Sensitivity of an Interferometer

Point-source sensitivity for a single antenna,

$$\sigma_S = \frac{2kT_s}{A_e(\Delta\nu\,\tau)^{1/2}} \qquad (3.201)$$

And for a two-element interferometer (where A_e is the effective collecting area of each element):

$$\sigma_S = \frac{2^{1/2}kT_s}{A_e(\Delta\nu\,\tau)^{1/2}} \qquad (3.202)$$

The point-source sensitivity is $2^{1/2}$ times better than the sensitivity of each antenna, but $2^{1/2}$ times worse than that of a single dish whose area is that of two antennas

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Two antennas multiply two independent sets of voltages together to make a visibility and thus there are two independent sets of noise multiplied

Information contained in the two independent square-law detector outputs have been discarded – together they have $2^{1/2}$ times the sensitivity of a single dish

Combined with the independent correlator output, the total sensitivity is $(2 + 2)^{1/2}$ which is 2x the sensitivity of the single dish

Sensitivity of an Interferometer

Fig. 3.34 (ERA)

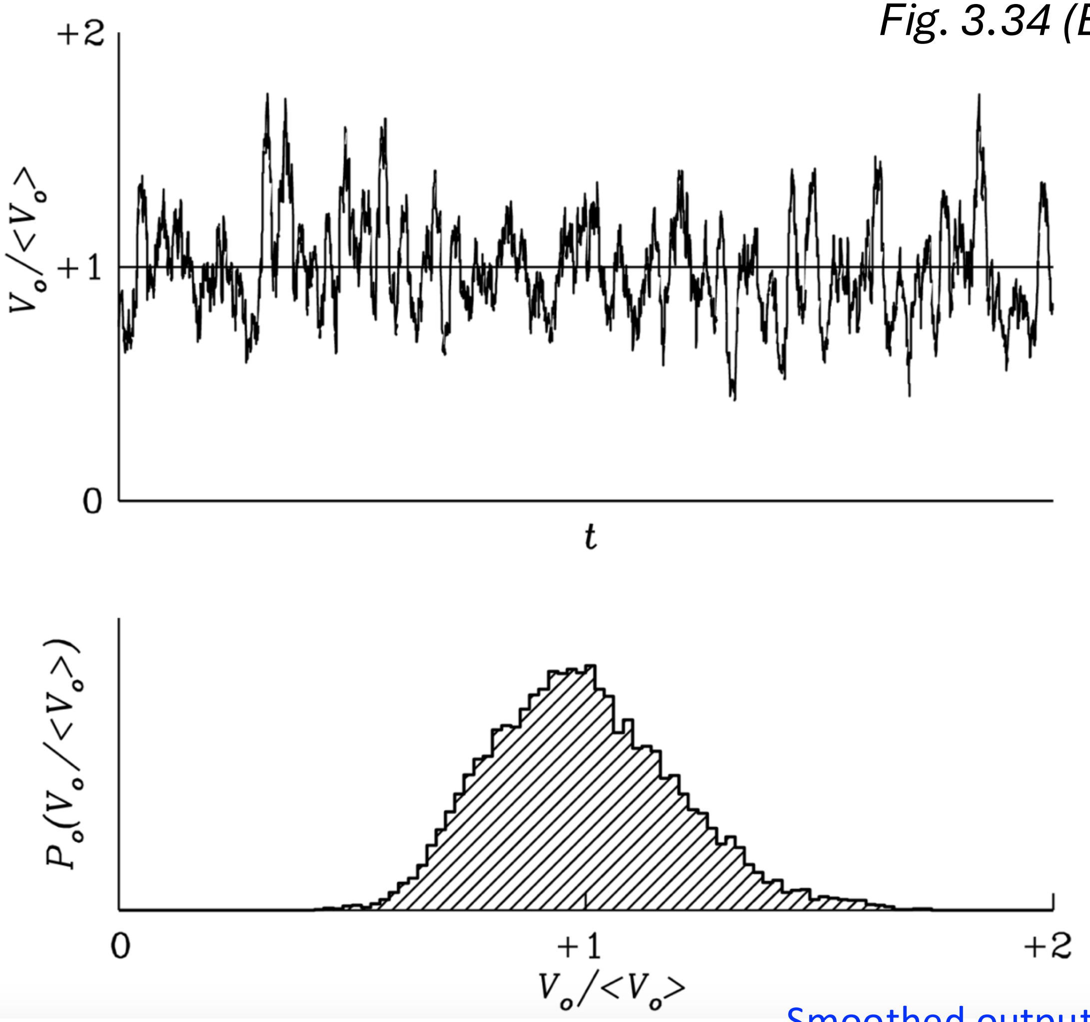
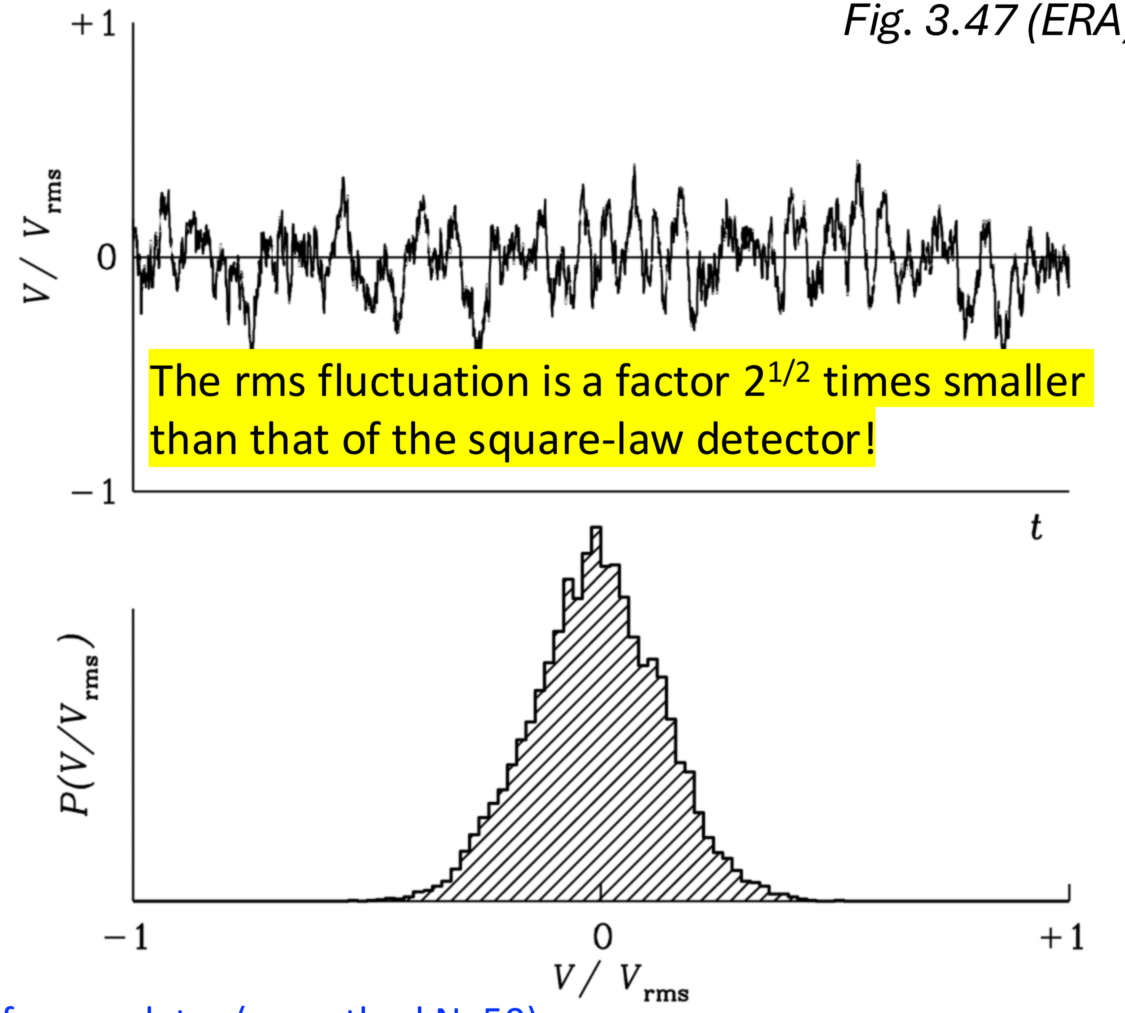


Fig. 3.47 (ERA)



The rms fluctuation is a factor $2^{1/2}$ times smaller than that of the square-law detector!

Smoothed output voltages of a correlator (smoothed N=50)

Sensitivity of an Interferometer

An interferometer with N dishes contains $N(N - 1)/2$ independent two-element interferometers. So long as the signal from each dish can be amplified *coherently* before it is spit up to be multiplied by the signals from the N-1 other antennas, its point-source rms noise (per beam) is

$$\sigma_S = \frac{2kT_s}{A_e[N(N-1)\,\Delta\nu\,\tau]^{1/2}}. \qquad (3.203)$$

The VLA with N = 27 dishes each d = 25 m in diameter has a sensitivity of a dish with $D = [N(N - 1)]^{1/4}\, d = [27(26)^{1/4}]$ 25 m = 129 m!

“Brightness” Sensitivity

BEWARE! The brightness sensitivity of an interferometer is **worse than a single dish** because the synthesized beam solid angle of an interferometer is much smaller than the beam solid angle of a single dish of the same total effective area

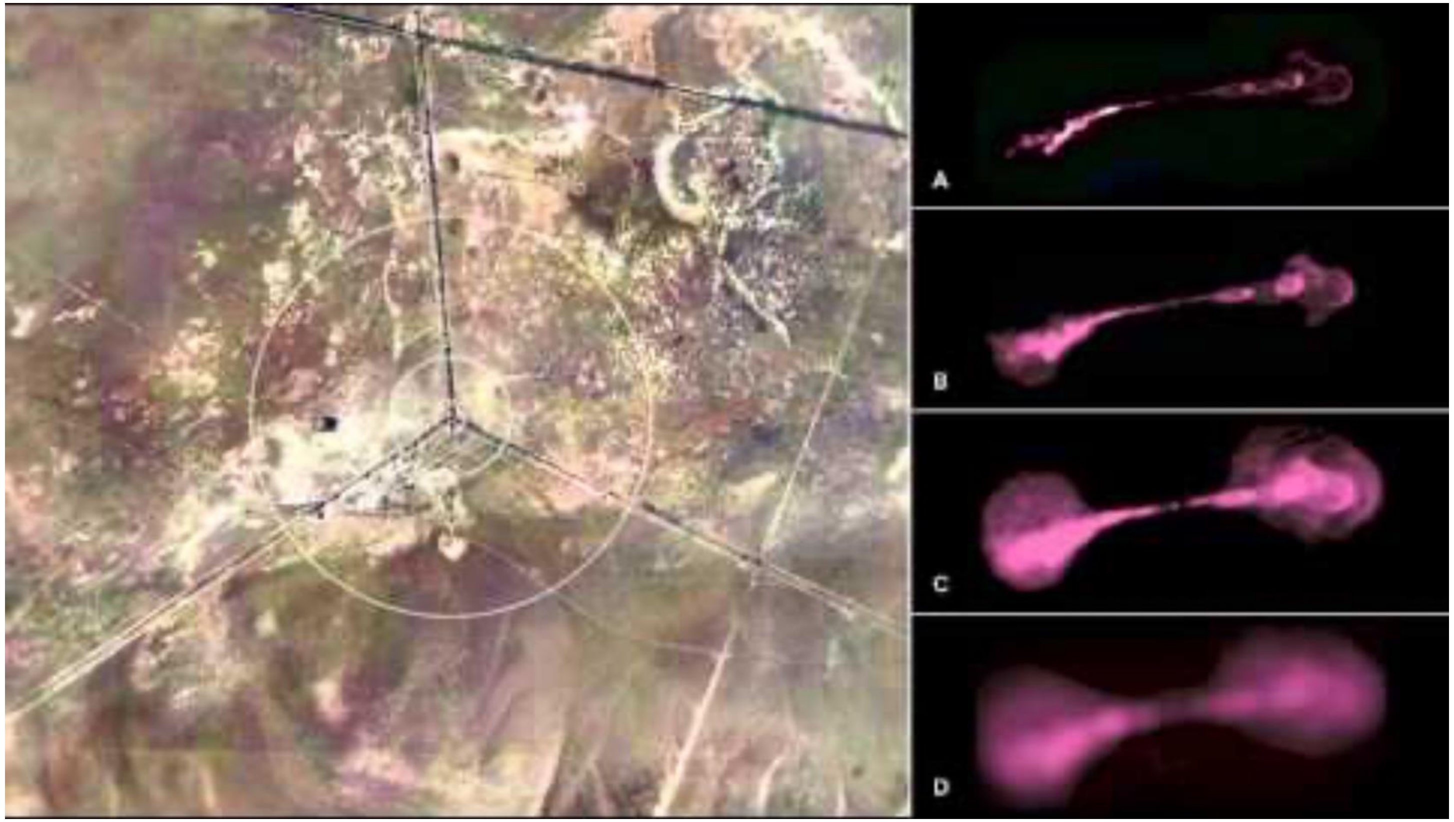
Interferometer resolution:

$\theta \sim \lambda/b$ radians

Single dish resolution:

$\theta \sim \lambda/D$ radians

Smaller by factor of $\sim (D/b)^2$ that defines the area **filling factor**



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$\theta \sim \lambda/b$ radians

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$\theta \sim \lambda/D$ radians

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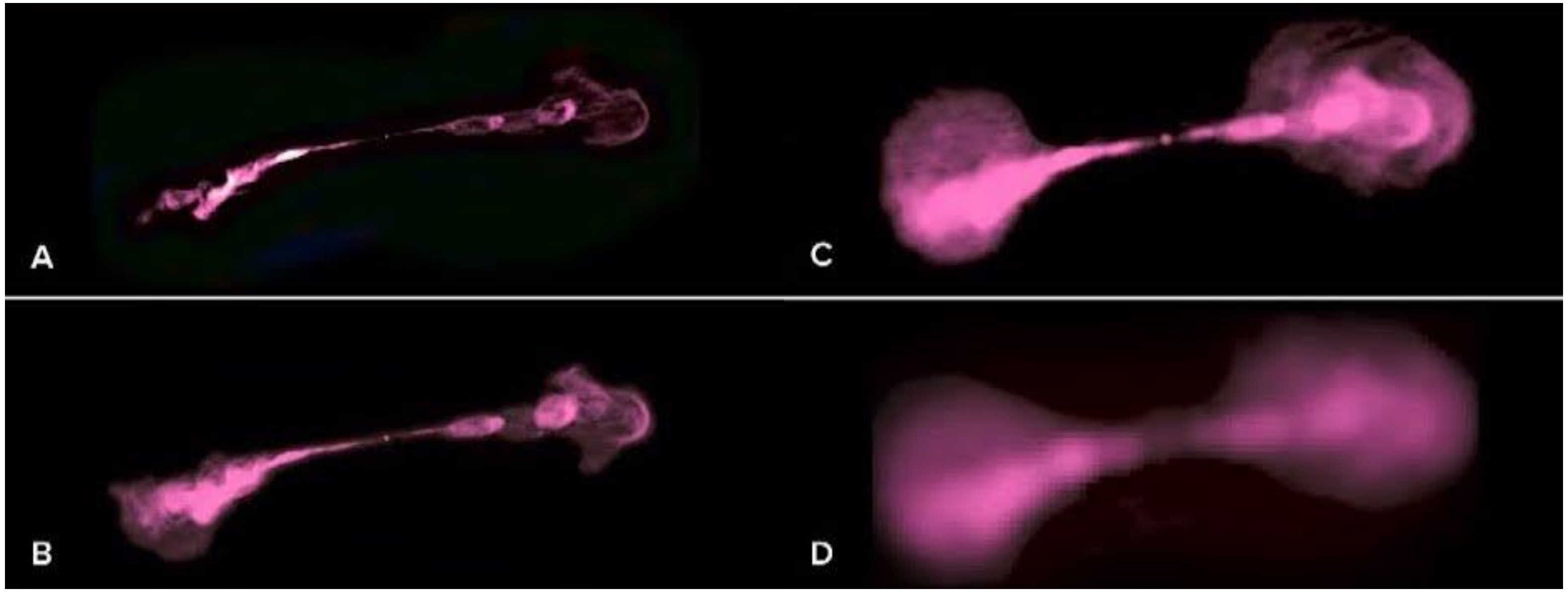


