- 1 year = 3.1536×10^7 s
- Proton mass = 1.6726×10^{-24} g
- Boltzmann's constant = 1.3807×10^{-16} erg K⁻¹
- Planck's constant = 6.6261×10^{-27} erg s
- see Tielens' book!

Lecture 1: Molecules in space

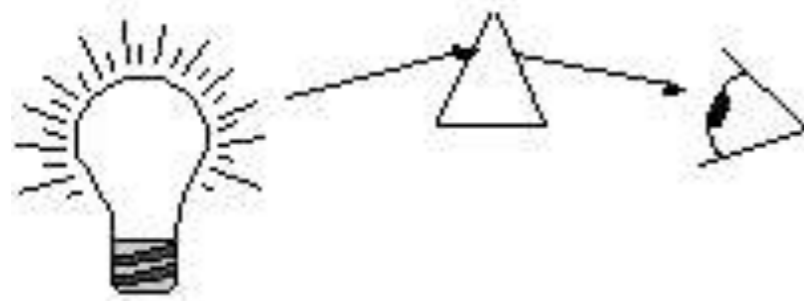


What is "molecular astrophysics"?

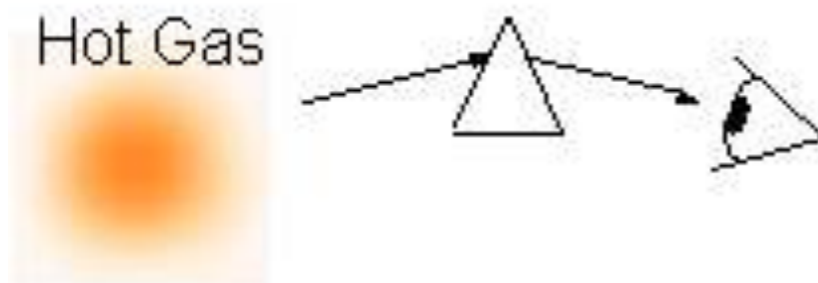
- Eddington: "Atoms are physics but molecules are chemistry"
- Molecular astrophysics (or astrochemistry) is the study of formation and destruction of molecules in the Universe, their interaction with radiation, and their feedback on physics of the environments"
- Interdisciplinary field: chemistry + physics + astronomy (+biology?)
- Observations (UV-millimeter), theoretical (astro)physics and chemistry, and laboratory astrochemistry

Detecting molecules

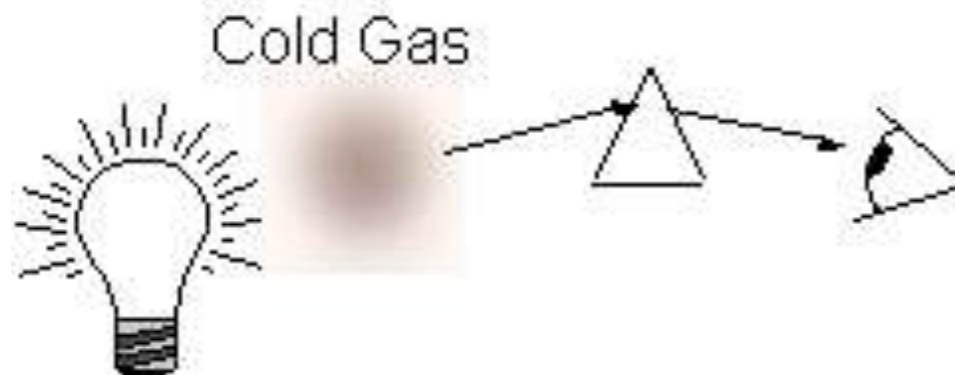
- Absorption: UV, optical, IR
- Emission: (sub-)millimeter
- Gas-phase & ices



Continuum Spectrum



Emission Line Spectrum

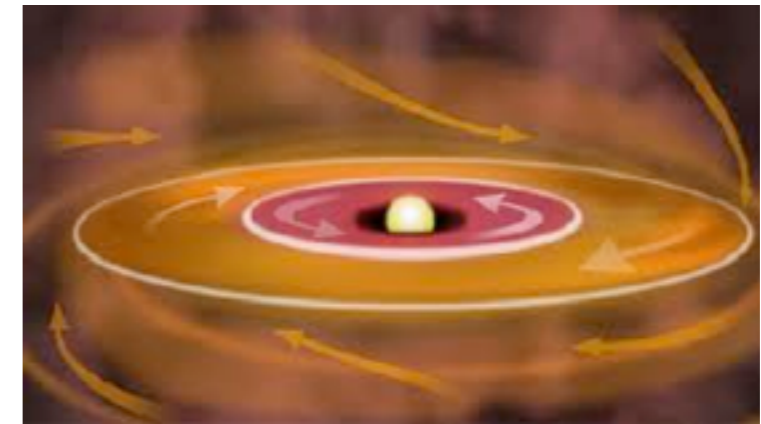
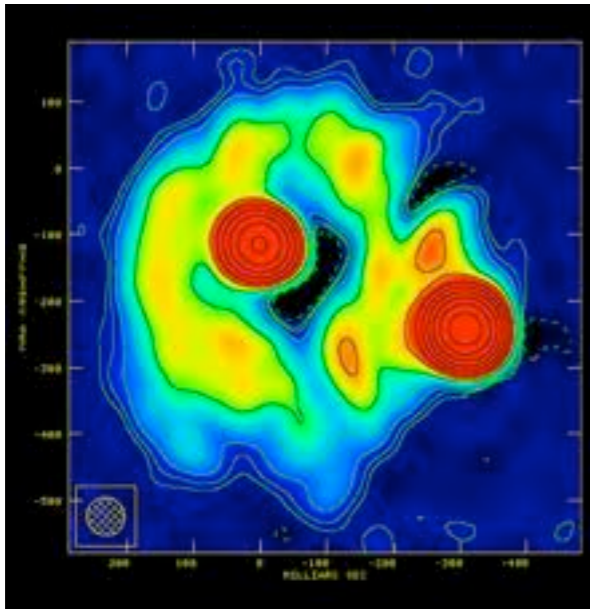


Absorption Line Spectrum



Molecules are everywhere!

- Molecules are found everywhere in the Universe:
 - Appeared in the Early Universe, \sim few min after Big Bang
 - High-z quasars and galaxies
 - Milky Way: interstellar and circumstellar medium
 - Solar system: solar photosphere, planetary atmospheres, comets, meteorites

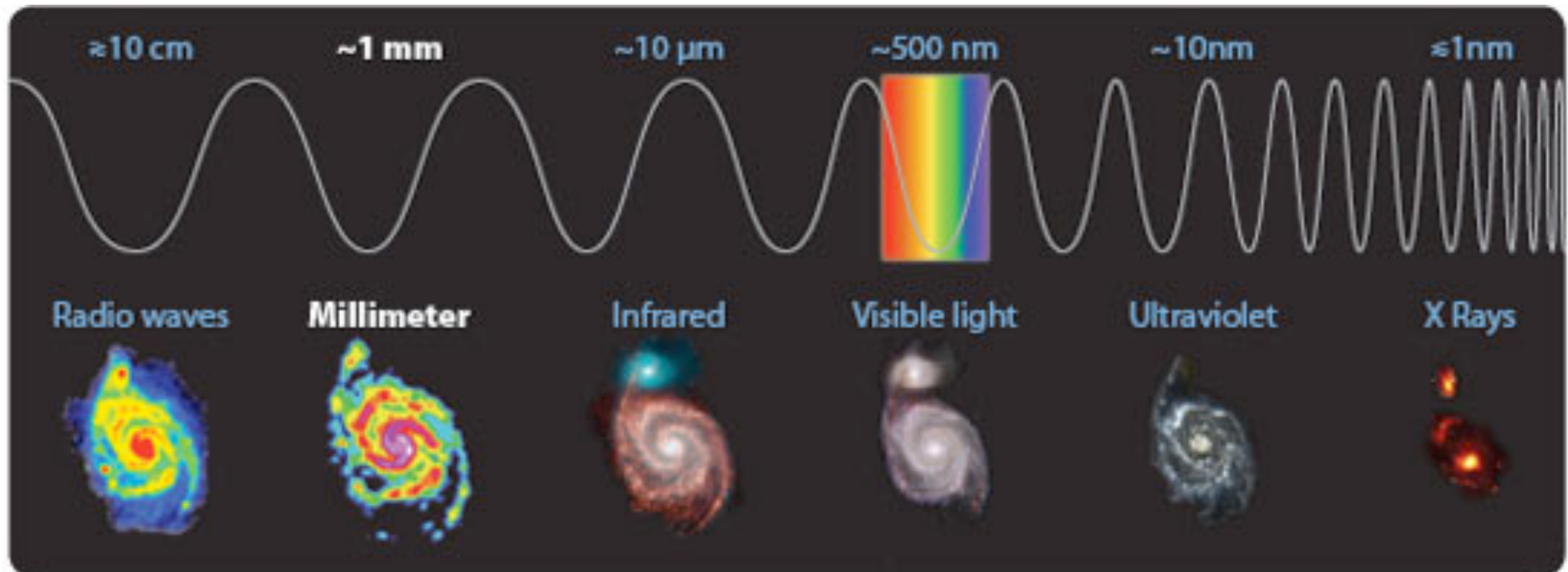


Importance of molecules

- Unique probes of physical conditions:
 - T_{kin} , density
 - Ionization
- Unique probes of kinematics
- Chemical composition and evolution
- Coolants of gas

Detecting molecules

- Molecular lines: (far-)UV–millimeter wavelengths
- Rotational, vibrational, electronic transitions (and their combination)
- Atmosphere transparency windows at IR: blocked by OH, H₂O, etc.



Physical conditions in various astrophysical objects

- Diffuse clouds: $T_{\text{kin}} \sim 100 \text{ K}$, $n \sim 100 \text{ cm}^{-3}$
- Dense clouds: $T_{\text{kin}} \sim 10\text{--}100 \text{ K}$, $n \sim 10^4\text{--}10^8 \text{ cm}^{-3}$
- Hot cores: $T_{\text{kin}} \sim 100\text{--}1000 \text{ K}$, $n \sim 10^6\text{--}10^8 \text{ cm}^{-3}$
- Protoplanetary disks: $T_{\text{kin}} \sim 10\text{--}1000 \text{ K}$, $n \sim 10^4\text{--}10^{13} \text{ cm}^{-3}$
- Circumstellar shells of evolved stars: $T_{\text{kin}} \sim 300\text{--}3,000 \text{ K}$, $n < 10^{14} \text{ cm}^{-3}$
- More: HII regions, photo-dissociation regions, supernova remnants, ...

- Earth atmosphere at sea level: $T_{\text{kin}} \sim 300 \text{ K}$, $n \sim 3 \cdot 10^{19} \text{ cm}^{-3}$

Typical timescales

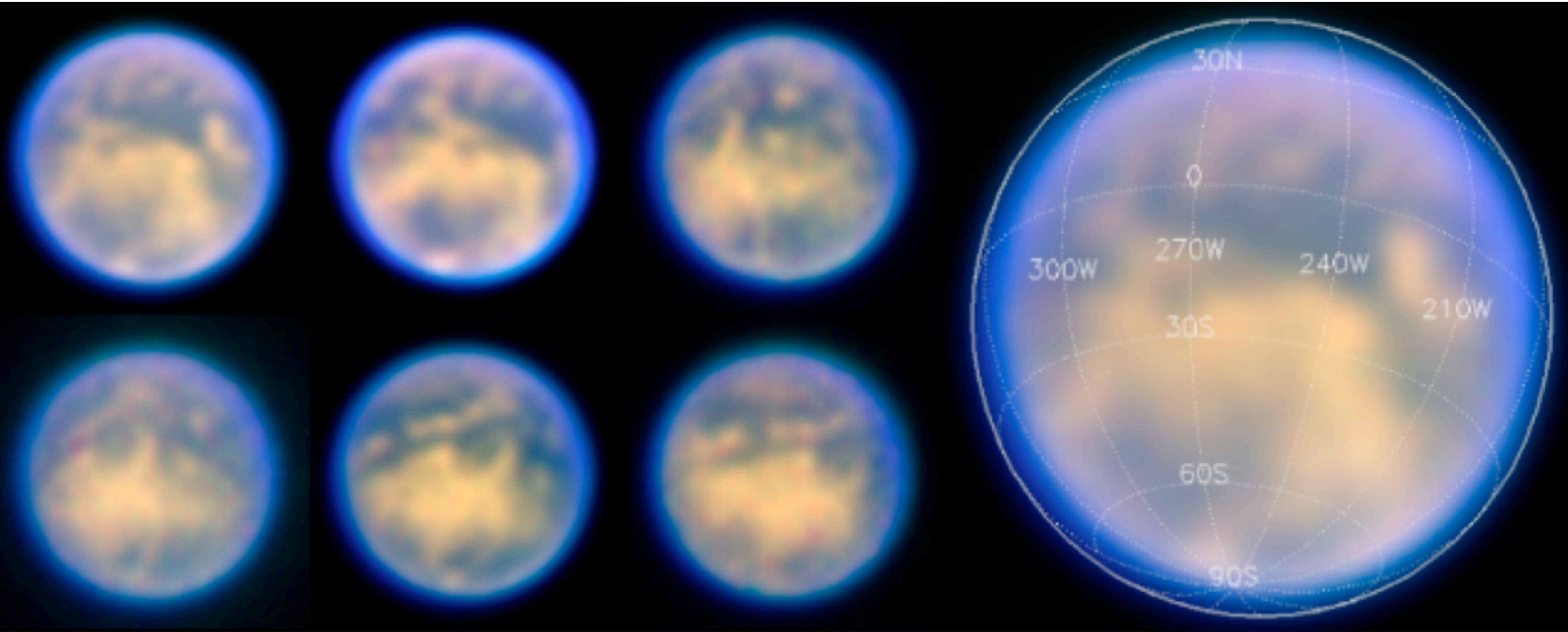
- Collision time: ~ 1 month at 10 K and 10^4 cm^{-3}
- Chemical time: $> 10^4 - 10^5$ years (molecular clouds)
- Life-time of a cloud: $\sim 1 - 10 \times 10^6$ years
- Low-mass star formation: $\sim 10^6$ years

Chemistry is slow yet there are many molecules in the interstellar medium!

Molecularly-rich environments

- Titan, 10 AU
- Taurus molecular complex (TMC): low-mass, 140 pc
- Orion molecular cloud: high-mass, ~450 pc
- AB Aur protoplanetary disk, ~140 pc
- IRC +10216 (CW Leo), evolved C-rich star, ~120–150 pc
- Sagittarius B2: a ring of molecular clouds, Galactic center, ~8.2 kpc
- Andromeda Galaxy (M31), nearest spiral galaxy, ~1 Mpc
- J 1148+5251, quasar at $z=6.4$ (~6.9 Gpc)

Titan



- Near-IR, NACO at the Very Large Telescope (VLT)

Taurus Molecular Cloud



- Optical + near-IR, Digitized Sky Survey (DSS) 2

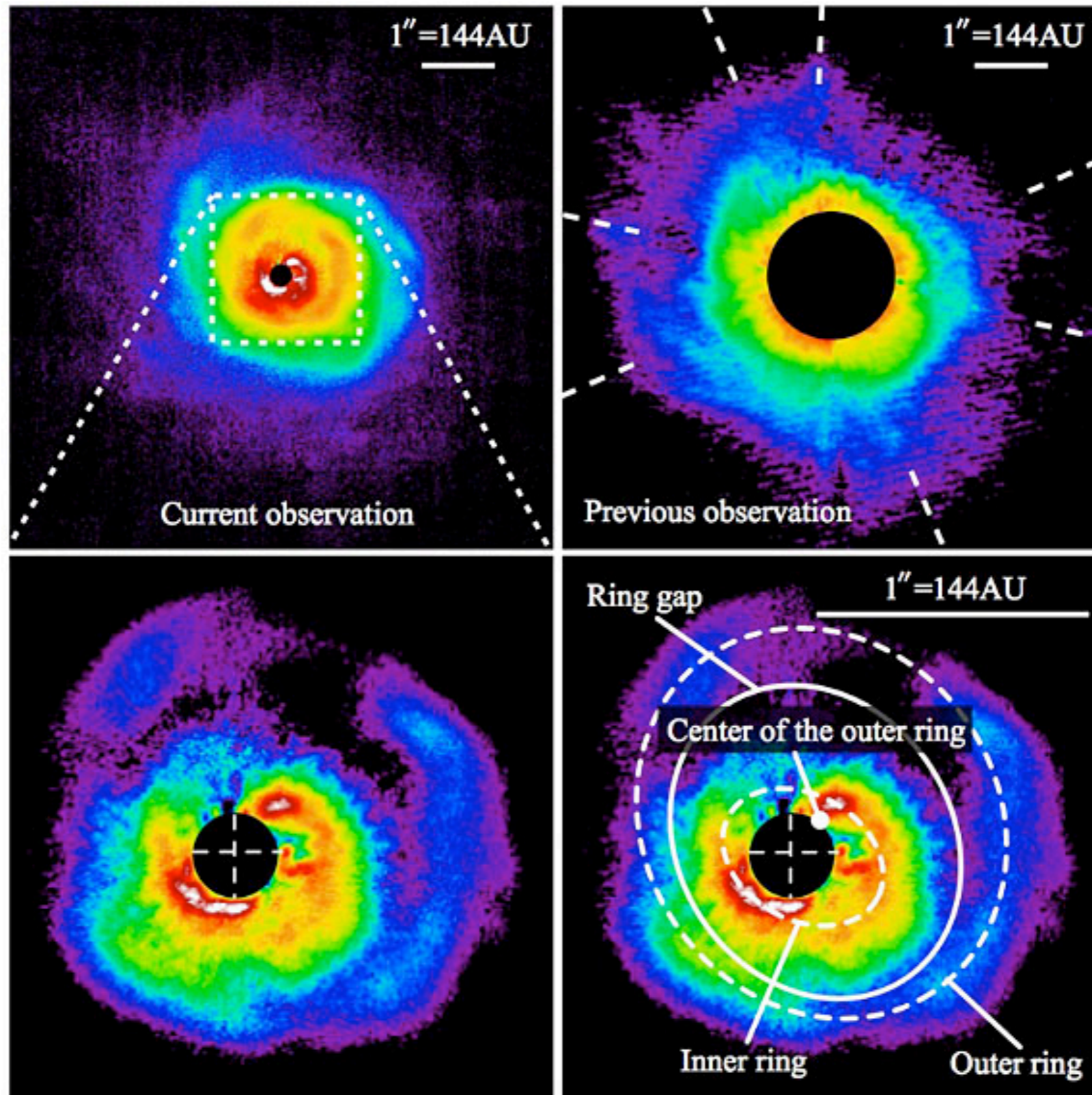
Orion Molecular Cloud



PANORAMICUNIVERSE.COM

- Optical, Hubble Space Telescope

Protoplanetary disk around AB Aur



- Near-IR, HiCIAO, Subaru

CW Leo (IRC +10216)