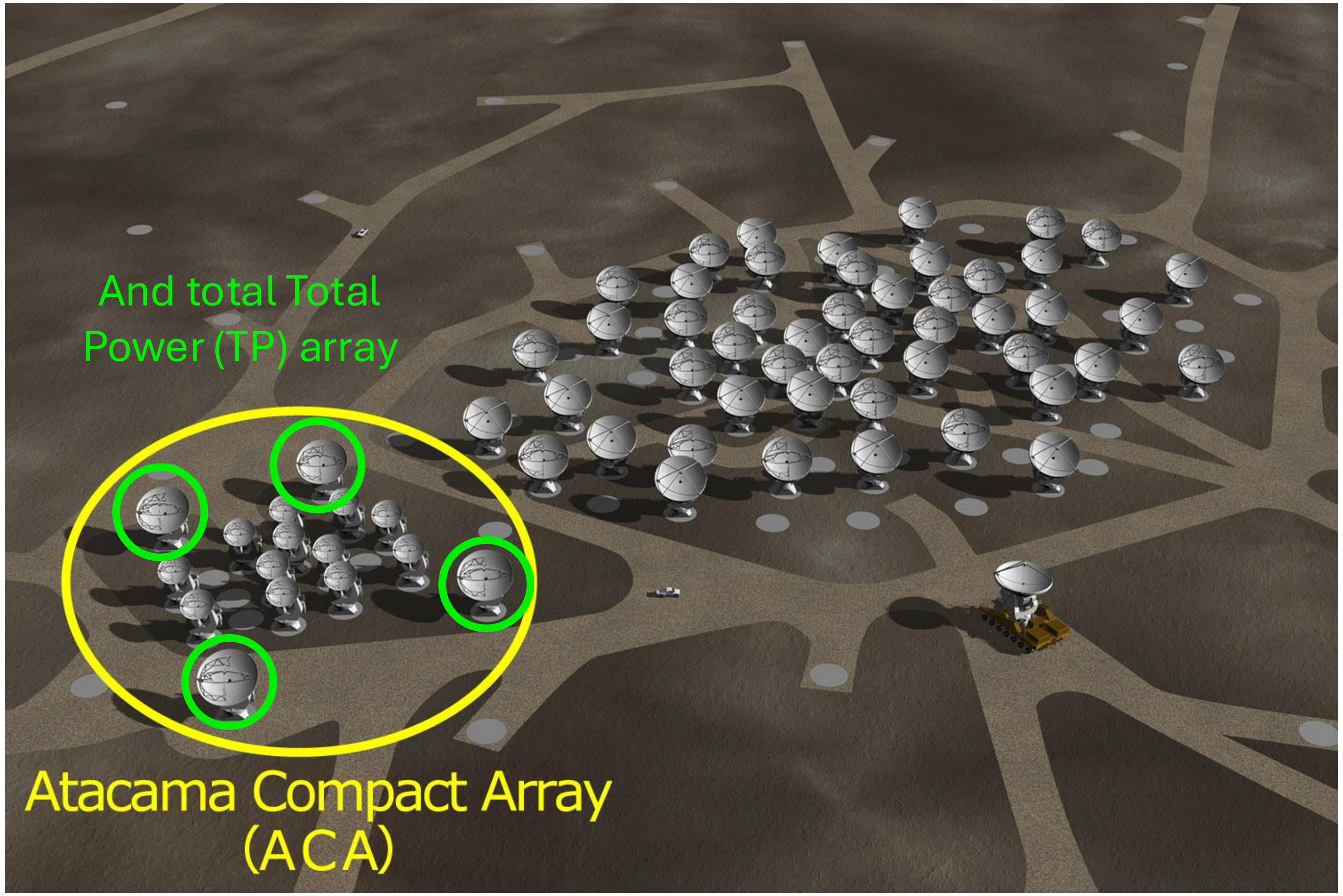
In order to be sensitive to emission at different scales, one often needs to **observe in different baseline configurations**

“Brightness” Sensitivity

ALMA tries to compensate to increase sensitivity and recover extended emission with, in addition to different ‘configurations’ of the 12m dishes:

- A compact ‘ACA’ setup with the use of 12 smaller 7m dishes
- A total power array made up of 4 of the 12m dishes

Ideally it would be best to combine with single-dish data, e.g., the GBT!

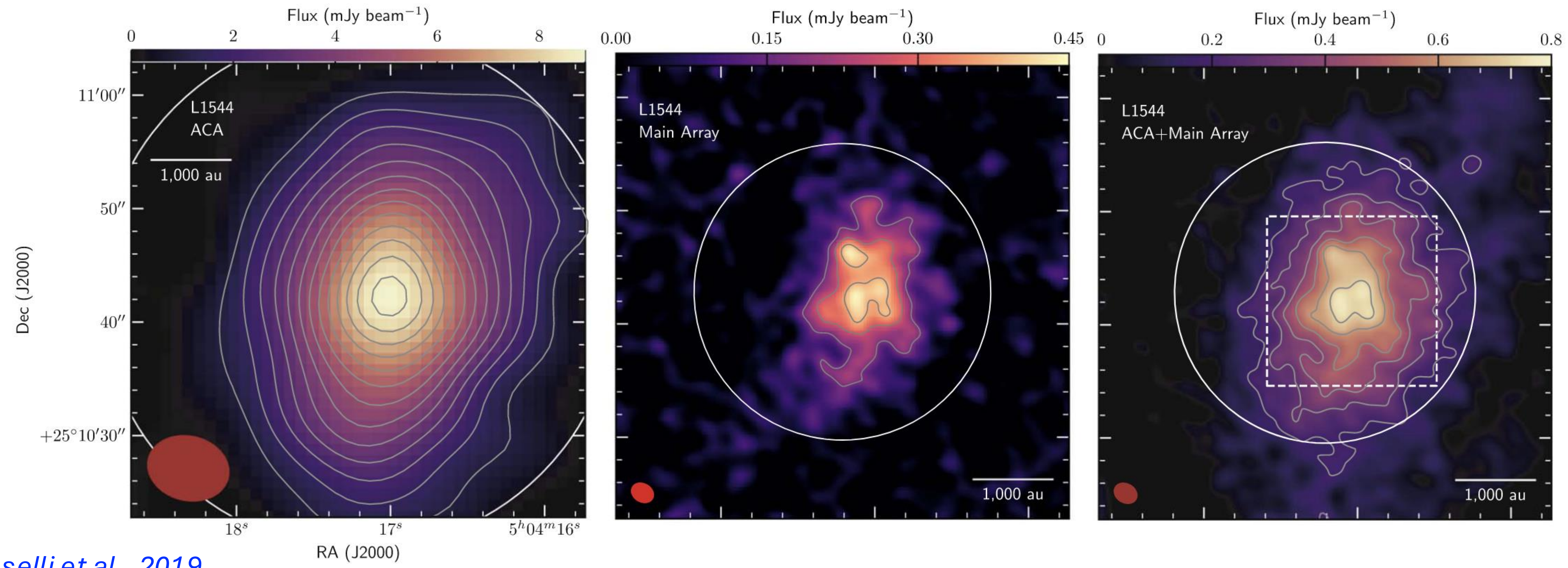


Credit: ALMA (ESO/NAOJ/NRAO)

“Brightness” Sensitivity

Keep in mind for Final Project!

ALMA ACA + 12m image of the Prestellar core L1544

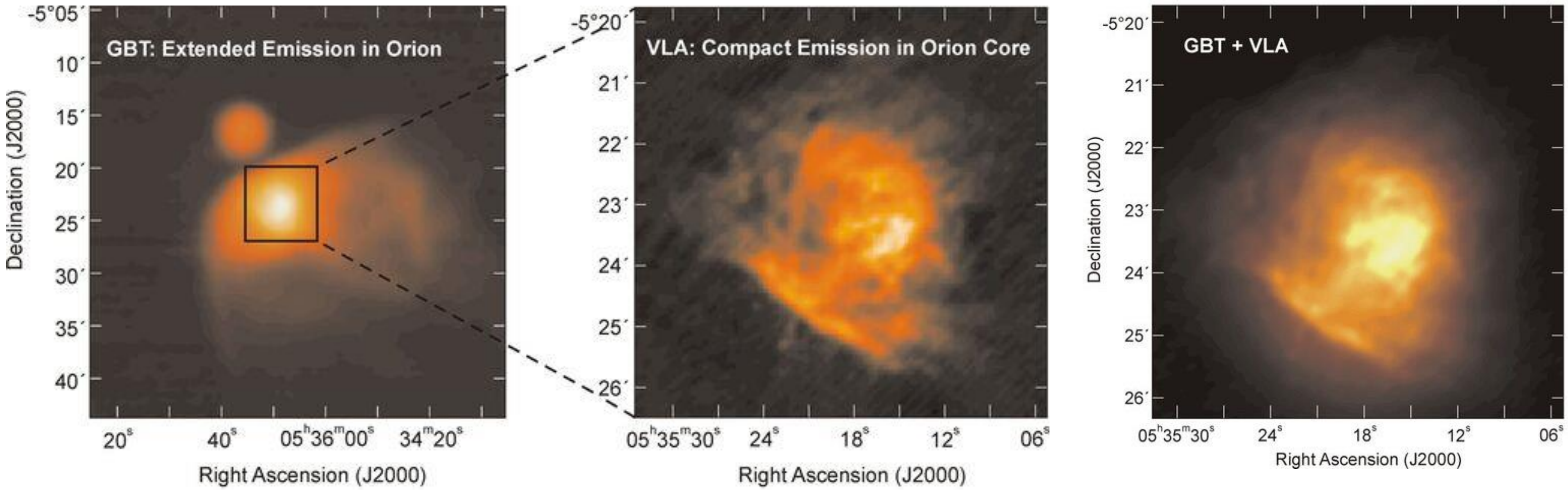


Caselli et al., 2019

“Brightness” Sensitivity

Keep in mind for Final Project!

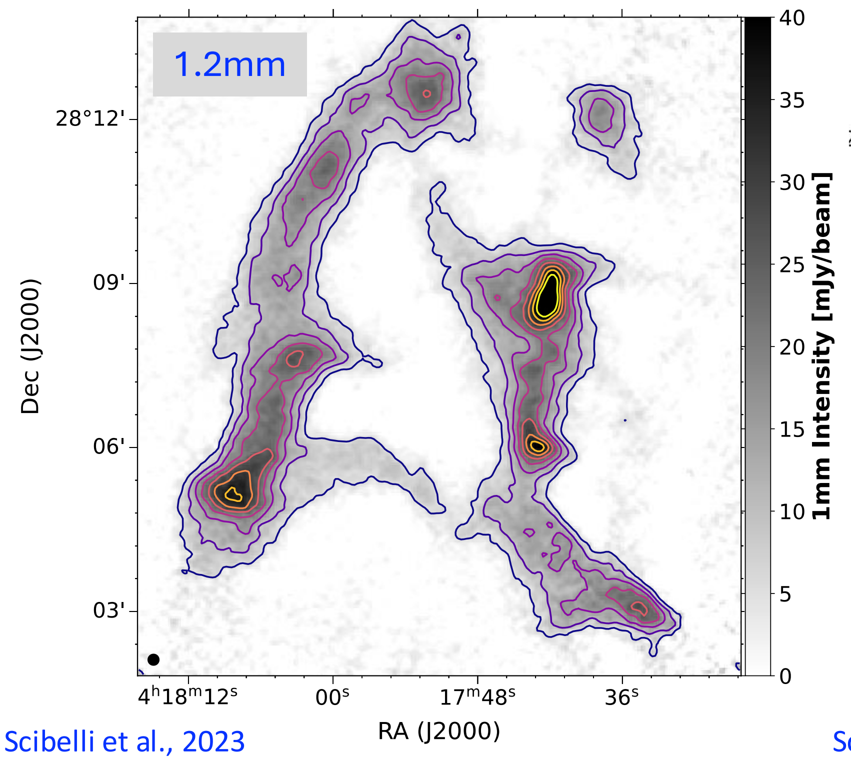
VLA+GBT image of the Orion Nebula HII region



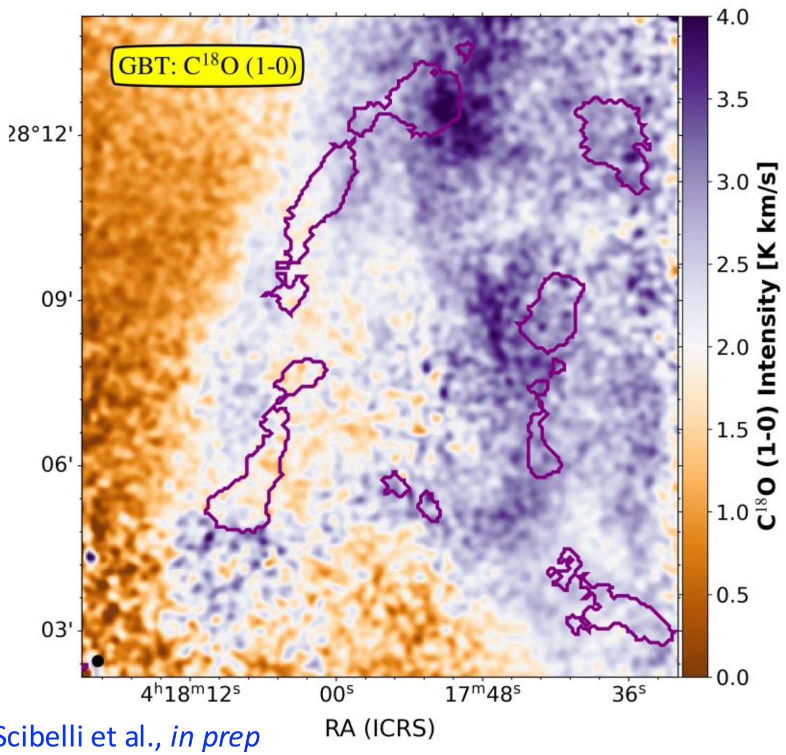
3.6 cm (8.435 GHz)
Combined with ‘feathering’ technique