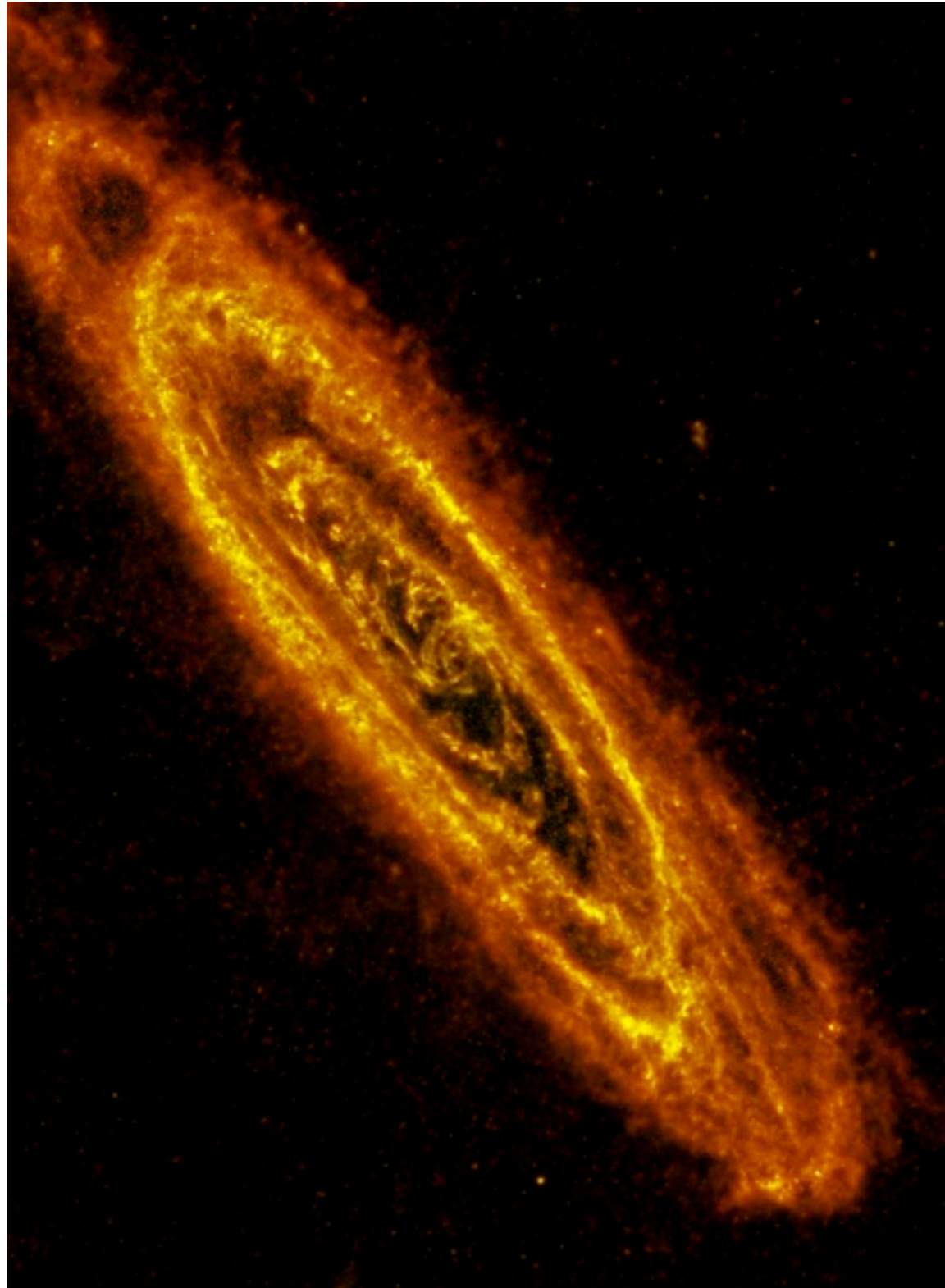
- 50-210 μm (FIR), PACS and SPIRE, Herschel

Sagittarius B2



ATLASGAL, submillimeter (red) + Midcourse Space Experiment (MSX), IR (green and blue)

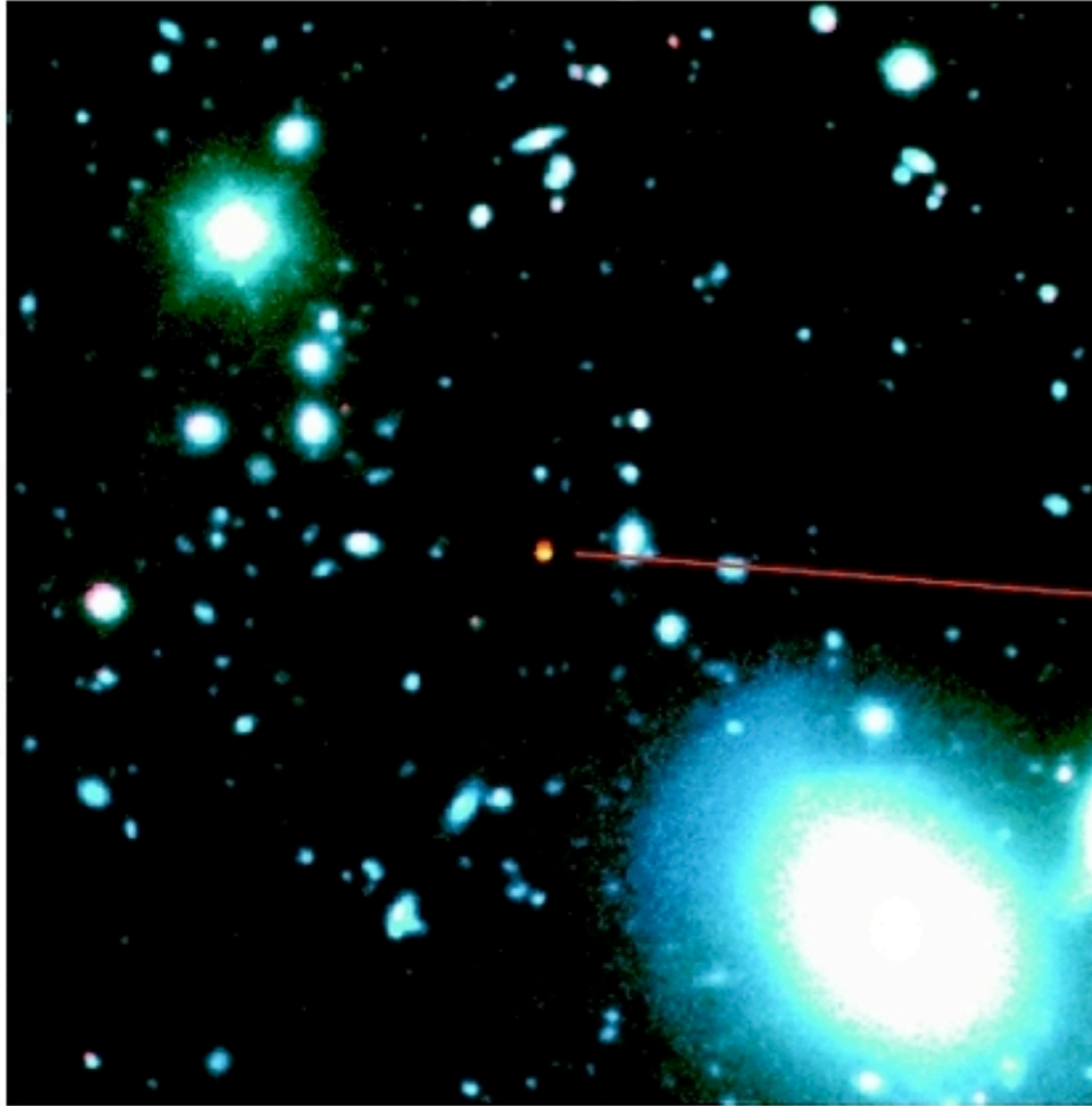
Andromeda Galaxy (M31)



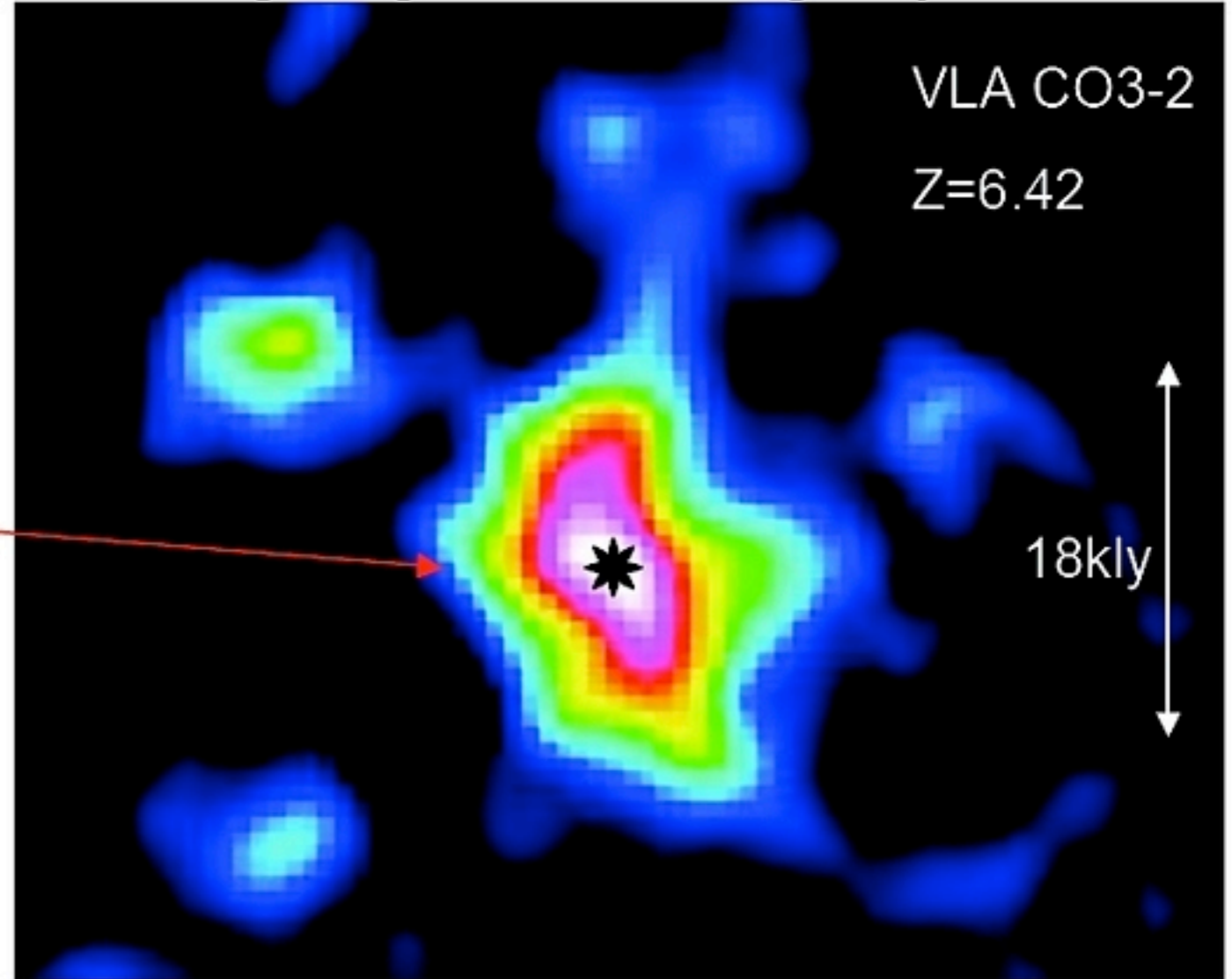
FIR, Spire, Herschel

J 1148+5251

Sloan Discovery Image



VLA image of giant molecular galaxy

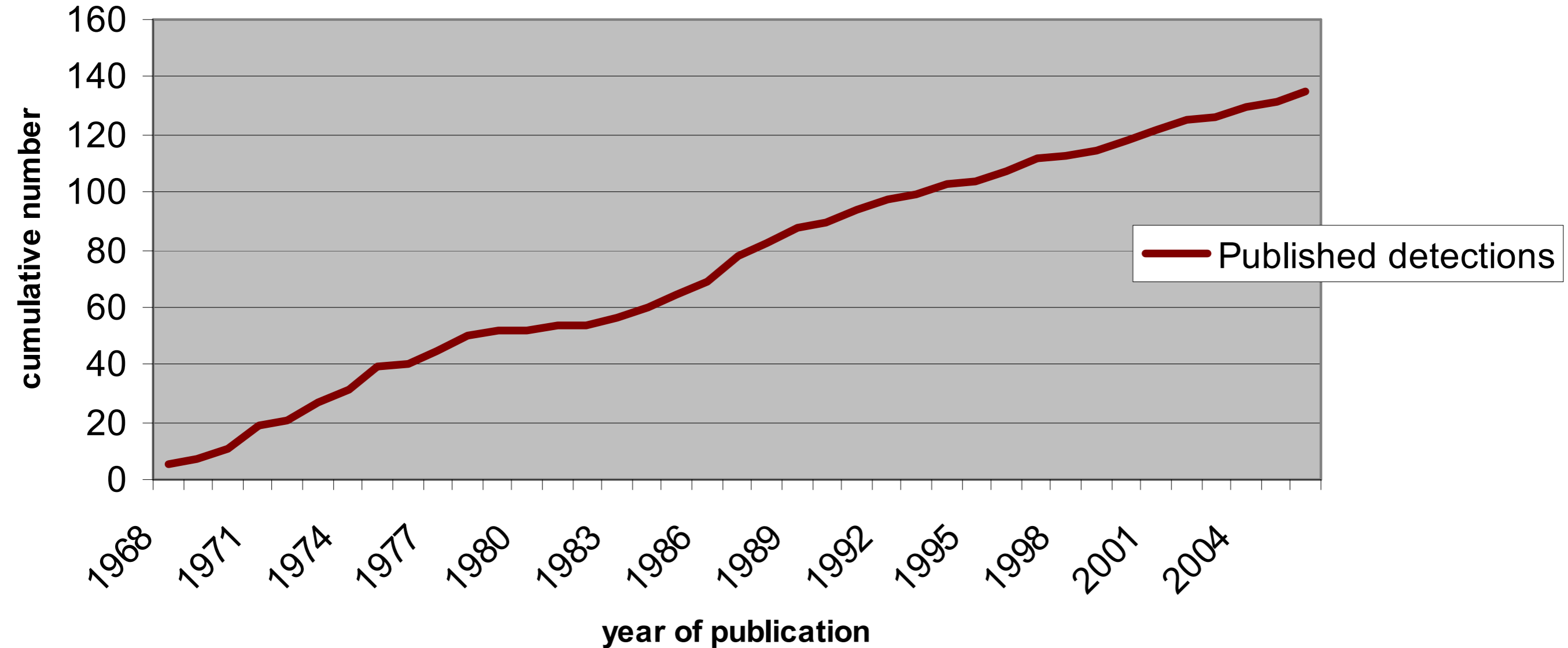


J1148+5251: Coeval formation of a super massive black hole and giant elliptical galaxy within 870Myr of the Big Bang

Pause

History of molecules in space

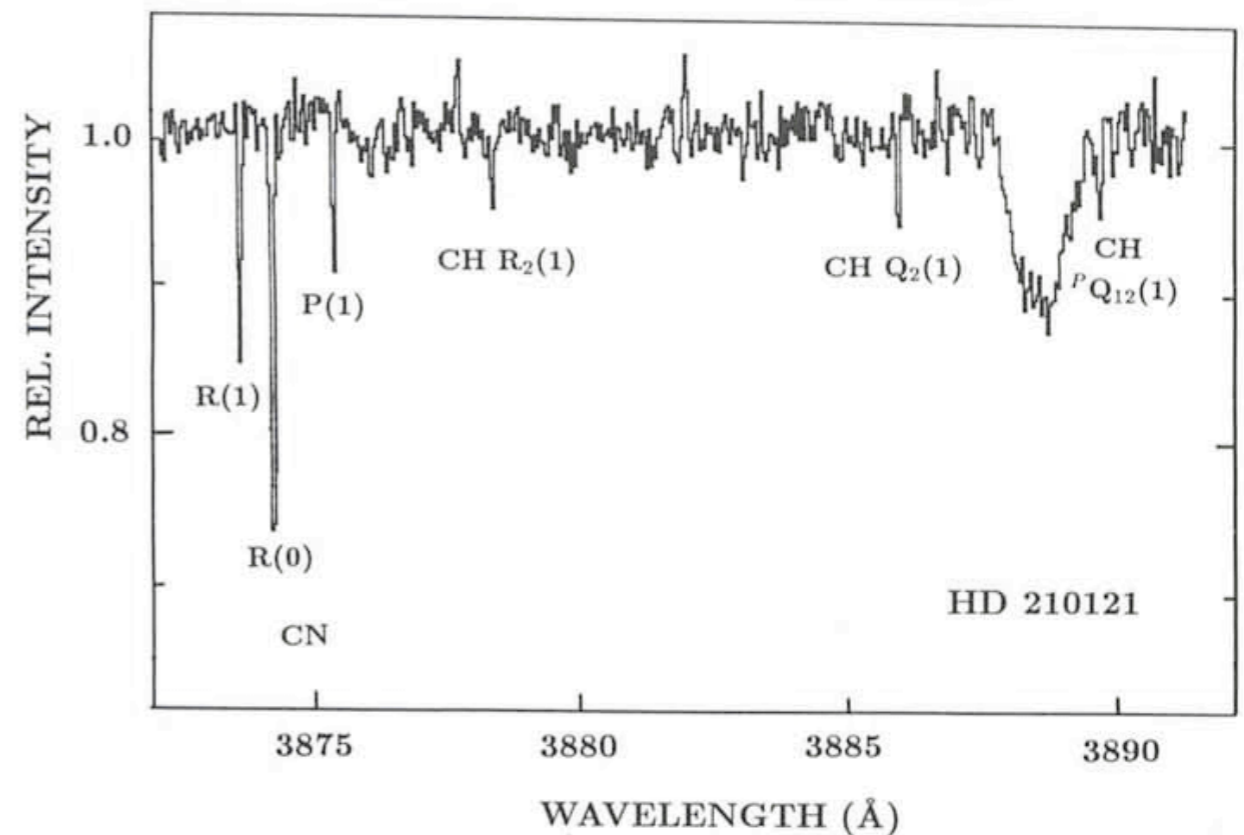
INTERSTELLAR & CIRCUMSTELLAR MOLECULES (May 2006)



History of molecules in space

- Diffuse Interstellar Bands (DIBs), optical:
 - Discovered by Heger (1922) and Merrill (1934):
 - Remains unidentified till 2012 (polyaromatic hydrocarbons?)

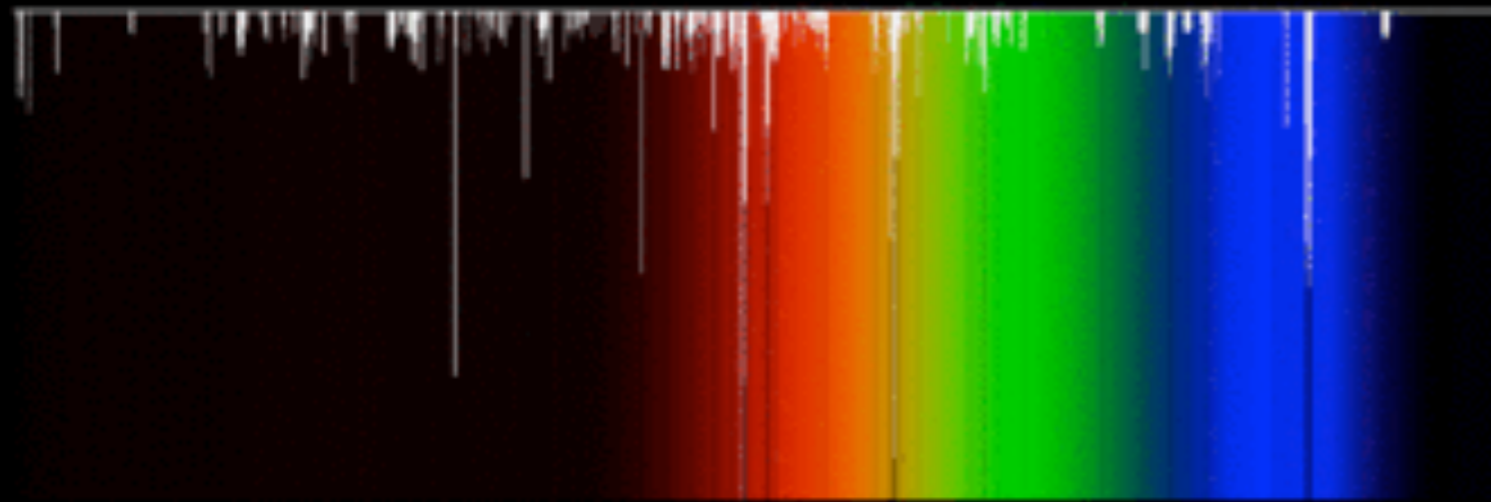
- Sharp absorption bands (optical):
 - CH: Swings & Rosenfeld (1937)
 - CN: McKellar (1940)
 - CH⁺: Douglas & Herzberg (1941)



- First theory by Bates and Spitzer (1951), Herbst & Klemperer (1973)