"Brightness" Sensitivity

Often, you'll see maps from any radio telescopes either listed with **units of 'Jy/beam' or 'K'**
Here I show single dish IRAM 30m and GBT maps in different units, mJy/beam and K km/s, respectively:



Scibelli et al., 2023



Scibelli et al., *in prep*

A proper "spectral brightness" depends only on the source, thus we often use **brightness temperature**, in Kelvin [K]

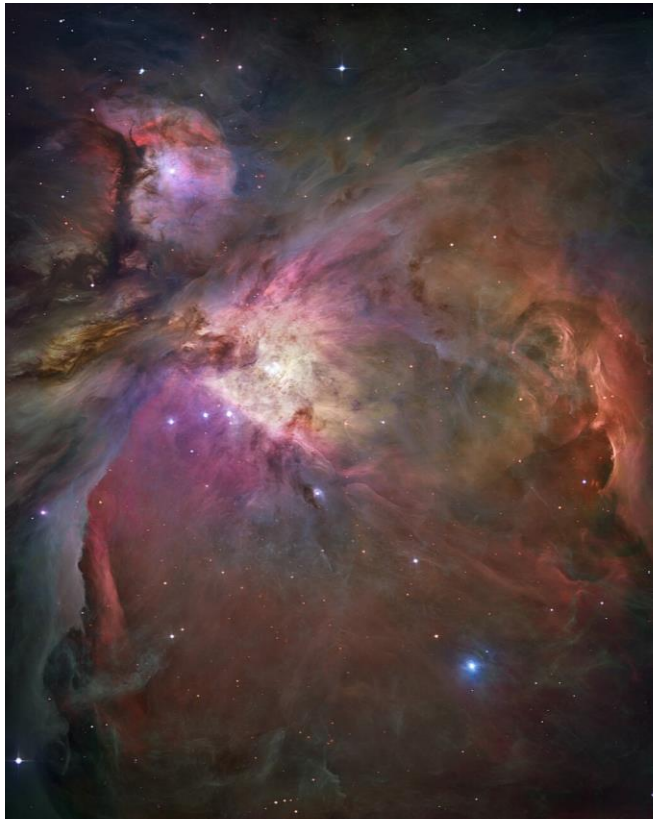
$$\sigma_T = \left(\frac{\sigma_S}{\Omega_A}\right)\frac{\lambda^2}{2k}. \quad (3.204)$$

https://science.nrao.edu/facilities/vla/proposing/TBconv

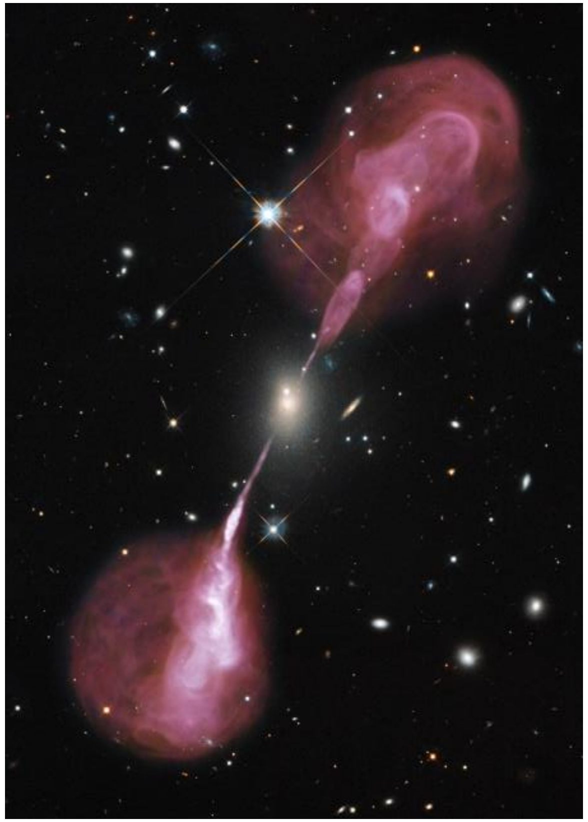
Emission Mechanisms

Spectral Lines (ERA Chap. 7)

Free-Free (ERA Chap. 4)



Synchrotron (ERA Chap. 5)



Pulsars (ERA Chap. 6)

Emission Mechanisms

Spectral Lines (ERA Chap. 7)

Free-Free (ERA Chap. 4)

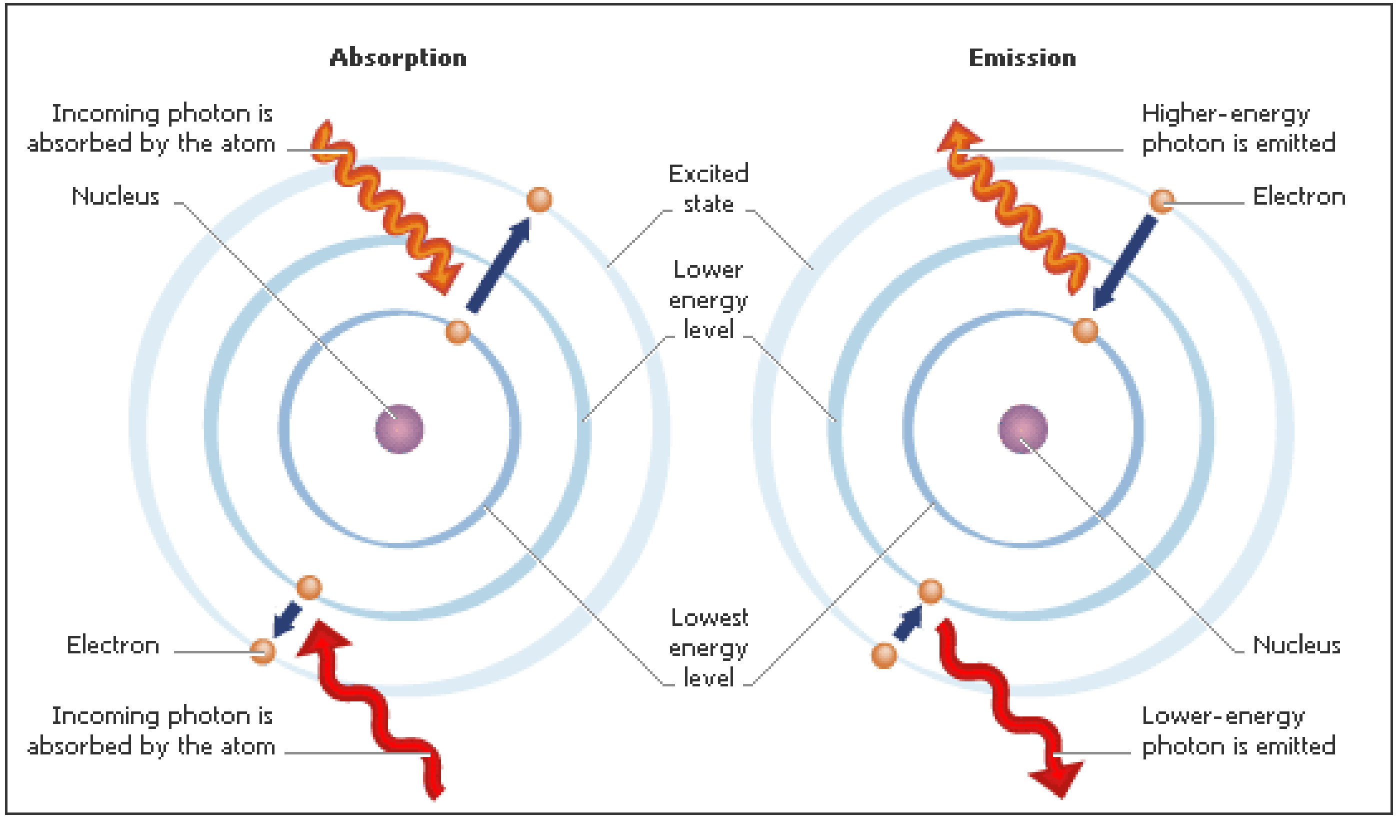
Synchrotron (ERA Chap. 5)

Pulsars (ERA Chap. 6)

GREEN BANK OBSERVATORY
AUI
NRAO National Radio Astronomy Observatory
NSF

Spectral Line Definition:

Spectral Lines are narrow ($\nu << \Delta\nu$) emission or absorption features in the spectra of gaseous and ionized sources and are intrinsically <u>quantum phenomena</u> because energy is quantized ($E = h\nu$) leading to lines occurring at specific frequencies



Main topics to cover:

- Molecular Emission
- Recombination Lines
- HI 21cm line
- Masers

Contact: sscibell@nrao.edu

Spectral Line Definition:

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Main topics to cover:

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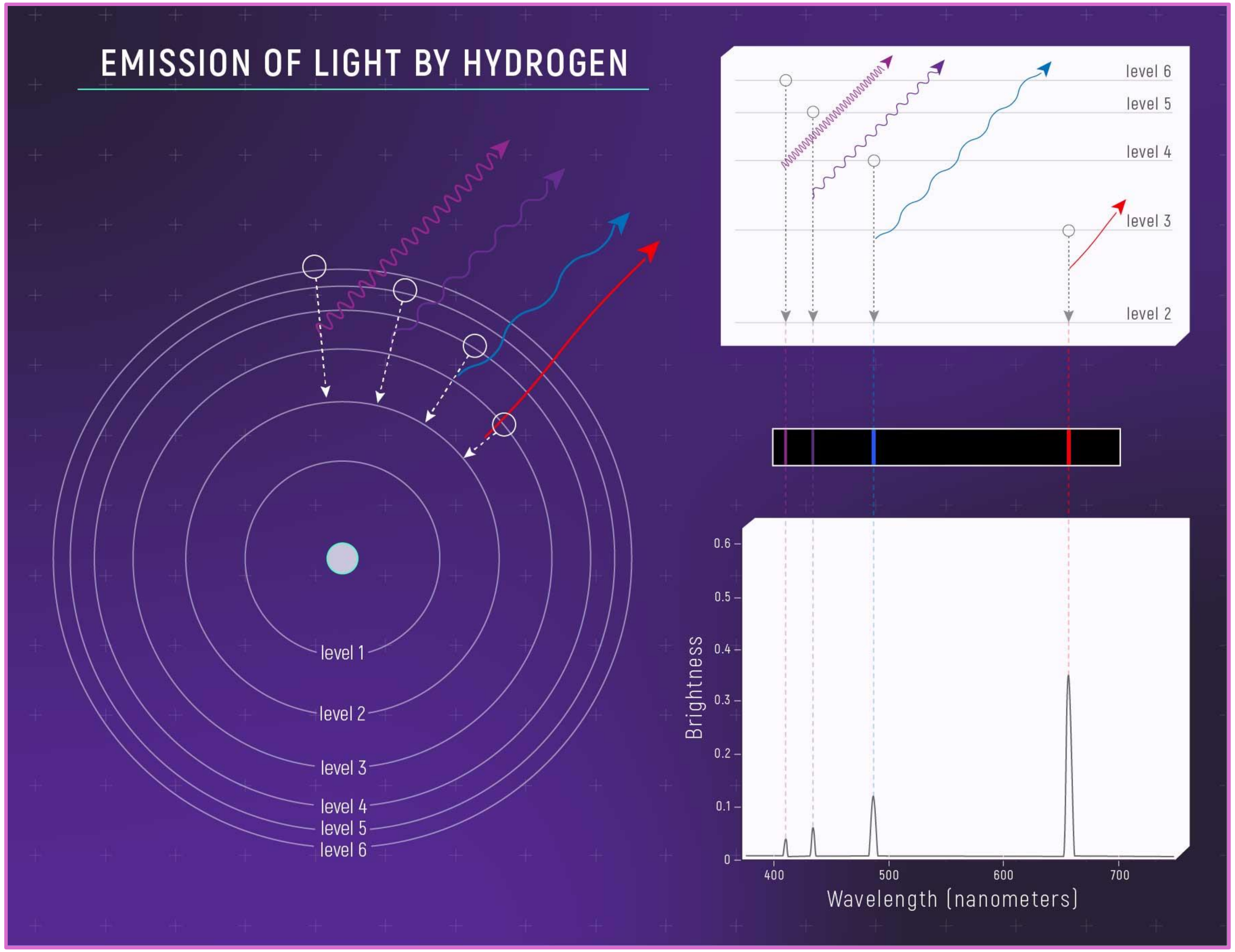

Spectral Line Definition:

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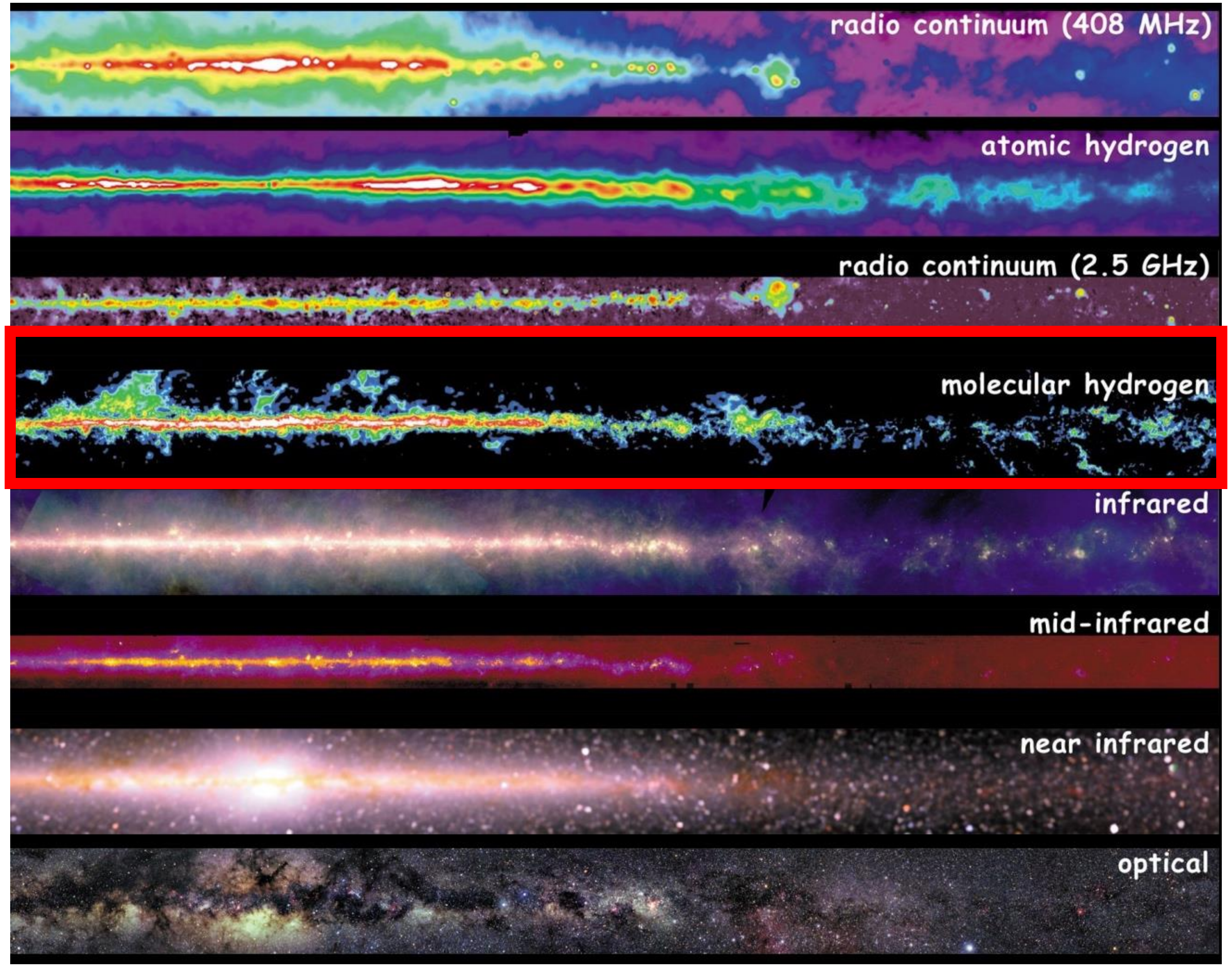
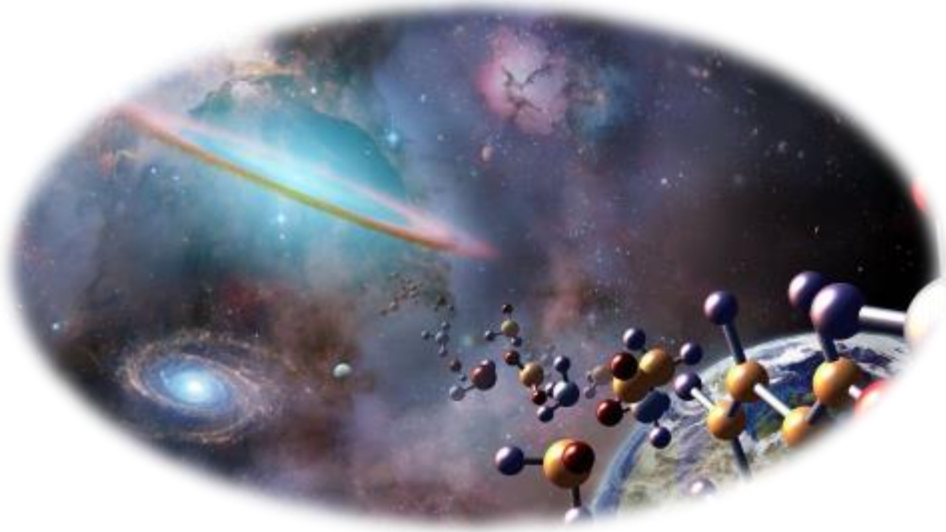
Main topics to cover:

- **Molecular Emission**
- Recombination Lines
- HI 21cm line
- Masers



"Molecular Astrophysics" or "Astrochemistry"

Definition: The study of the formation and destruction of molecules in the Universe, their interaction with radiation, and their feedback on physics of the environments

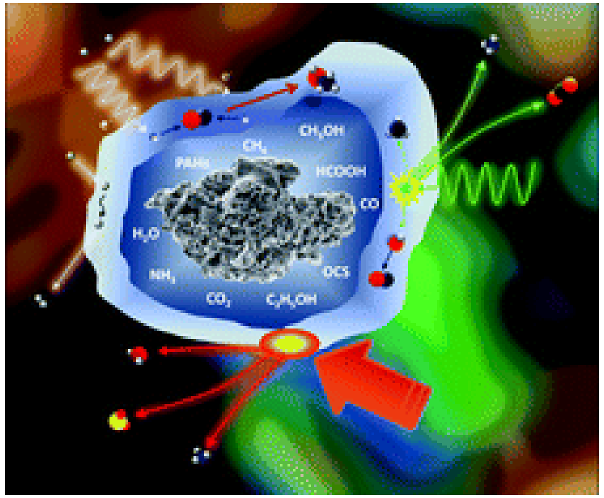


I write about molecules with great diffidence, having not yet rid myself of the tradition that ***atoms are physics, but molecules are chemistry****, but the new conclusions that hydrogen is abundant seems to make it likely that the above mentioned elements H, O, and N will frequency form molecules*

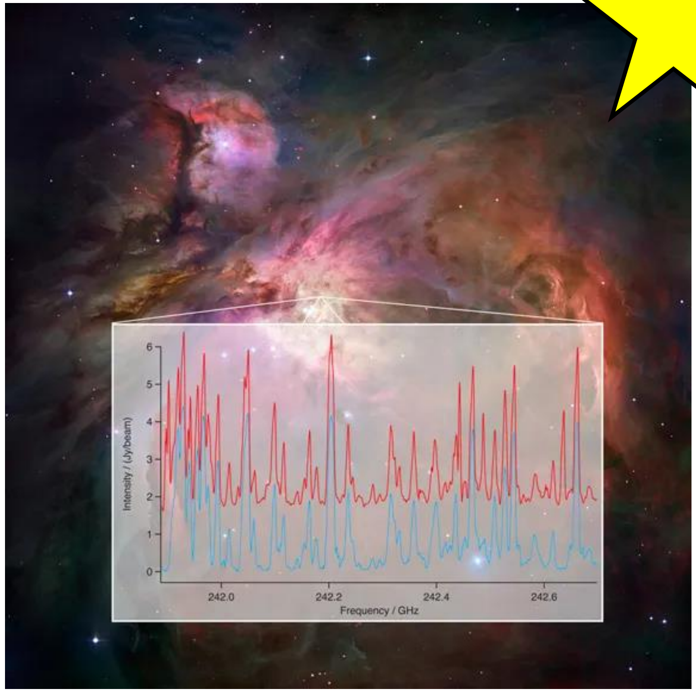
- *Sir A. Eddington, 1937*

Astrochemistry is an interdisciplinary field! Including, chemistry, physics, astronomy, biology, etc.,

Modeling



Observations



Things an astro**chemist** does

Laboratory

“Molecular Astrophysics” or “Astrochemistry”

Known Interstellar Molecules

Created with **ASTROMOL** v2021.8.0
bmcguir2.github.io/astromol
McGuire 2022 *ApJS* 259, 30

2 Atoms

CH, CN, CH^+, OH, CO, H_2, SiO, CS, SO, SiS, NS, C_2, NO, HCl, $NaCl$, $AlCl$, KCl, AlF, PN, SiC, CP, NH, SiN, SO^+, CO^+, HF, N_2, CF^+, PO, O_2, AlO, CN^-, OH^+, SH^+, HCl^+, SH, TiO, ArH^+, NS^+, HeH^+, VO, PO^+, SiP, FeC

3 Atoms

H_2O, HCO^+, HCN, OCS, HNC, H_2S, N_2H^+, C_2H, SO_2, HCO, HNO, HCS^+, HOC^+, SiC_2, C_2S, C_3, CO_2, CH_2, C_2O, $MgNC$, NH_2, $NaCN$, N_2O, $MgCN$, H_3^+, $SiCN$, $AlNC$, $SiNC$, HCP, CCP, $AlOH$, H_2O^+, H_2Cl^+, KCN, $FeCN$, HO_2, TiO_2, CCN, $SiCSi$, S_2H, HCS, HSC, NCO, $CaNC$, NCS, MgC_2, HSO

4 Atoms

NH_3, H_2CO, $HNCO$, H_2CS, C_2H_2, C_3N, $HNCS$, $HOCO^+$, C_3O, *l*-C_3H, $HCNH^+$, H_3O^+, C_3S, *c*-C_3H, HC_2N, H_2CN, SiC_3, CH_3, C_3N^-, PH_3, $HCNO$, $HOCN$, $HSCN$, $HOOH$, *l*-C_3H^+, $HMgNC$, $HCCO$, $CNCN$, $HONO$, $MgCCH$, $HCCS$, $HNCN$, H_2NC, $HCCS^+$, CH_3^+

5 Atoms

HC_3N, $HCOOH$, CH_2NH, NH_2CN, H_2CCO, C_4H, SiH_4, *c*-C_3H_2, CH_2CN, C_5, SiC_4, H_2CCC, CH_4, $HCCNC$, $HNCCC$, H_2COH^+, C_4H^-, $CNCHO$, $HNCNH$, CH_3O, NH_3D^+, H_2NCO^+, $NCCNH^+$, CH_3Cl, MgC_3N, HC_3O^+, NH_2OH, HC_3S^+, H_2CCS, C_4S, $CHOSH$, $HCSCN$, HC_3O, $NaCCCN$, MgC_3N^+

6 Atoms

CH_3OH, CH_3CN, NH_2CHO, CH_3SH, C_2H_4, C_5H, CH_3NC, HC_2CHO, H_2C_4, C_5S, HC_3NH^+, C_5N, HC_4H, HC_4N, *c*-H_2C_3O, CH_2CNH, C_5N^-, $HNCHCN$, SiH_3CN, MgC_4H, CH_3CO^+, H_2CCCS, CH_2CCH, $HCSCCH$, C_5O, $HCCNCH^+$, C_5H^+, *c*-C_5H, HC_4S, $HMgCCCN$, MgC_4H^+, $H_2C_3H^+$, $HOCOOH$, H_2C_3N

7 Atoms

CH_3CHO, CH_3CCH, CH_3NH_2, CH_2CHCN, HC_5N, C_6H, *c*-C_2H_4O, CH_2CHOH, C_6H^-, CH_3NCO, HC_5O, $HOCH_2CN$, HC_4NC, HC_3HNH, *c*-C_3HCCH, MgC_5N, CH_2C_3N, *l*-H_2C_5, NC_4NH^+, MgC_5N^+

12 Atoms

C_6H_6, *n*-C_3H_7CN, *i*-C_3H_7CN, $C_2H_5OCH_3$, 1-C_5H_5CN, 2-C_5H_5CN, *n*-$CH_3CH_2CH_2OH$, *i*-$CH_3CH_2CH_2OH$, *i*-C_4H_8, 1-C_5H_4CCH, 2-C_5H_4CCH

8 Atoms

$HCOOCH_3$, CH_3C_3N, C_7H, CH_3COOH, H_2C_6, CH_2OHCHO, HC_6H, CH_2CHCHO, CH_2CCHCN, NH_2CH_2CN, CH_3CHNH, CH_3SiH_3, NH_2CONH_2, $HCCCH_2CN$, CH_2CHCCH, MgC_6H, $C_2H_3NH_2$, $HOCHCHOH$, $HCCCHCCC$, C_7N^-, CH_3CHCO, MgC_6H^+

9 Atoms

CH_3OCH_3, CH_3CH_2OH, CH_3CH_2CN, HC_7N, CH_3C_4H, C_8H, CH_3CONH_2, C_8H^-, CH_2CHCH_3, CH_3CH_2SH, HC_7O, CH_3NHCHO, $H_2CCCHCCH$, $HCCCHCHCN$, H_2CCHC_3N

10 Atoms

CH_3COCH_3, $HOCH_2CH_2OH$, CH_3CH_2CHO, CH_3C_5N, CH_3CHCH_2O, CH_3OCH_2OH, H_2CCCHC_3N, C_6H_4, C_2H_5NCO, HC_7NH^+, $CH_3CHCHCN$, CH_2CCH_3CN, CH_2CHCH_2CN, NH_2COCH_2OH

11 Atoms

HC_9N, CH_3C_6H, C_2H_5OCHO, CH_3COOCH_3, CH_3COCH_2OH, C_5H_6, $NH_2CH_2CH_2OH$, CH_2CCHC_4H, $C_{10}H^-$, C_4H_5CN

13+ Atoms

C_6H_5CN, $HC_{11}N$, *c*-$C_5H_4CCH_2$, *c*-C_6H_5CCH, 1-$C_{10}H_7CN$, 2-$C_{10}H_7CN$, C_9H_8, 2-C_9H_7CN, C_{60}, C_{60}^+, C_{70}

>300!

~~298 Molecules~~

Last Updated: 2 Jan 2024

McGuire 2022

"Molecular Astrophysics" or "Astrochemistry"

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2 Atoms

CH, CN, CH^+, OH, CO, H_2, SiO, CS, SO, SiS, NS, C_2, NO, HCl, NaCl, AlCl, KCl, AlF, PN, SiC, CP, NH, SiN, SO^+, CO^+, HF, N_2, CF^+, PO, O_2, AlO, CN^-, OH^+, SH^+, HCl^+, SH, TiO, ArH^+, NS^+, HeH^+, VO, PO^+, SiP, FeC

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4 Atoms

NH_3, H_2CO, HNCO, H_2CS, C_2H_2, C_3N, HNCS, $HOCO^+$, C_3O, l-C_3H, $HCNH^+$, H_3O^+, C_3S, c-C_3H, HC_2N, H_2CN, SiC_3, CH_3, C_3N^-, PH_3, HCNO, HOCN, HSCN, HOOH, l-C_3H^+, HMgNC, HCCO, CNCN, HONO, MgCCH, HCCS, HNCN, H_2NC, $HCCS^+$, CH_3^+

5 Atoms

HC_3N, HCOOH, CH_2NH, NH_2CN, H_2CCO, C_4H, SiH_4, c-C_3H_2, CH_2CN, C_5, SiC_4, H_2CCC, CH_4, HCCNC, HNCCC, H_2COH^+, C_4H^-, CNCHO, HNCNH, CH_3O, NH_3D^+, H_2NCO^+, $NCCNH^+$, CH_3Cl, MgC_3N, HC_3O^+, NH_2OH, HC_3S^+, H_2CCS, C_4S, CHOSH, HCSCN, HC_3O, NaCCCN, MgC_3N^+

6 Atoms

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7 Atoms

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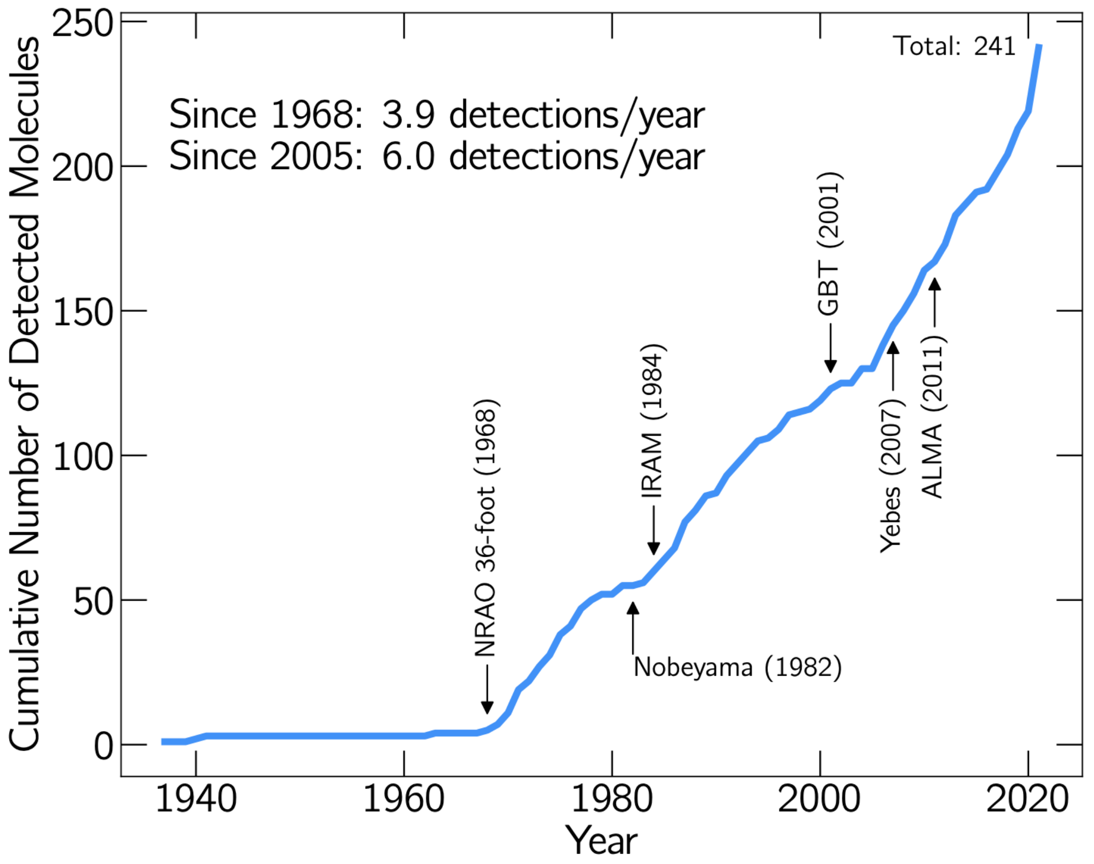
~~298 Molecules~~ >300!