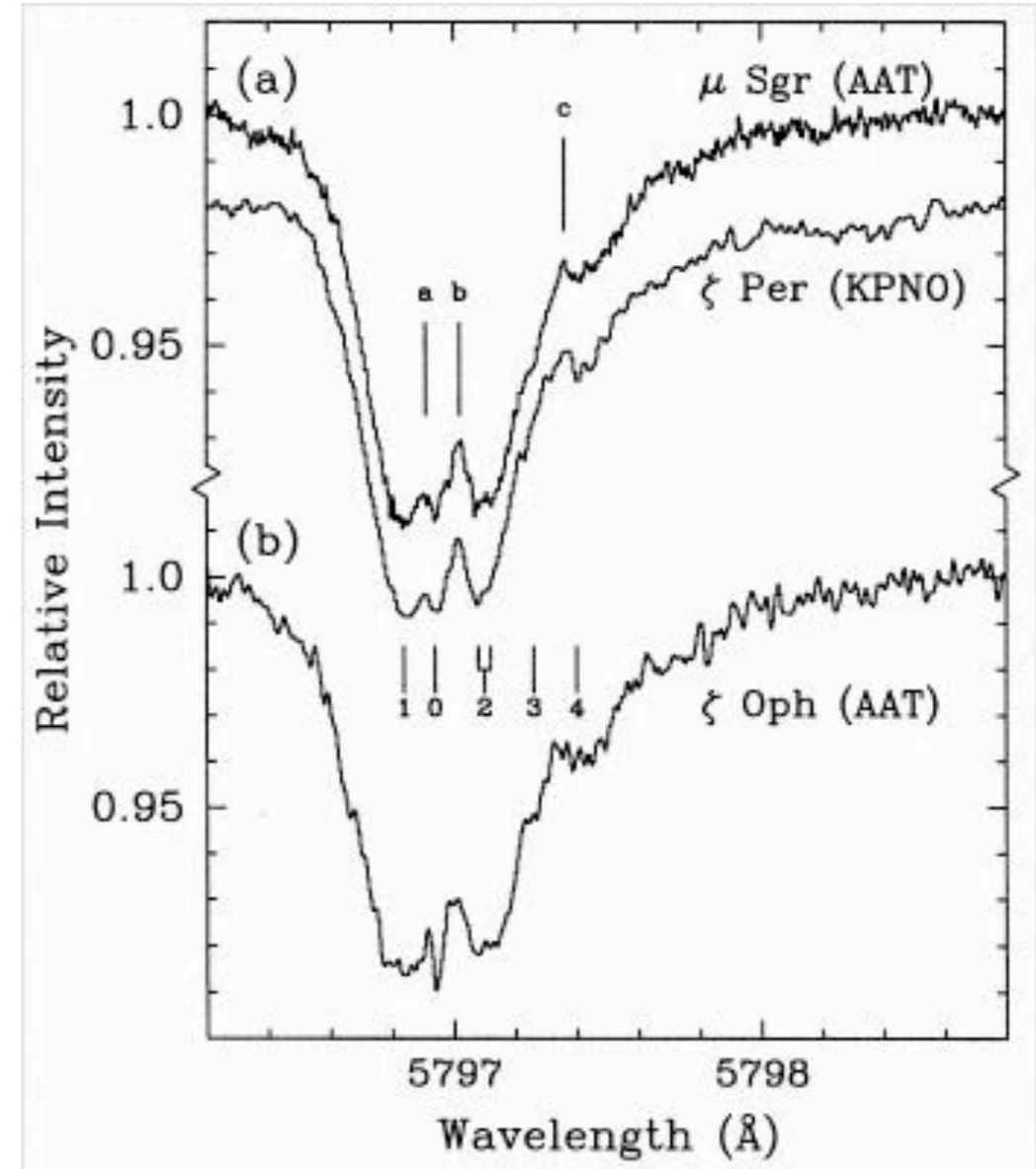
Diffuse Interstellar Bands

The Diffuse Interstellar Bands



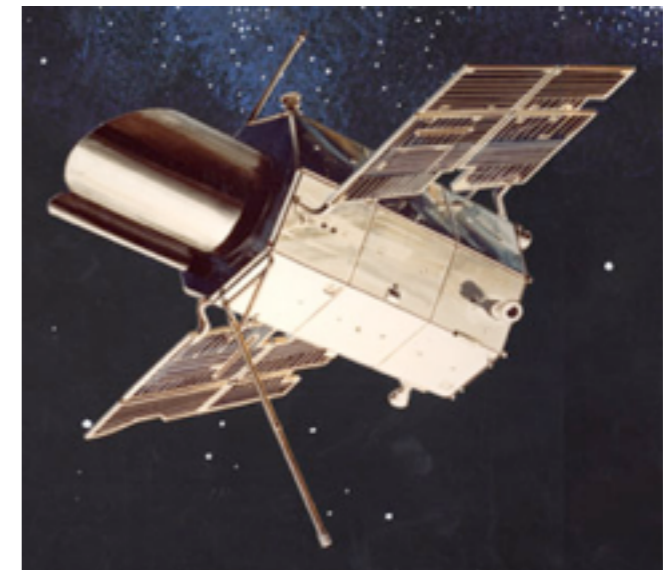
Courtesy P. Jenniskens, F.-K. Deort

- >400 (UV–near IR), very sharp, <1 nm
- Strengths of DIBs do not correlate
- Present consensus:
 - large gas-phase molecules (PAHs?)
 - likely carbon-based
 - not dust (fine structures in spectra), albeit correlate with A_V

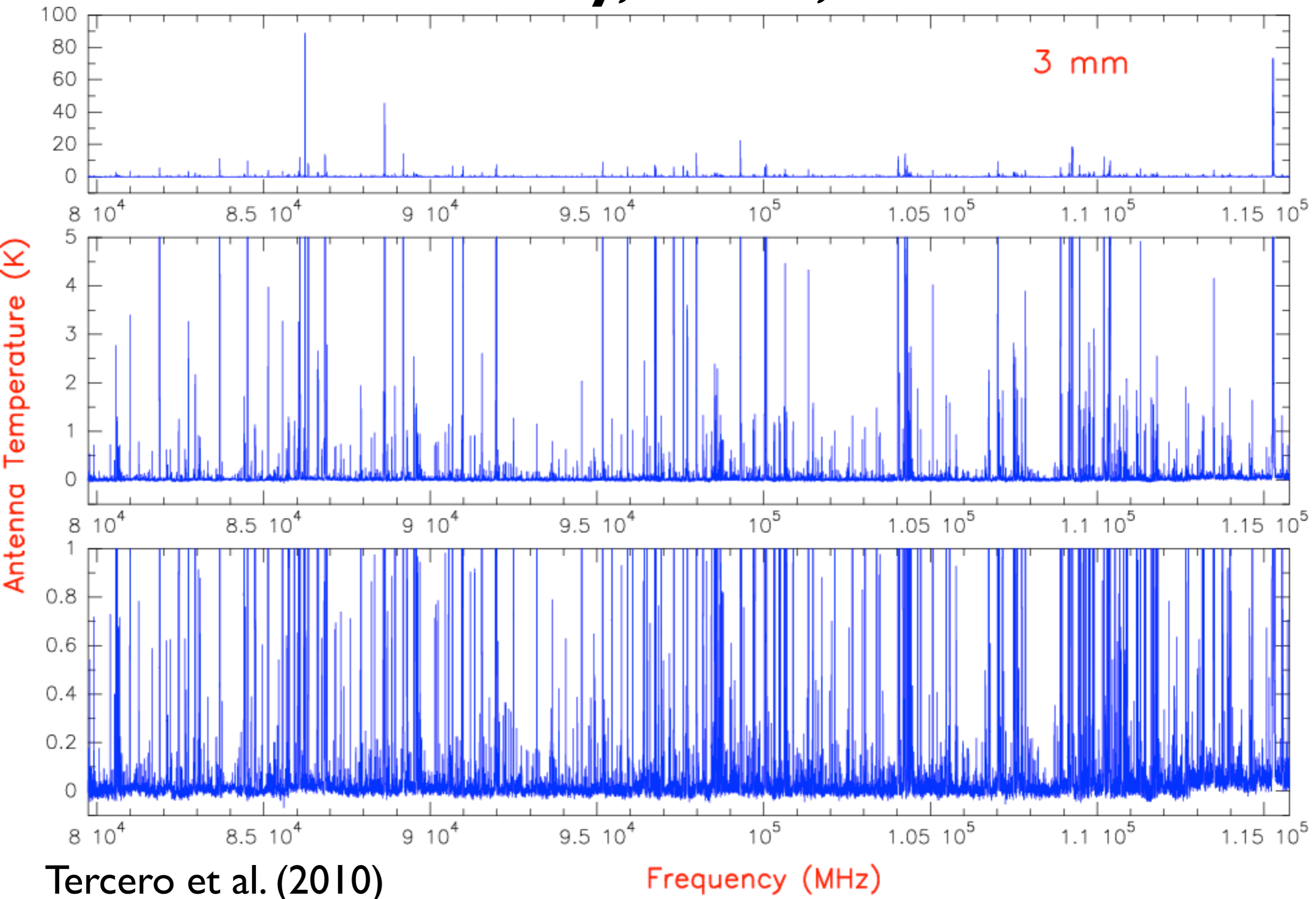


History of molecules in space

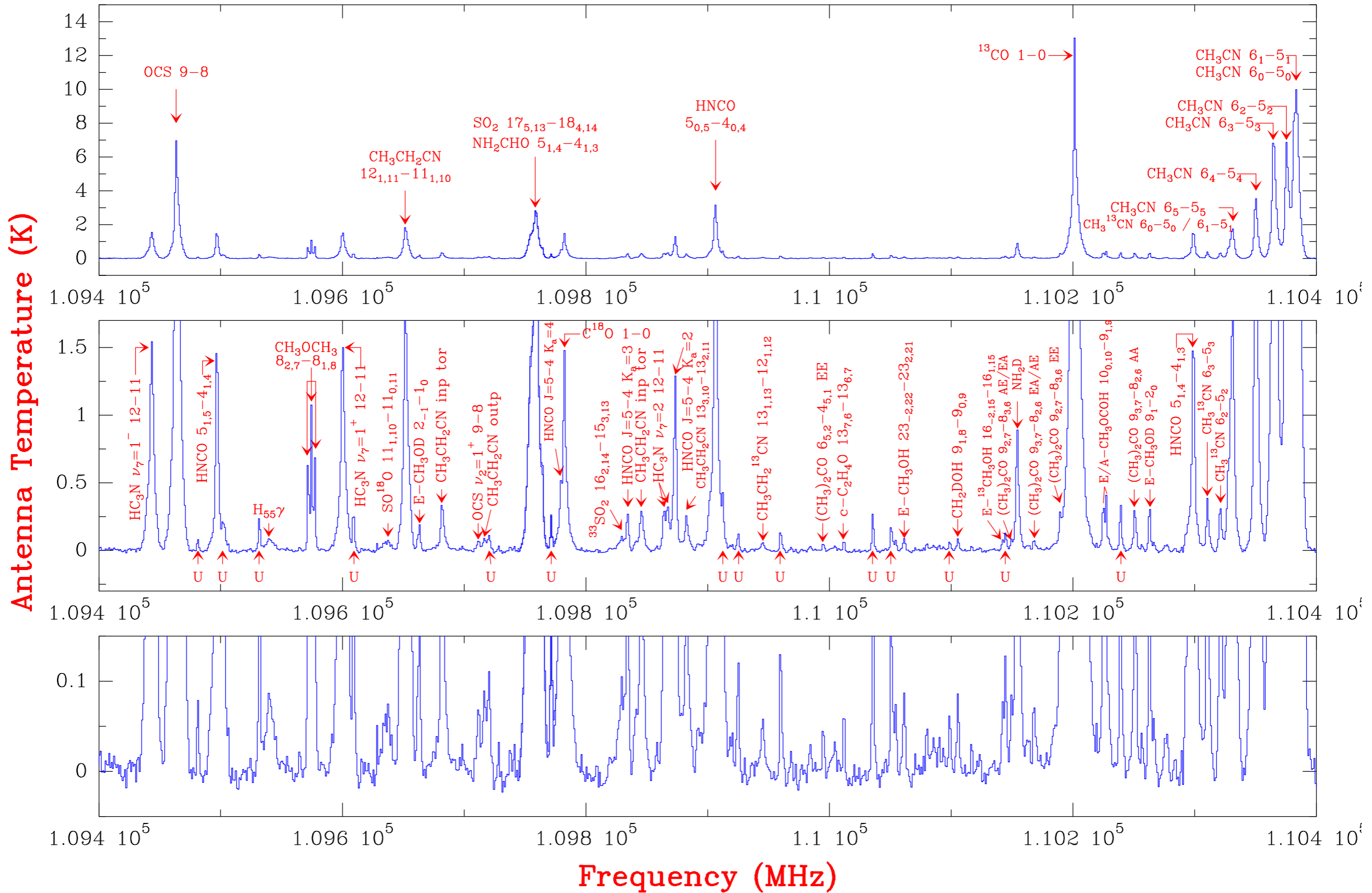
- Radio telescopes:
 - H I 21 cm: Ewen & Purcell (1951)
 - OH 18 cm: Weinreb et al. (1963)
 - NH₃ 1 cm: Cheung, Townes et al. (1968)
 - H₂O 1 cm: Cheung et al. (1969)
- UV telescopes: Copernicus (1970): H₂ at ~125nm (1970), later N₂
- (Sub-)millimeter telescopes: CO at 115 GHz (1970), H₂CO (1970), and many others