Last Updated: 2 Jan 2024



McGuire 2022

“Molecular Astrophysics” or “Astrochemistry”

Known Interstellar Molecules

Created with **ASTROMOL** v2021.8.0
bmcguir2.github.io/astromol
McGuire 2022 *ApJS* 259, 30

2 Atoms

CH, CN, CH^+, OH, CO, H_2, SiO, CS, SO, SiS, NS, C_2, NO, HCl, NaCl, AlCl, KCl, AlF, PN, SiC, CP, NH

SiN, SO^+, CO^+, HF, N_2, CF^+, PO, O_2, AlO, CN^-, OH^+, SH^+, HCl^+, SH, TiO, ArH^+, NS^+, HeH^+, VO, PO^+, SiP, FeC

3 Atoms

H_2O, HCO^+, HCN, OCS, HNC, H_2S, N_2H^+, C_2H, SO_2, HCO, HNO, HCS^+, HOC^+, SiC_2, C_2S, C_3, CO_2, CH_2, C_2O, MgNC, NH_2, NaCN, N_2O, MgCN

H_3^+, SiCN, AlNC, SiNC, HCP, CCP, AlOH, H_2O^+, H_2Cl^+, KCN, FeCN, HO_2, TiO_2, CCN, SiCSi, S_2H, HCS, HSC, NCO, CaNC, NCS, MgC_2, HSO

4 Atoms

NH_3, H_2CO, HNCO, H_2CS, C_2H_2, C_3N, HNCS, $HOCO^+$, C_3O, *l*-C_3H, $HCNH^+$, H_3O^+, C_3S, *c*-C_3H, HC_2N, H_2CN, SiC_3, CH_3

C_3N^-, PH_3, HCNO, HOCN, HSCN, HOOH, *l*-C_3H^+, HMgNC, HCCO, CNCN, HONO, MgCCH, HCCS, HNCN, H_2NC, $HCCS^+$, CH_3^+

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HC_3N, HCOOH, CH_2NH, NH_2CN, H_2CCO, C_4H, SiH_4, *c*-C_3H_2, CH_2CN, C_5, SiC_4, H_2CCC, CH_4, HCCNC, HNCCC, H_2COH^+, C_4H^-, CNCHO

HNCNH, CH_3O, NH_3D^+, H_2NCO^+, $NCCNH^+$, CH_3Cl, MgC_3N, HC_3O^+, NH_2OH, HC_3S^+, H_2CCS, C_4S, CHOSH, HCSCN, HC_3O, NaCCCN, MgC_3N^+

6 Atoms

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7 Atoms

CH_3CHO, CH_3CCH, CH_3NH_2, CH_2CHCN, HC_5N, C_6H, *c*-C_2H_4O, CH_2CHOH, C_6H^-, CH_3NCO, HC_5O, $HOCH_2CN$, HC_4NC, HC_3HNH, *c*-C_3HCCH, MgC_5N, CH_2C_3N, *l*-H_2C_5, NC_4NH^+, MgC_5N^+

8 Atoms

$HCOOCH_3$, CH_3C_3N, C_7H, CH_3COOH, H_2C_6, CH_2OHCHO, HC_6H, CH_2CHCHO, CH_2CCHCN, NH_2CH_2CN, CH_3CHNH, CH_3SiH_3, NH_2CONH_2, $HCCCH_2CN$, CH_2CHCCH, MgC_6H, $C_2H_3NH_2$, HOCHCHOH, HCCCHCCC, C_7N^-, CH_3CHCO, MgC_6H^+

9 Atoms

CH_3OCH_3, CH_3CH_2OH, CH_3CH_2CN, HC_7N, CH_3C_4H, C_8H, CH_3CONH_2, C_8H^-

CH_2CHCH_3, CH_3CH_2SH, HC_7O, CH_3NHCHO, $H_2CCCHCCH$, HCCCHCHCN, H_2CCHC_3N

10 Atoms

CH_3COCH_3, $HOCH_2CH_2OH$, CH_3CH_2CHO, CH_3C_5N, CH_3CHCH_2O, CH_3OCH_2OH, H_2CCCHC_3N, C_6H_4, C_2H_5NCO, HC_7NH^+, $CH_3CHCHCN$, CH_2CCH_3CN, CH_2CHCH_2CN, NH_2COCH_2OH

11 Atoms

HC_9N, CH_3C_6H, C_2H_5OCHO, CH_3COOCH_3, CH_3COCH_2OH, C_5H_6, $NH_2CH_2CH_2OH$, CH_2CCHC_4H, $C_{10}H^-$, C_4H_5CN

12 Atoms

C_6H_6, *n*-C_3H_7CN, *i*-C_3H_7CN, $C_2H_5OCH_3$, 1-C_5H_5CN, 2-C_5H_5CN, *n*-$CH_3CH_2CH_2OH$, *i*-$CH_3CH_2CH_2OH$, *i*-C_4H_8, 1-C_5H_4CCH, 2-C_5H_4CCH

13+ Atoms

C_6H_5CN, $HC_{11}N$, *c*-$C_5H_4CCH_2$, *c*-C_6H_5CCH, 1-$C_{10}H_7CN$, 2-$C_{10}H_7CN$

C_9H_8, 2-C_9H_7CN, C_{60}, C_{60}^+, C_{70}

>300!

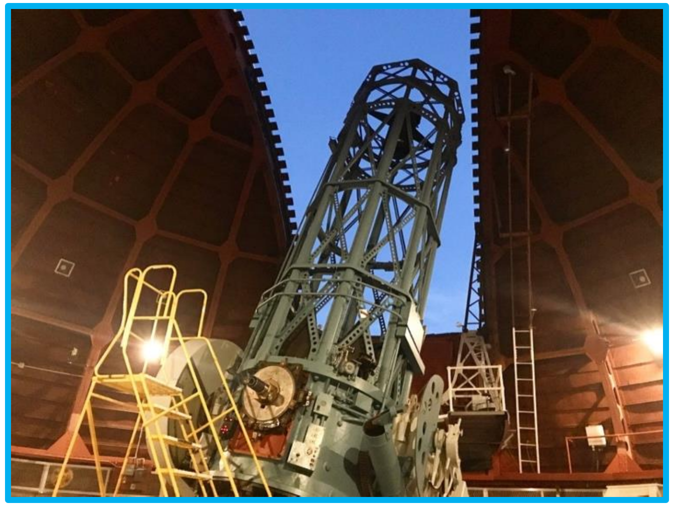
298 Molecules

Last Updated: 2 Jan 2024

McGuire 2022

Facility	#	Facility	#
IRAM 30-m	64	SMA	2
NRAO 36-ft	33	SEST	2
GBT 100-m	28	SOFIA	2
NRAO/ARO 12-m	27	Hat Creek 20-ft	2
Yebes 40-m	19	IRTF	2
Nobeyama 45-m	15	PdBI	2
NRAO 140-ft	13	OVRO	2
Bell 7-m	8	MWO 4.9-m	2
ALMA	8	Hubble	1
SMT	7	IRAS	1
Herschel	7	BIMA	1
Parkes	5	NRL 85-ft	1
FCRAO 14-m	5	ATCA	1
ISO	5	Mitaka 6-m	1
APEX	4	McMath Solar Telescope	1
Onsala 20-m	4	UKIRT	1
KPNO 4-m	4	Odin	1
Effelsberg 100-m	4	FUSE	1
Algonquin 46-m	3	KAO	1
Mt. Wilson	3	Mt. Hopkins 60-in	1
Spitzer	3	Aerobee-150 Rocket	1
Haystack	3	Millstone Hill 84-ft	1
CSO	2	Goldstone	1

“Molecular Astrophysics” or “Astrochemistry”



The first molecules detected in the ISM were CH, CN and CH+ during the mid- twentieth century via an **optical** absorption spectroscopy (McKellar, 1940)

McGuire 2022

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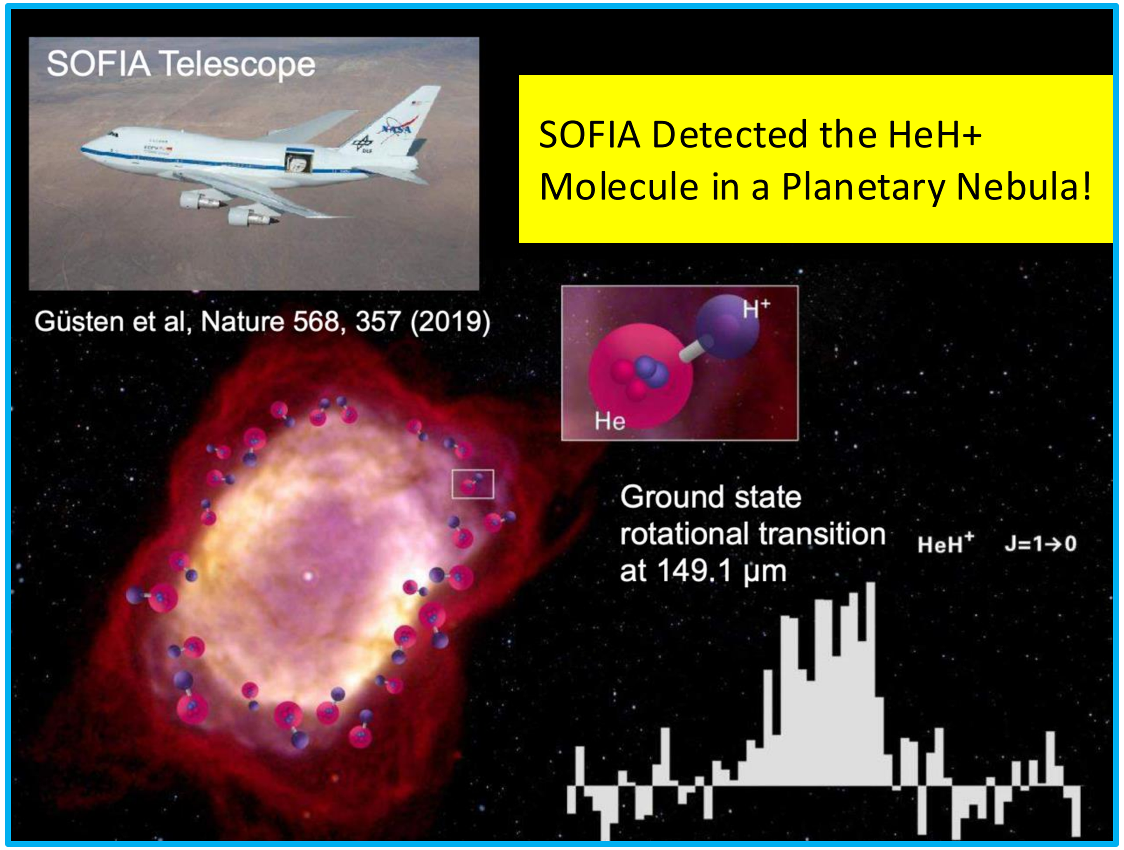

McGuire 2022

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“Molecular Astrophysics” or “Astrochemistry”

> 90% of Molecules Identified by Radio Astronomy!

Green Bank Radio Telescope, 100m, in West Virginia


Yebes 40m outside of Madrid, Spain


IRAM 30m, Granada, Spain


Arizona 12m, Kitt Peak, AZ


Control Room @ SMT, Mt. Graham, AZ

McGuire 2022

Facility	#	Facility	#
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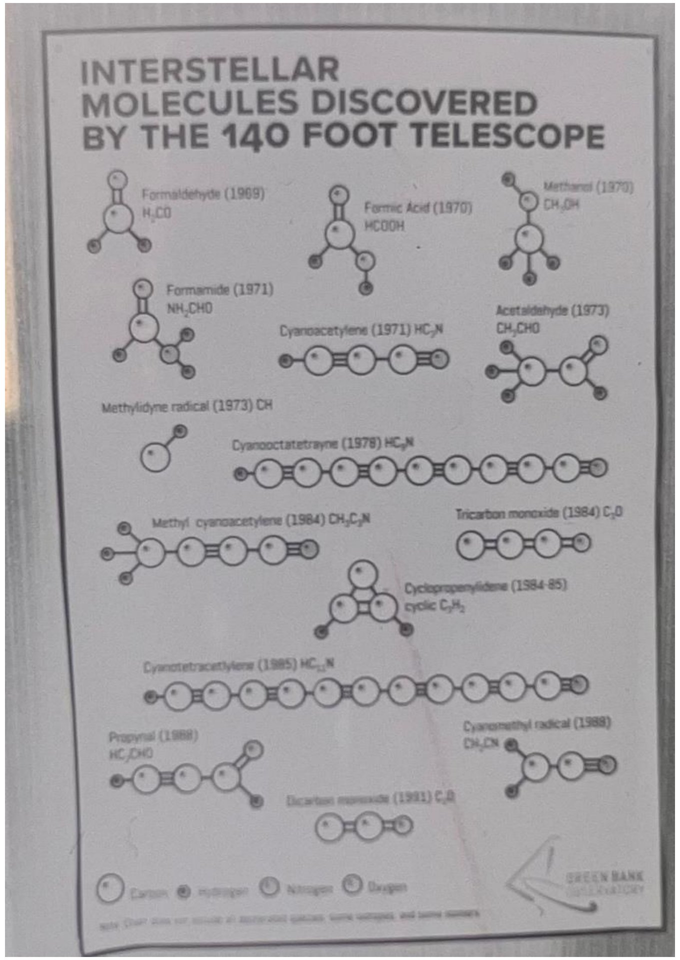