Orion KL Survey, 3 mm, IRAM 30-m

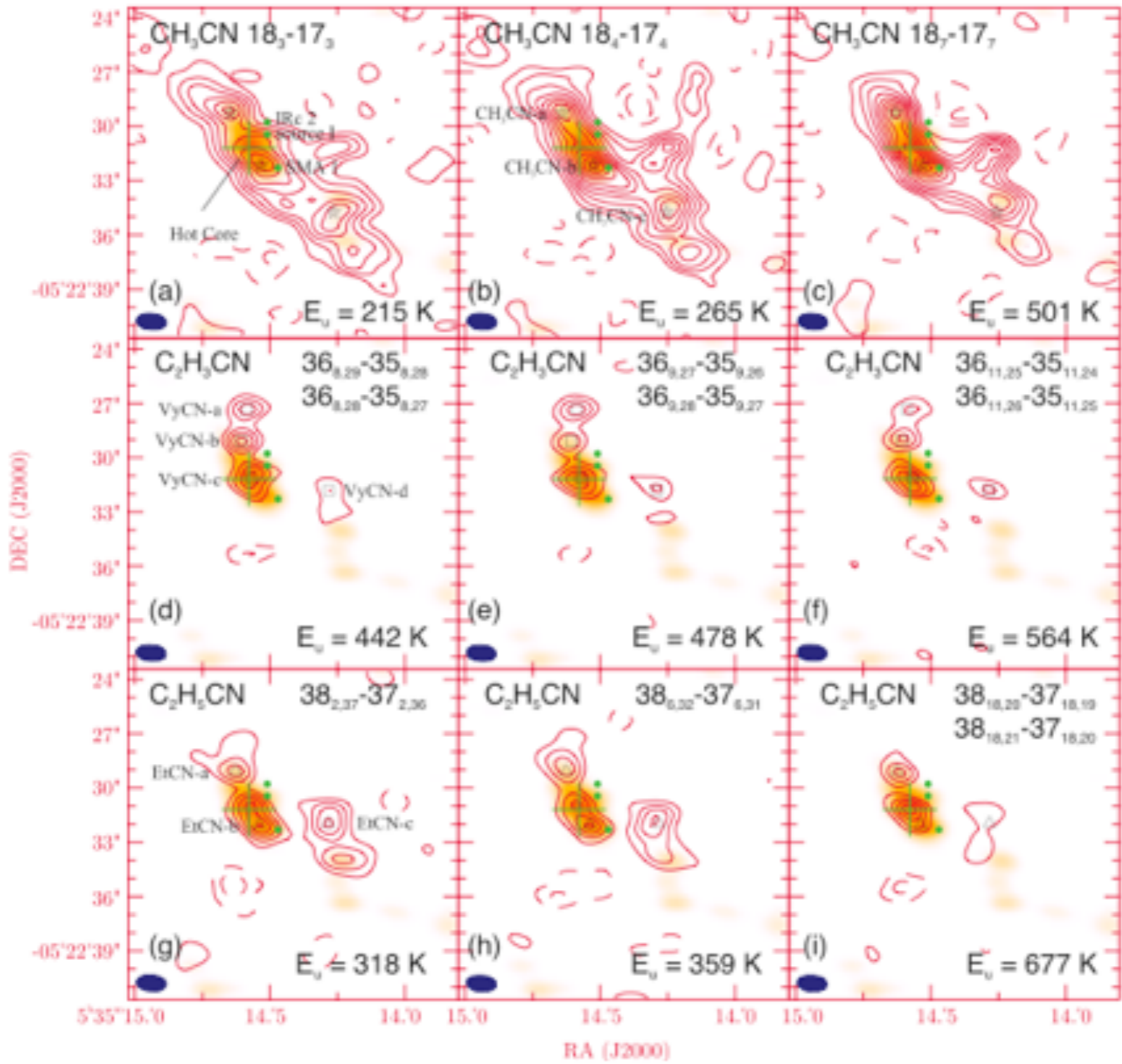


Orion KL Survey, 3 mm, IRAM 30-m



Tercero et al. (2010)

Orion KL map, Imm, Submillimeter Array

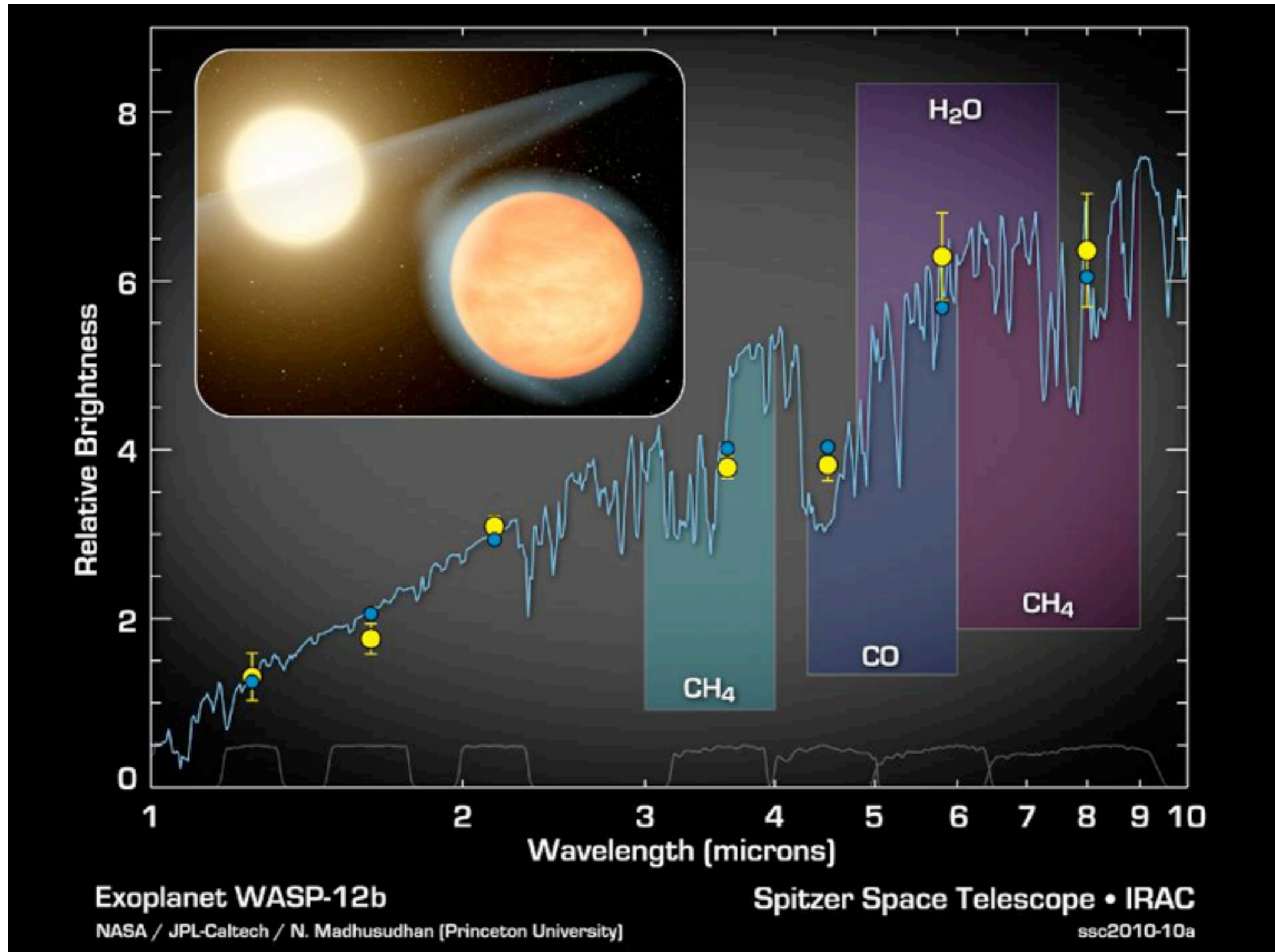


Wang et al. (2008)