140 foot telescope

Facility	#	Facility	#
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NRAO 36-ft	33	SEST	2
GBT 100-m	28	SOFIA	2
NRAO/ARO 12-m	27	Hat Creek 20-ft	2
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Onsala 20-m	4	UKIRT	1
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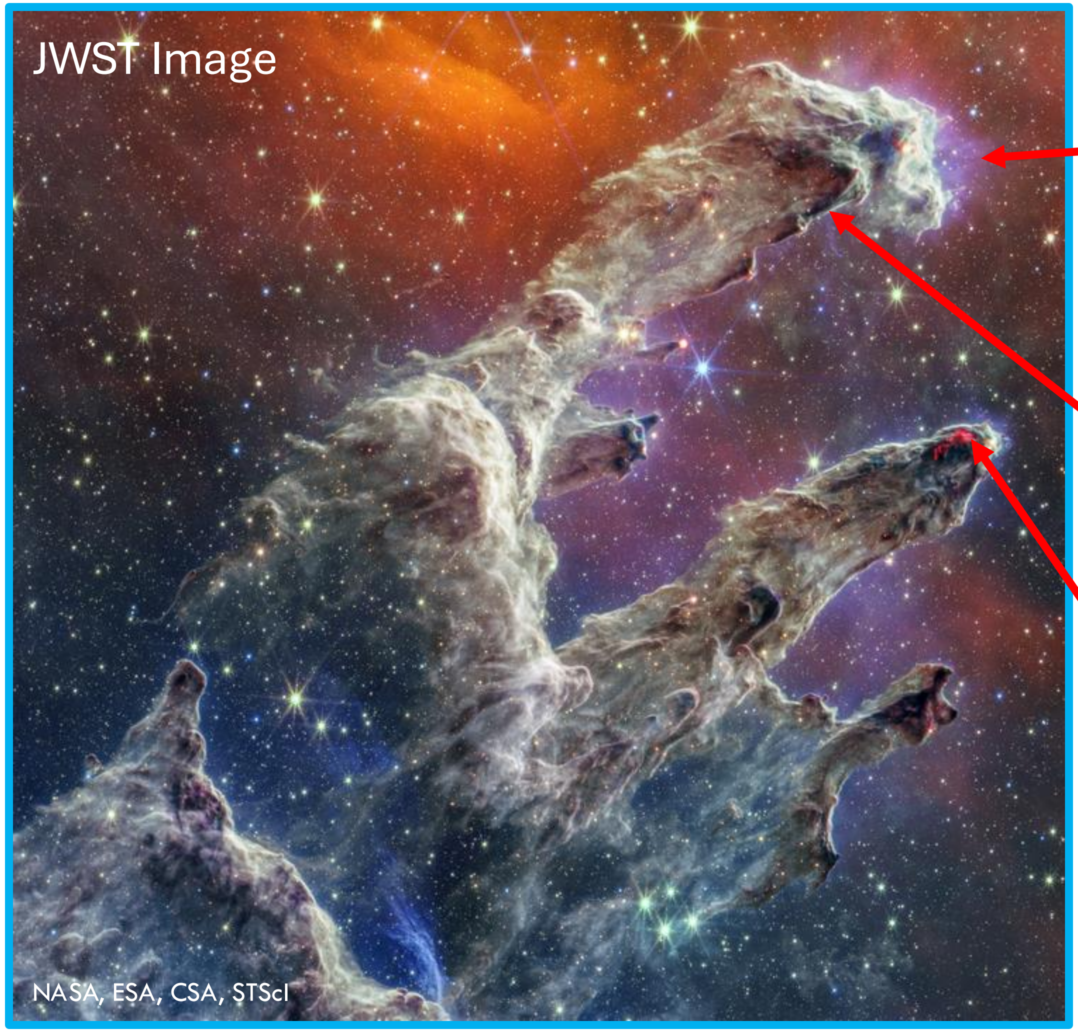
Importance of molecules in space!



Probes of a variety of **physical** (temperature, density, ionization, gas kinematics) and **environmental** (heating and cooling gas) **conditions**!

Diffuse Clouds:

- densities ~ 1- 10 cm^{-3}
- T ~ 100 K
- Starlight (UV radiation) can penetrate

Dense Clouds:

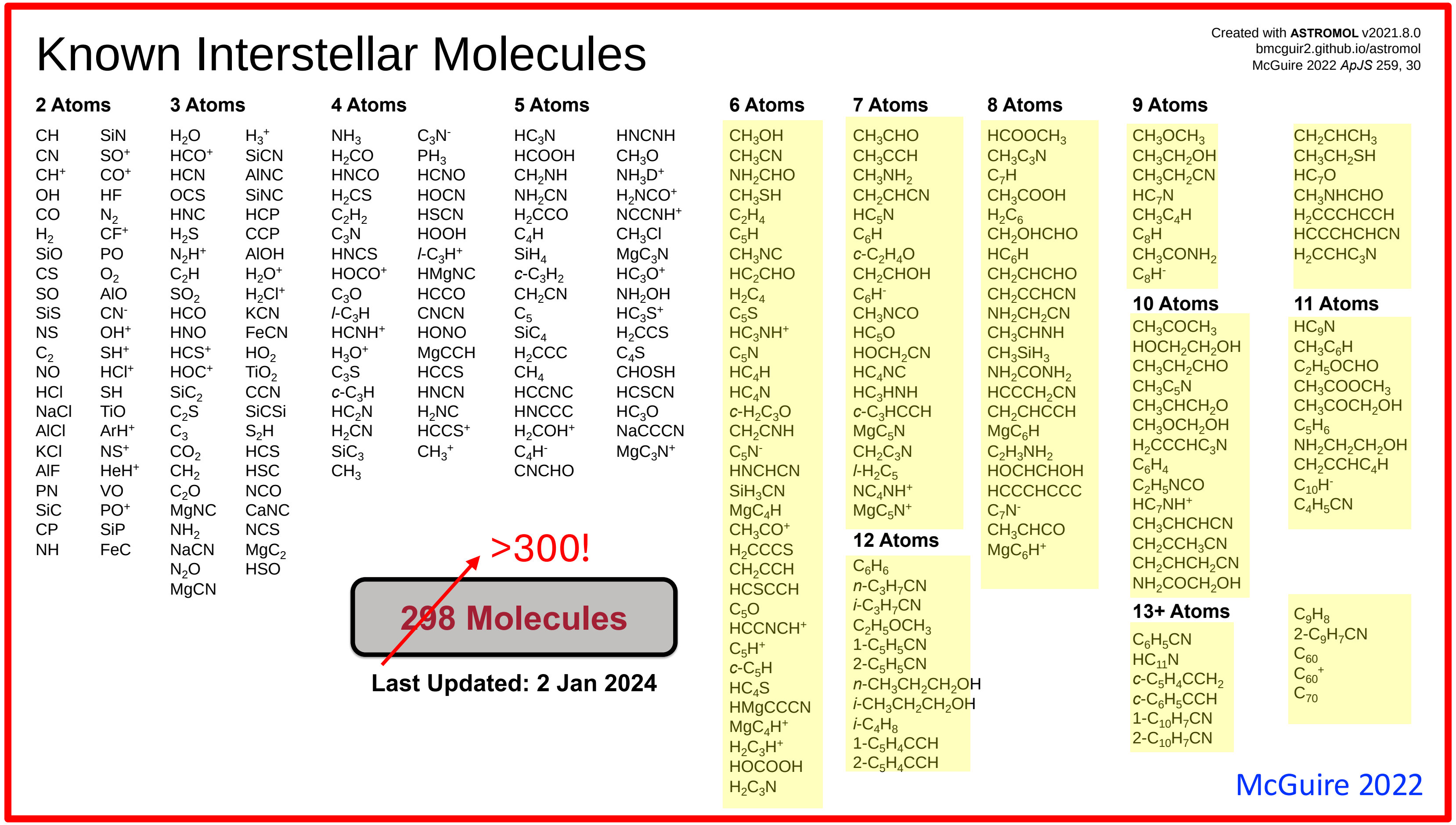
- densities ~ 10^3 - 10^6 cm^{-3}
- T ~ 10 - 100 K
- Starlight cannot penetrate

“Hot Cores”:

- densities ~ 10^3 - 10^6 cm^{-3}
- T ~ 10 - 300 K
- An embedded forming star

Importance of molecules in space!

Probes of a variety of **chemical conditions** (chemical processes, "Age" indicators, prebiotic chemistry (origin of life?)



Complex Organic Molecules

- Contains at least 6 or more atoms
- Contains at least one carbon atom

Herbst & van Dishoeck 2009

Of interest to astrochemists and astrobiologists, COMs are the **precursor molecules of prebiotic chemistry**

Understanding the formation of COMs in the various physical conditions throughout our universe is an active area of research!

Importance of molecules in space!

Probes of a variety of **chemical conditions** (chemical processes, "Age" indicators, prebiotic chemistry (origin of life?)

Known Interstellar Molecules

Created with **ASTROMOL** v2021.8.0
bmcguir2.github.io/astromol
McGuire 2022 *ApJS* 259, 30

2 Atoms

CH, CN, CH^+, OH, CO, H_2, SiO, CS, SO, SiS, NS, C_2, NO, HCl, $NaCl$, $AlCl$, KCl, AlF, PN, SiC, CP, NH

SiN, SO^+, CO^+, HF, N_2, CF^+, PO, O_2, AlO, CN^-, OH^+, SH^+, HCl^+, SH, TiO, ArH^+, NS^+, HeH^+, VO, PO^+, SiP, FeC

3 Atoms

H_2O, HCO^+, HCN, OCS, HNC, H_2S, N_2H^+, C_2H, SO_2, HCO, HNO, HCS^+, HOC^+, SiC_2, C_2S, C_3, CO_2, CH_2, C_2O, $MgNC$, NH_2, $NaCN$, N_2O, $MgCN$

H_3^+, $SiCN$, $AlNC$, $SiNC$, HCP, CCP, $AlOH$, H_2O^+, H_2Cl^+, KCN, $FeCN$, HO_2, TiO_2, CCN, $SiCSi$, S_2H, HCS, HSC, NCO, $CaNC$, NCS, MgC_2, HSO

4 Atoms

NH_3, H_2CO, $HNCO$, H_2CS, C_2H_2, C_3N, $HNCS$, $HOCO^+$, C_3O, *l*-C_3H, $HCNH^+$, H_3O^+, C_3S, *c*-C_3H, HC_2N, H_2CN, SiC_3, CH_3

C_3N^-, PH_3, $HCNO$, $HOCN$, $HSCN$, $HOOH$, *l*-C_3H^+, $HMgNC$, $HCCO$, $CNCN$, $HONO$, $MgCCH$, $HCCS$, $HNCN$, H_2NC, $HCCS^+$, CH_3^+

5 Atoms

HC_3N, $HCOOH$, CH_2NH, NH_2CN, H_2CCO, C_4H, SiH_4, *c*-C_3H_2, CH_2CN, C_5, SiC_4, H_2CCC, CH_4, $HCCNC$, $HNCCC$, H_2COH^+, C_4H^-, $CNCHO$

$HNCNH$, CH_3O, NH_3D^+, H_2NCO^+, $NCCNH^+$, CH_3Cl, MgC_3N, HC_3O^+, NH_2OH, HC_3S^+, H_2CCS, C_4S, $CHOSH$, $HCSCN$, HC_3O, $NaCCCN$, MgC_3N^+

6 Atoms

CH_3OH, CH_3CN, NH_2CHO, CH_3SH, C_2H_4, C_5H, CH_3NC, HC_2CHO, H_2C_4, C_5S, HC_3NH^+, C_5N, HC_4H, HC_4N, *c*-H_2C_3O, CH_2CNH, C_5N^-, $HNCHCN$, SiH_3CN, MgC_4H, CH_3CO^+, H_2CCCS, CH_2CCH, $HCSCCH$, C_5O, $HCCNCH^+$, C_5H^+, *c*-C_5H, HC_4S, $HMgCCCN$, MgC_4H^+, $H_2C_3H^+$, $HOCOOH$, H_2C_3N

7 Atoms

CH_3CHO, CH_3CCH, CH_3NH_2, CH_2CHCN, HC_5N, C_6H, *c*-C_2H_4O, CH_2CHOH, C_6H^-, CH_3NCO, HC_5O, $HOCH_2CN$, HC_4NC, HC_3HNH, *c*-C_3HCCH, MgC_5N, CH_2C_3N, *l*-H_2C_5, NC_4NH^+, MgC_5N^+

12 Atoms

C_6H_6, *n*-C_3H_7CN, *i*-C_3H_7CN, $C_2H_5OCH_3$, 1-C_5H_5CN, 2-C_5H_5CN, *n*-$CH_3CH_2CH_2OH$, *i*-$CH_3CH_2CH_2OH$, *i*-C_4H_8, 1-C_5H_4CCH, 2-C_5H_4CCH

8 Atoms

$HCOOCH_3$, CH_3C_3N, C_7H, CH_3COOH, H_2C_6, CH_2OHCHO, HC_6H, CH_2CHCHO, CH_2CCHCN, NH_2CH_2CN, CH_3CHNH, CH_3SiH_3, NH_2CONH_2, $HCCCH_2CN$, CH_2CHCCH, MgC_6H, $C_2H_3NH_2$, $HOCHCHOH$, $HCCCHCCC$, C_7N^-, CH_3CHCO, MgC_6H^+

9 Atoms

CH_3OCH_3, CH_3CH_2OH, CH_3CH_2CN, HC_7N, CH_3C_4H, C_8H, CH_3CONH_2, C_8H^-

CH_2CHCH_3, CH_3CH_2SH, HC_7O, CH_3NHCHO, $H_2CCCHCCH$, $HCCCHCHCN$, H_2CCHC_3N

10 Atoms

CH_3COCH_3, $HOCH_2CH_2OH$, CH_3CH_2CHO, CH_3C_5N, CH_3CHCH_2O, CH_3OCH_2OH, H_2CCCHC_3N, C_6H_4, C_2H_5NCO, HC_7NH^+, $CH_3CHCHCN$, CH_2CCH_3CN, CH_2CHCH_2CN, NH_2COCH_2OH

11 Atoms

HC_9N, CH_3C_6H, C_2H_5OCHO, CH_3COOCH_3, CH_3COCH_2OH, C_5H_6, $NH_2CH_2CH_2OH$, CH_2CCHC_4H, $C_{10}H^-$, C_4H_5CN

13+ Atoms

C_6H_5CN, $HC_{11}N$, *c*-$C_5H_4CCH_2$, *c*-C_6H_5CCH, 1-$C_{10}H_7CN$, 2-$C_{10}H_7CN$

C_9H_8, 2-C_9H_7CN, C_{60}, C_{60}^+, C_{70}

>300!