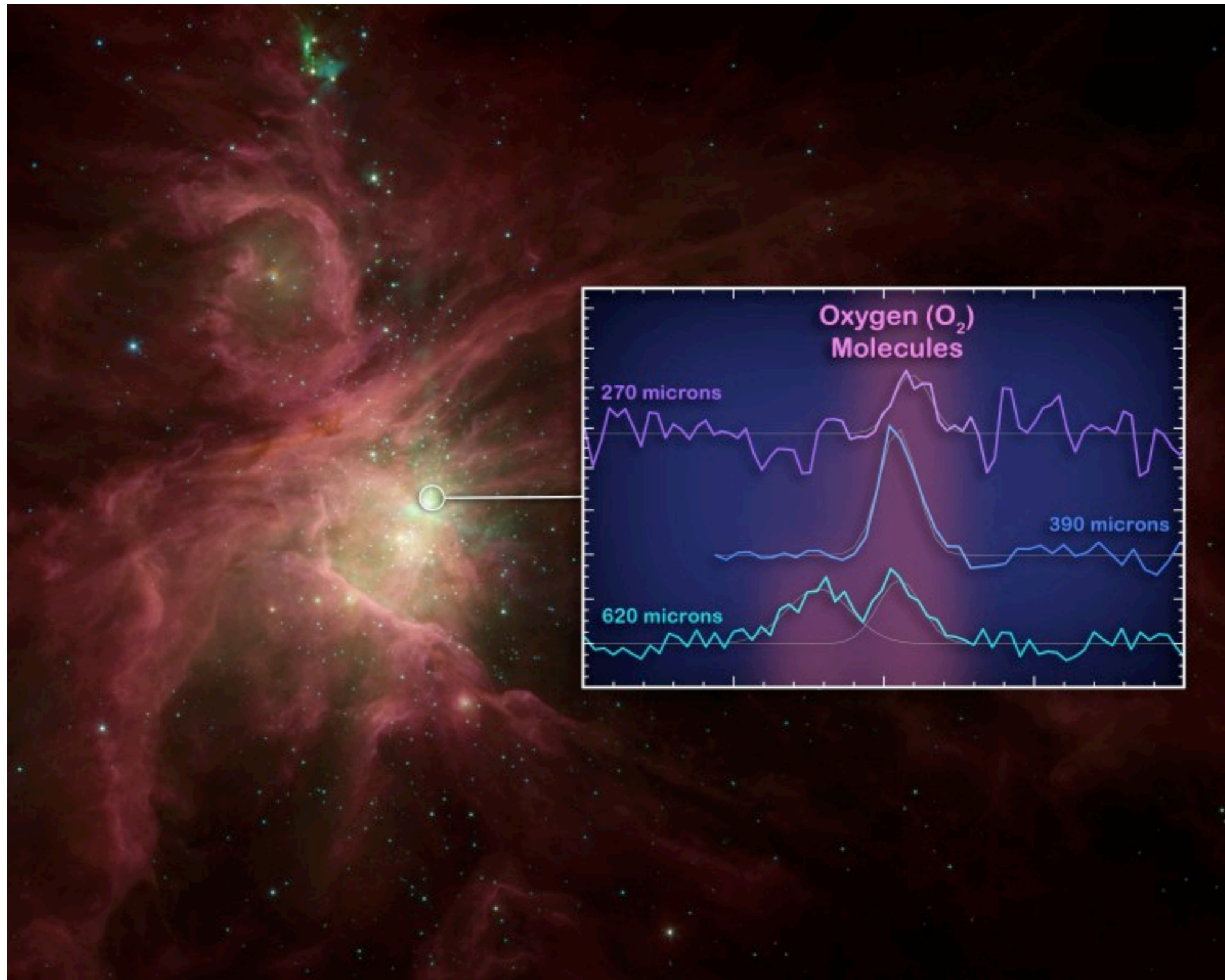
History of molecules in space

- IR telescopes:
 - IRAS (1983): 0.6 m, 12–100 μm , first sky survey, dust (β Pictoris disk)
 - Infrared Space Observatory (1995–1998): 0.6 m, 2.5–240 μm , dust & molecules (H_2O , HF, OH, OI, C_6H_6 , CH_3 , CO_2 , ...), infrared cirrus clouds
 - Spitzer Space Telescope (2003–2009): 0.8 m, 3–180 μm , high-sensitivity imaging and mapping, dust & molecules (OH, H_2O , C_2H_2 , ...)
 - Herschel Space Observatory (2009–2012): 2.4 m, 60–670 μm , high-sensitivity imaging and mapping, dust & molecules (CH_3OH , H_2S , HCN, SO_2 , H_2CO , H_2O , ...)
 - Ground-based: Keck, VLT, ...

Molecules, exoplanet WASP-12b, Spitzer



O₂ in Orion, 487–1121 GHz, Herschel



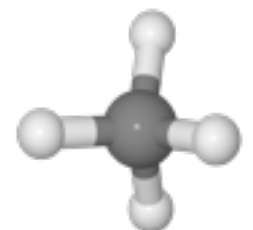
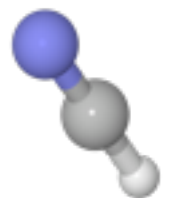
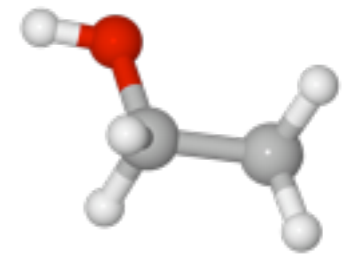
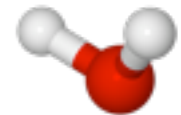
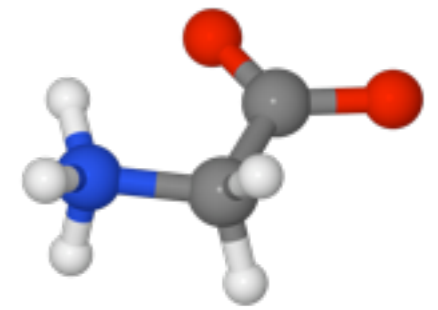
Goldsmith et al. (2011)

Detected molecules (~170)

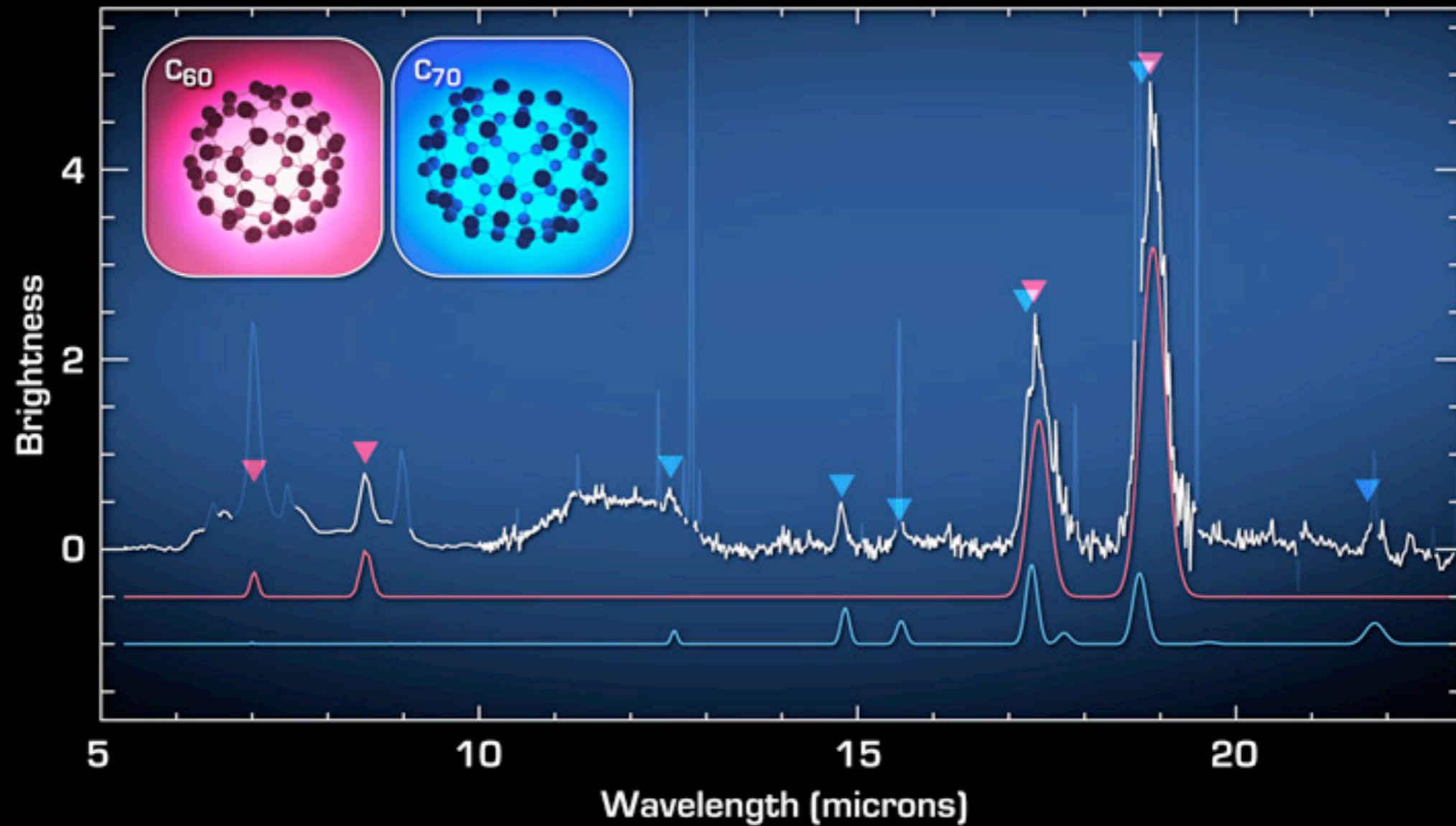
H2	H3+	CH3	CH4	CH3OH	CH3NH2	HCOOCH3	(CH3)2O	(CH3)2CO
CO	CH2	NH3	CH2NH	CH3SH	CH3CCH	CH3C3N	C2H5OH	CH3C5N
CS	NH2	H3O+	H2CCC	C2H4	CH3CHO	HC6H	C2H5CN	CH3CH2CHO
CN	H2O	H2CO	c-C3H2	CH3CN	c-CH2OCH2	C7H	CH3C4H	(CH2OH)2
C2	H2S	H2CS	CH2CN	CH3NC	CH2CHCN	HOCH2CHO	C8H	HCOOC2H5
CH	CCH	c-C3H	NH2CN	CH2CHO	HC5N	CH3COOH	HC7N	HC9N
CH+	HCN	I-C3H	CH2CO	NH2CHO	C6H	H2CCCHCN	CH3CONH2	CH3C6H
HF	HNC	C2H2	HCOOH	HC3NH+	CH2CHOH	H2C6	CH3CHCH2	C6H6
CF+	HCO	HCNH+	C4H	H2CCCC	C6H-	CH2CHCHO	C8H-	C3H7CN
SiO	HCO+	H2CN	HC3N	C5H		NH2CH2CN		HCIIN
SiS	HOC+	HCCN	HCCNC	HC4H				C2H5OCH3
SiC	N2H+	HNCO	HNCCC	HC4N				
SiN	HNO	HOCN	H2COH+	c-C3H2O				
NH	HCS+	HCNO	C4H-	CH2CNH				
NO	C3	HNCS	SiH4	C5N-				
SO	C2O	HSCN	C5	C5N				
SO+	C2S	C3N	SiC4					
CP	SO2	C3O	CNCHO					
PO	N2O	C3S						
PN	CO2	C3N-						
HCl	H2O+	HCO2+						
KCl	H2Cl+	CNCHO						
AlCl	OCS	C-SiC2						
OH	MgNC				AlF	AlNC	AlOH	NaCl
OH+	MgCN				SiNC	CCP	HCP	FeO
SH	NaCN				CO+	O2	N2	
CN-	SiCN							

Detected molecules

- 170 interstellar & circumstellar molecules
- 41 extragalactic molecules
- Up to 11 atoms (since 2010 => 70)!
- 20 positive ions (cations)
- 6 negative ions (anions)
- ~30 free radicals
- ~20 isomers
- 6 linear and 6 cyclic species (including simplest PAH, C₆H₆)
- 11 Si-, 6 P-, and 5 Cl-bearing species
- 11 metal-bearing species
- 10 species with deuterium
- Organic molecules: ethers, acids, alcohols, aldehydes, ...



Detection of fullerenes (C_{60} & C_{70})



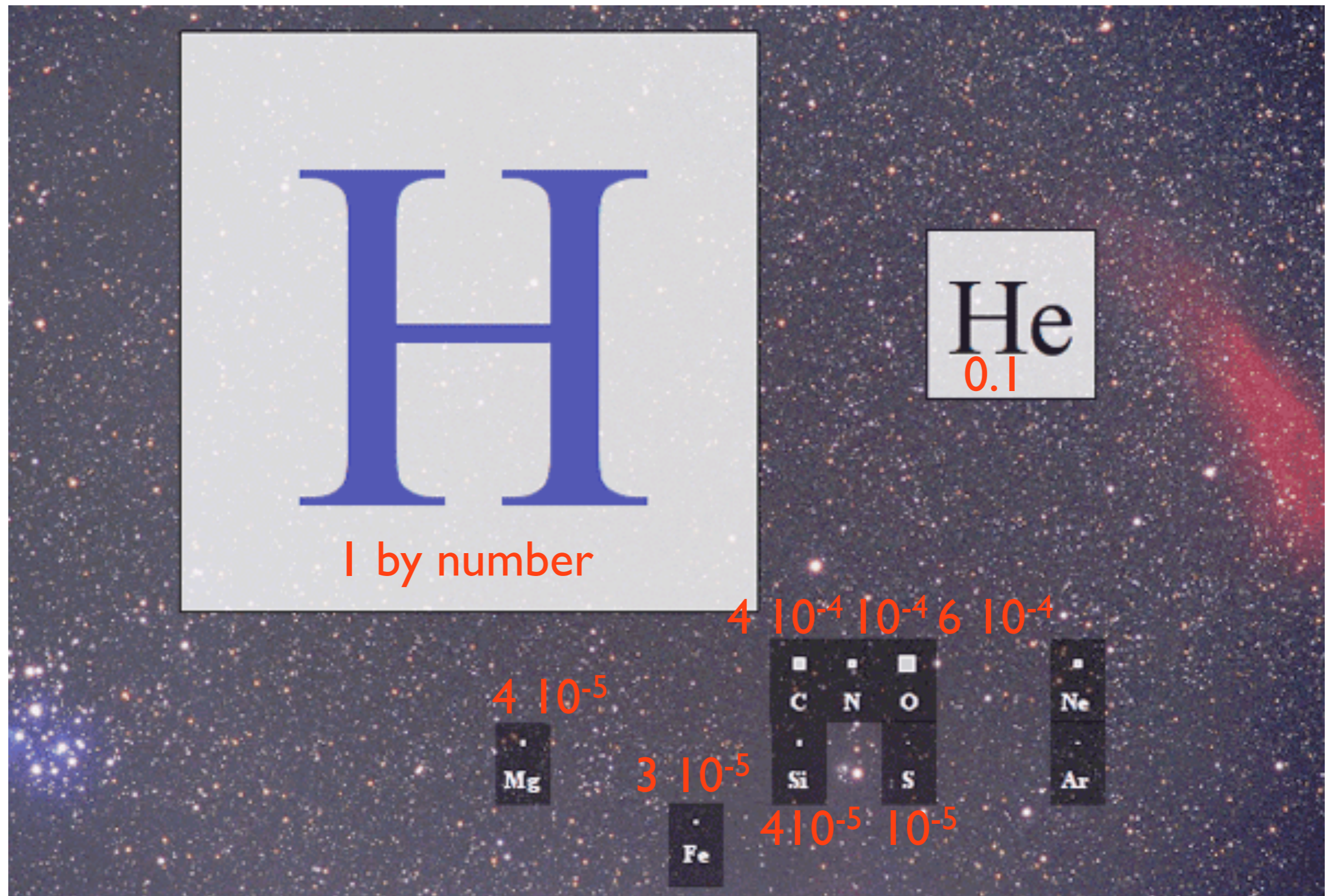
Buckyballs In A Young Planetary Nebula

NASA / JPL-Caltech / J. Cami (Univ. of Western Ontario/SETI Institute)

Spitzer Space Telescope • IRS

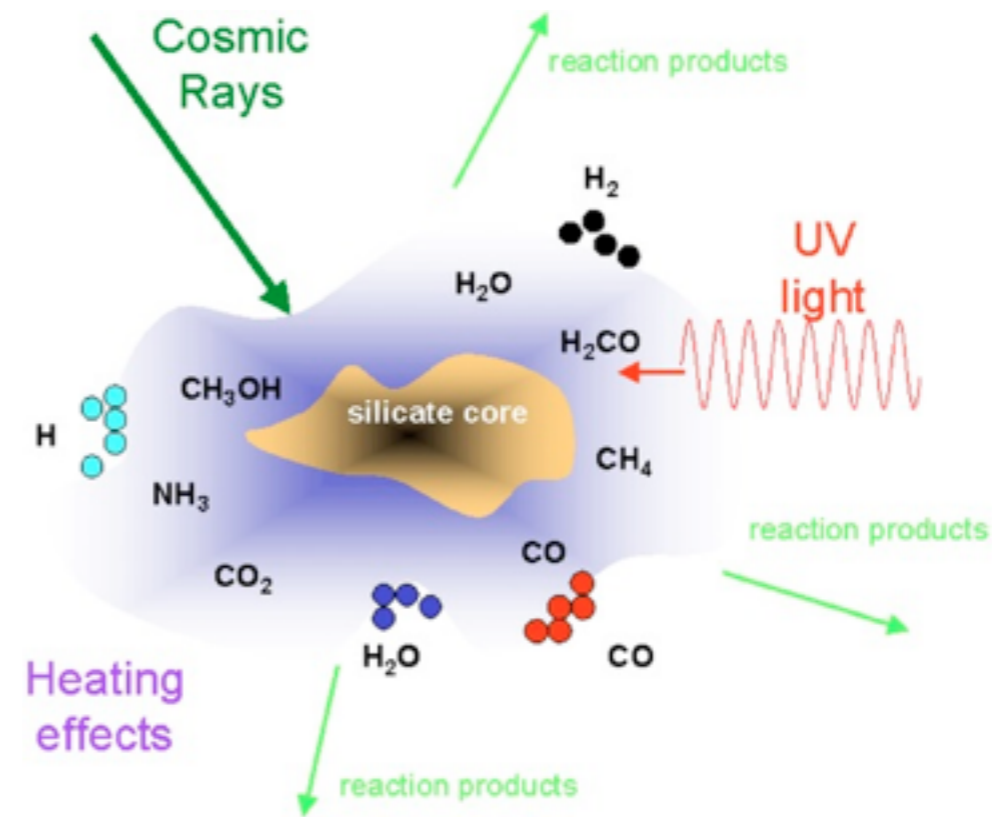
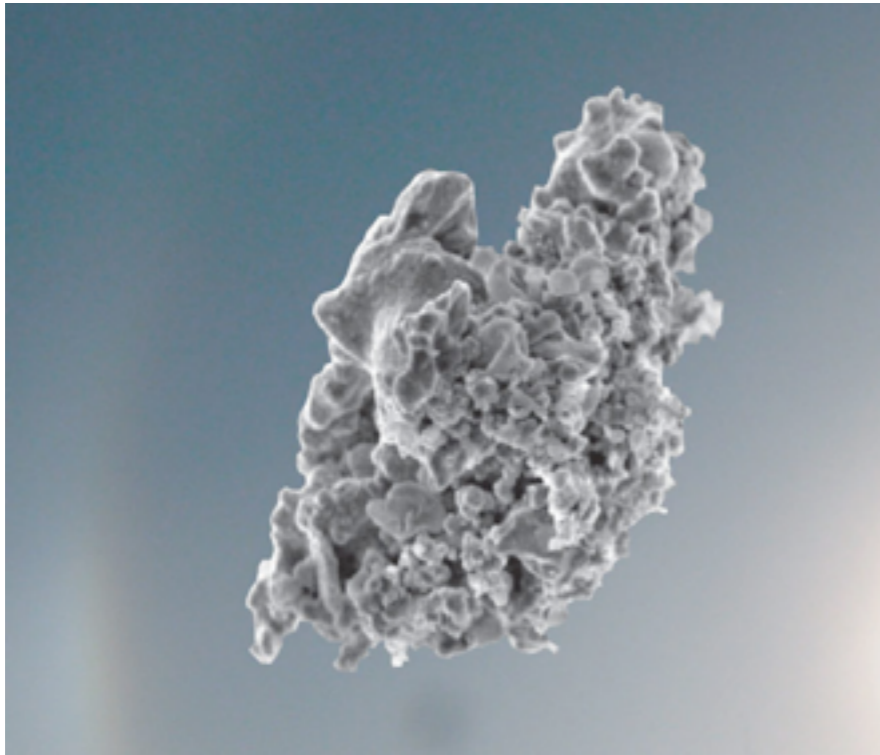
ssc2010-06a

Astronomer's periodic table



- 99% gas, 1% dust (by mass), depletion of refractory elements

Interstellar Dust



- Formed in AGB stars & grow in the ISM/CSM
- Small, $\sim 0.01\text{--}1\ \mu\text{m}$
- Silicate core, with refractory materials (most of Si, Mg, Fe)
- Carbonaceous material ($\sim 30\%$ of O, $\sim 60\%$ of C)
- Abundance $\sim 10^{-12}$ wrt to H_2
- $T_{\text{kin}} < 150\ \text{K}$: condensation of gas \Rightarrow icy mantles

How molecules form, survive, and "shine"?

Next lectures!