~~298~~ Molecules

Last Updated: 2 Jan 2024

McGuire 2022

Complex Organic Molecules

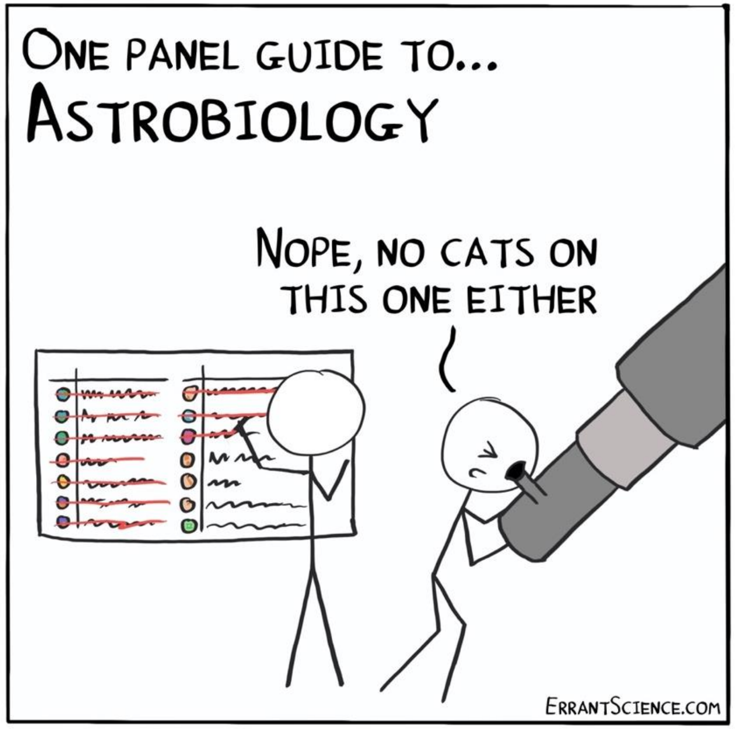
- Contains at least 6 or more atoms
- Contains at least one carbon atom

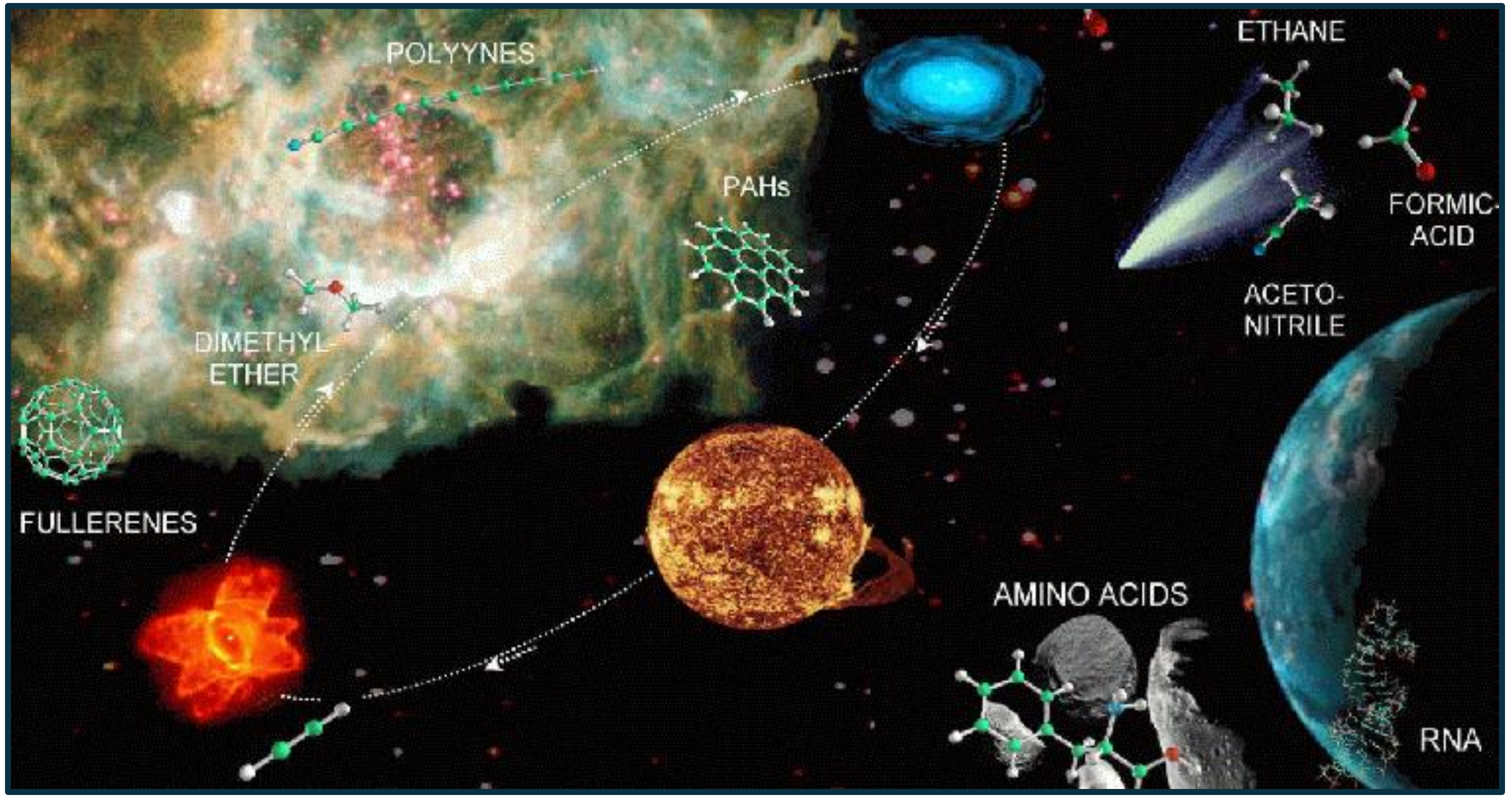
Herbst & van Dishoeck 2009

CH_3OH: Methyl or wood alcohol, is extremely toxic!

CH_3CHO: Green apple smell! Found in fermented foods, including yogurt and aged wines

Big Questions in Astrochemistry: COMs as Prebiotic Precursors?



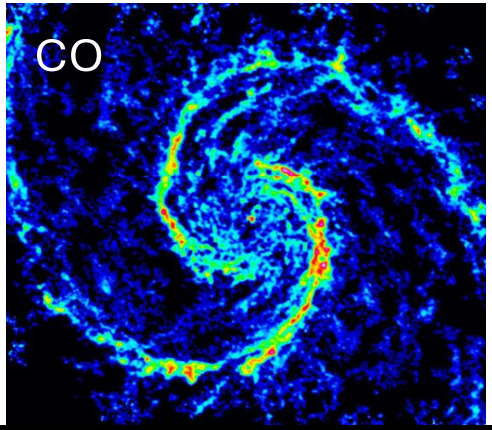


http://www.esa.int/spaceinimages/Images/2001/05/Astrobiology

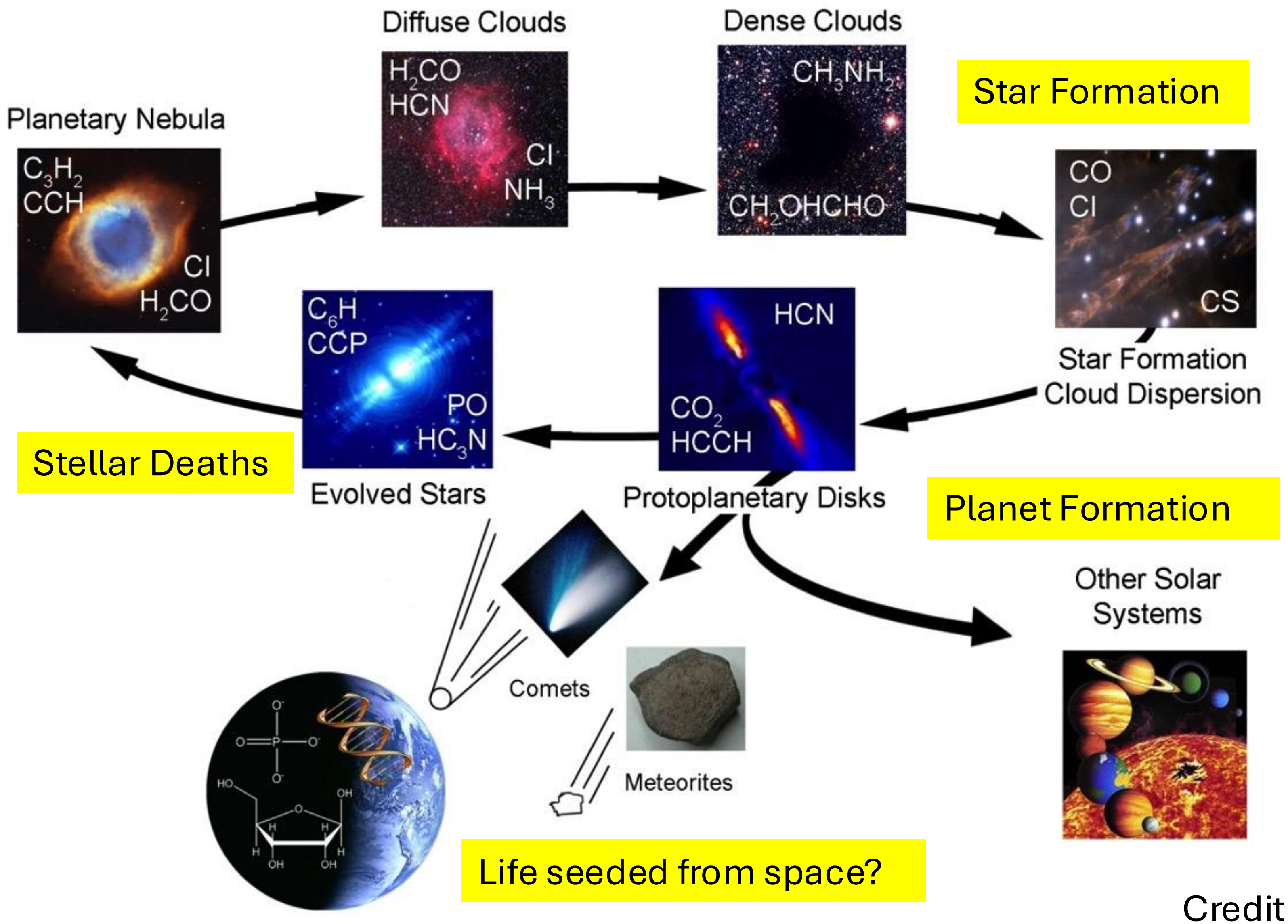
Do organic molecules synthesized in space contribute to the chemical evolution needed for the ***emergence of life on Earth***?

Molecular Life Cycle

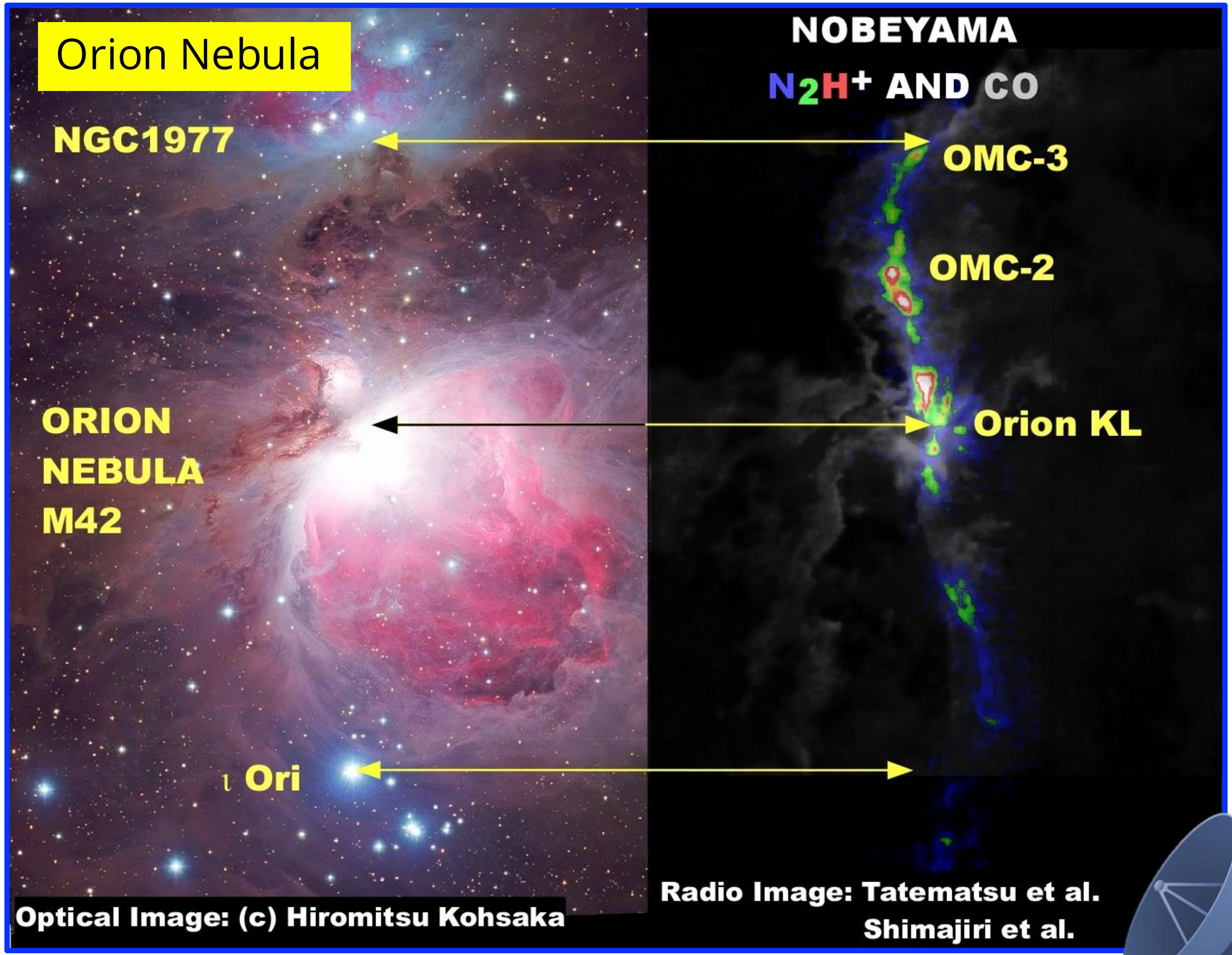
Within Galaxies... →



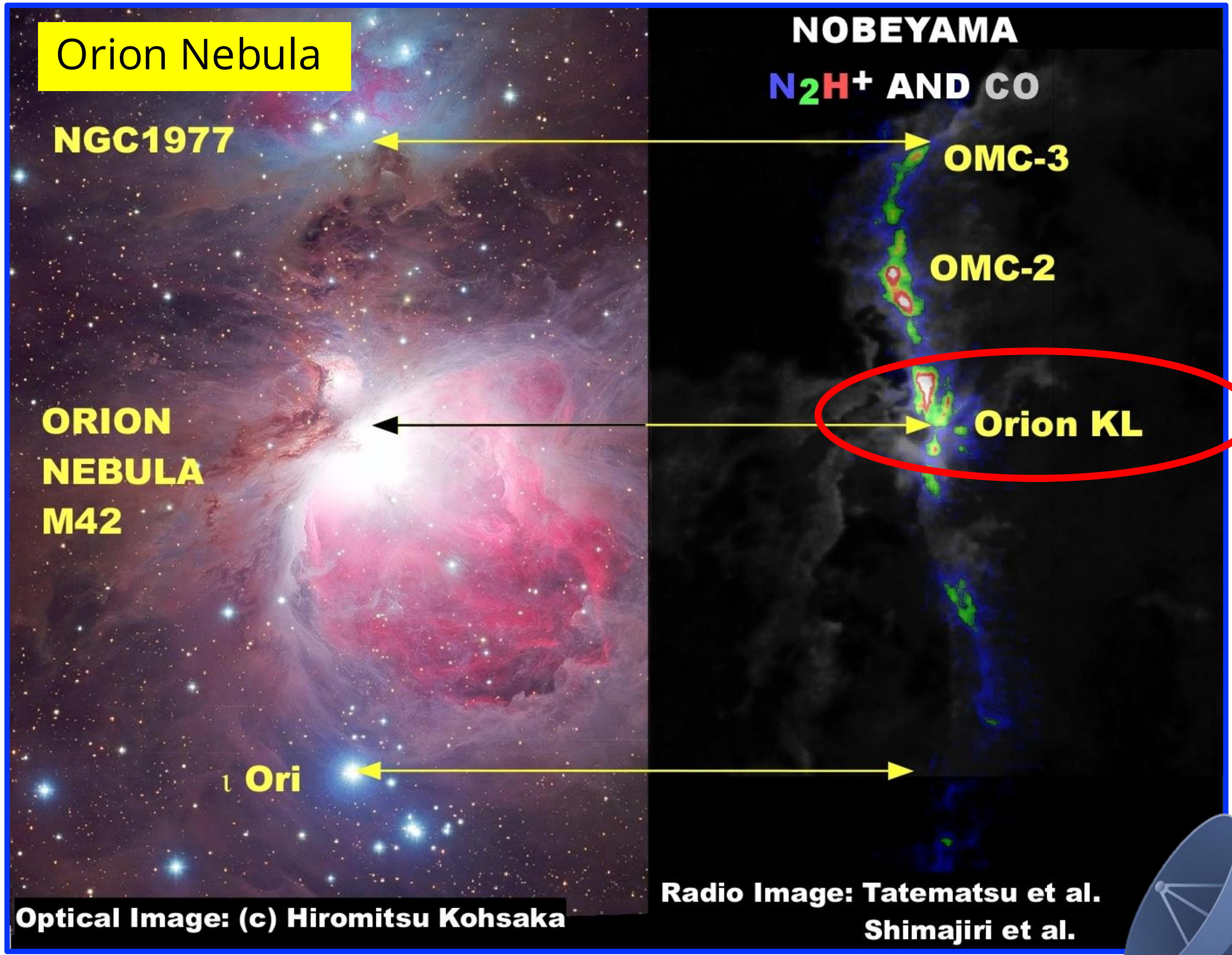
M51 – Whirlpool Galaxy



Credit: L. Ziurys



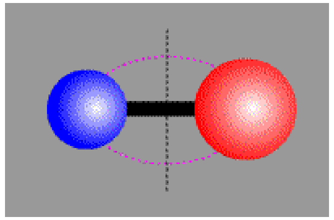
https://www.nro.nao.ac.jp/~kt/html/kt-e.html

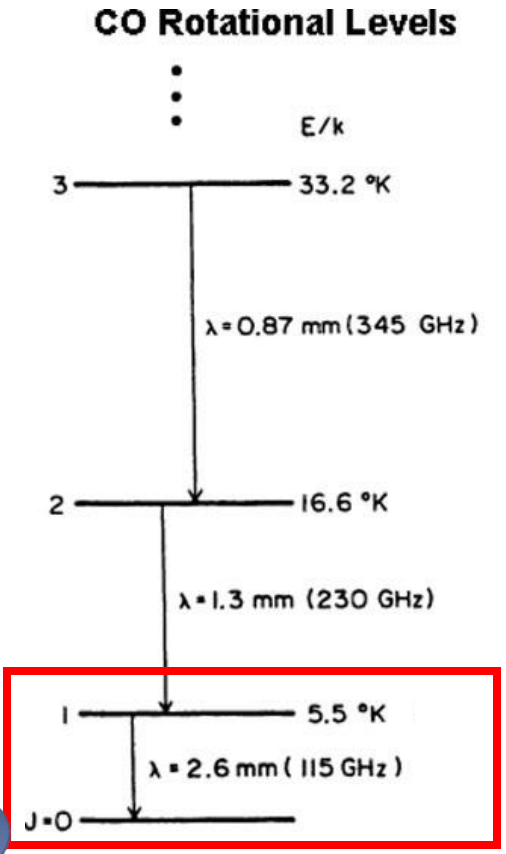


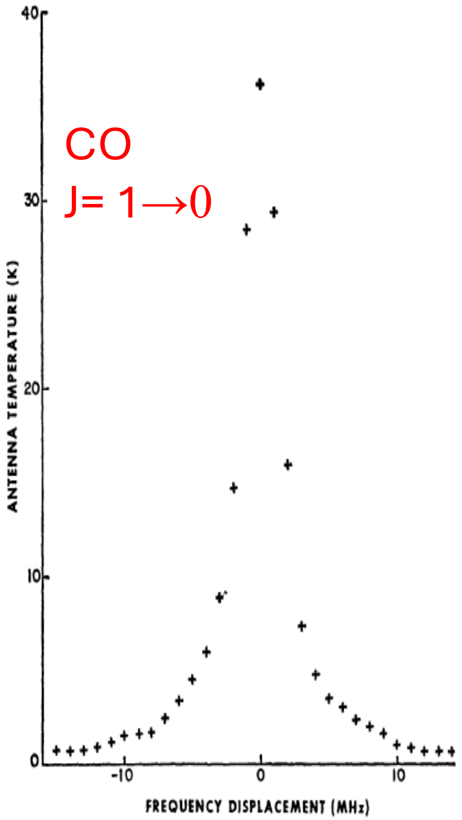
https://www.nro.nao.ac.jp/~kt/html/kt-e.html

Discovery of CO

in the Star Forming Region,
Orion KL at 115 GHz
(J = 1 → 0 transition)
in 1970 at **Kitt Peak, Arizona!**





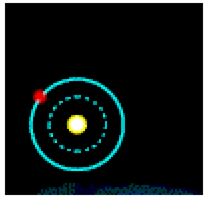


Wilson et al., 1970

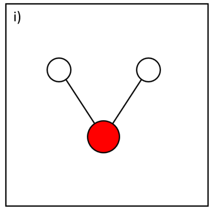
Spectroscopy: Primary Molecule Identification Method!

- Molecular Energy Levels consist of:

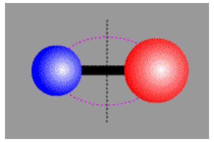
Credit: L. Ziurys



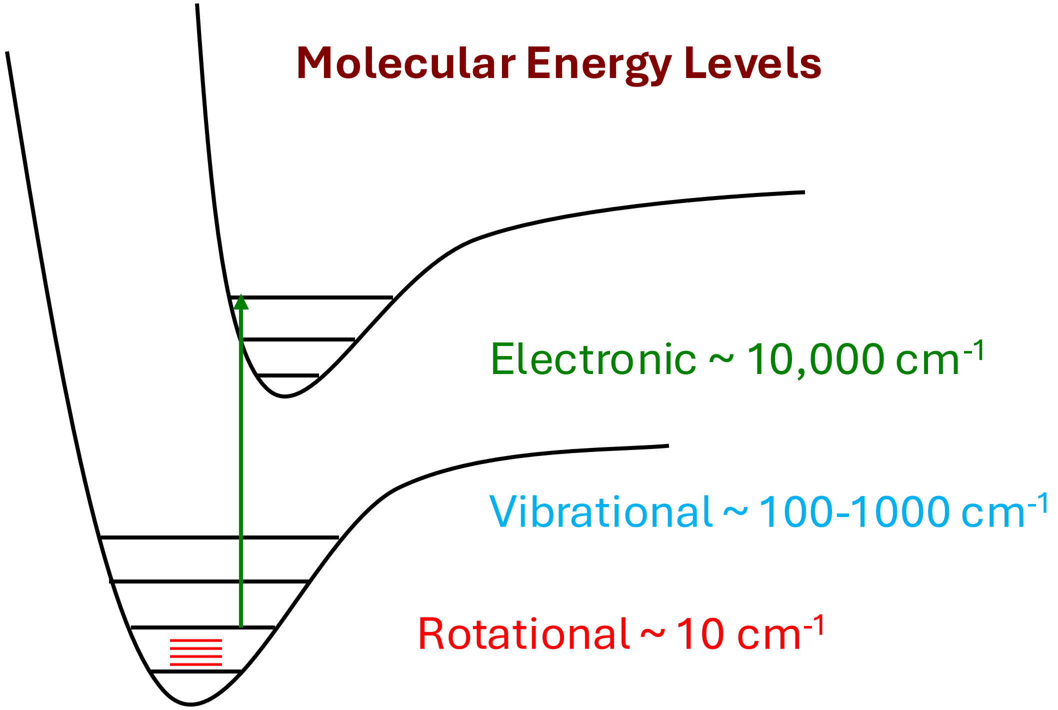
1) ELECTRONIC STATES
   - electrons change levels
   - energies in visible, UV



2) VIBRATIONAL STATES
   - normal modes of nuclear motions
   - occur in infrared region



3) ROTATIONAL STATES
   - end-on-end motion of nuclei
   - energies in microwave/millimeter-wave regions



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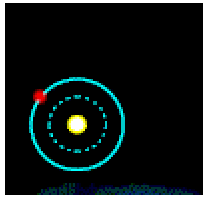

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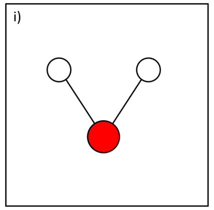

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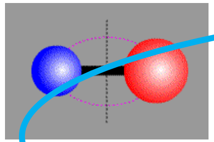

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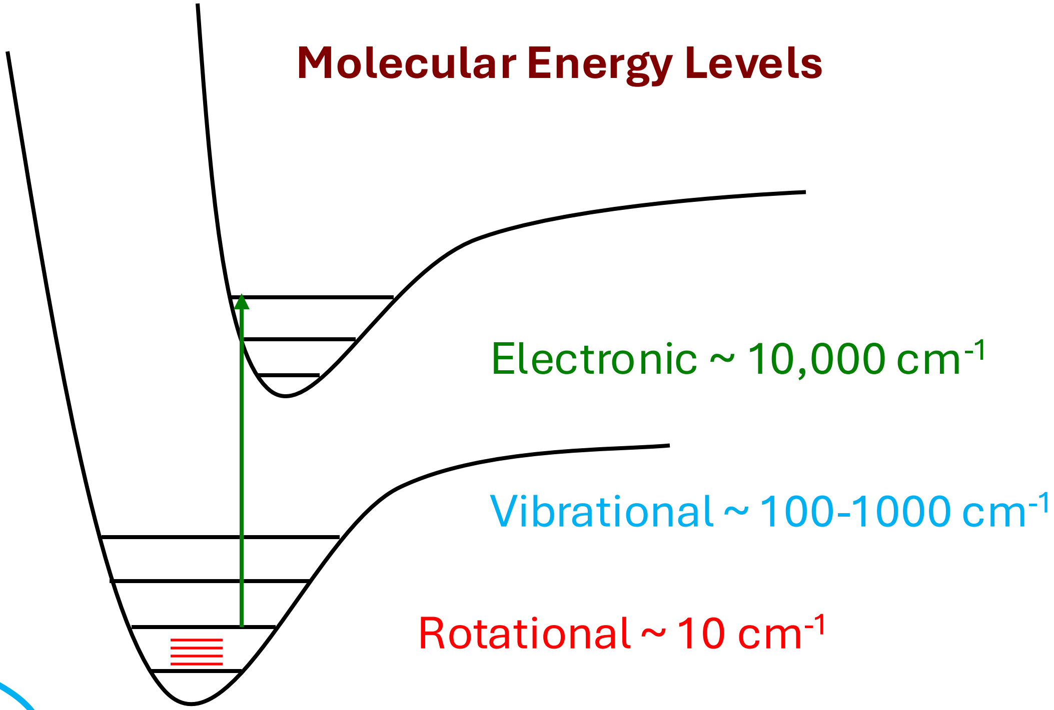


- Electronic states have **vibrational/rotational structure**
- Vibrational states have **rotational structure**

Spectroscopy: Primary Molecule Identification Method!

ELECTRONIC STATES

Credit: L. Ziurys

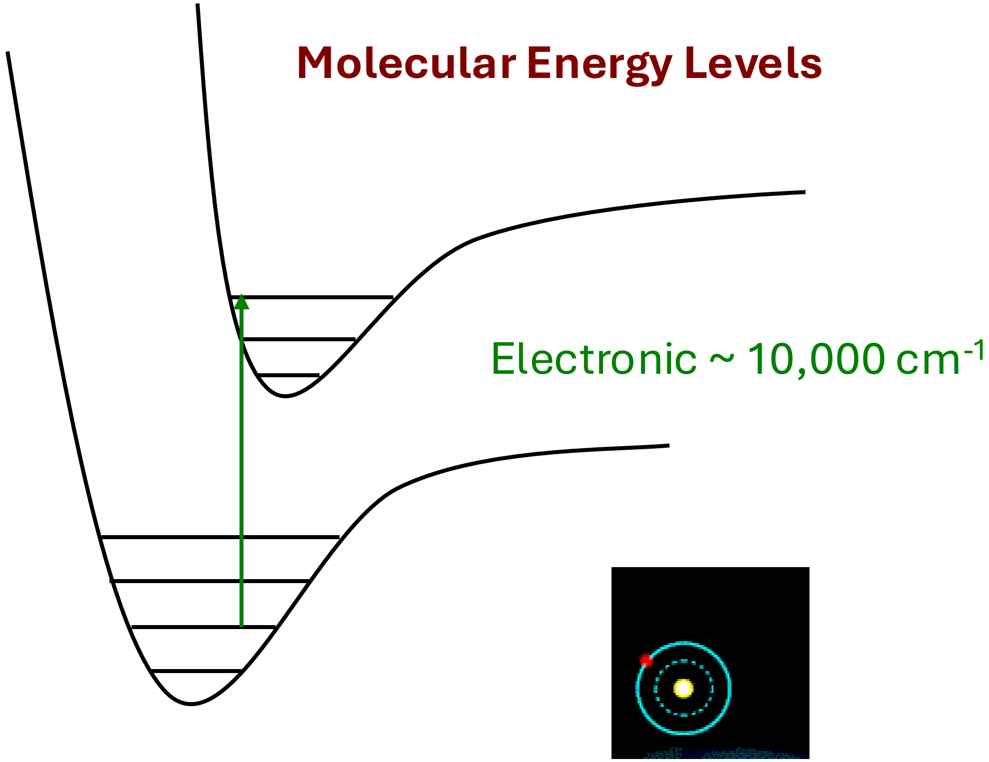
- Need energies ~ 0.5 – 1 eV to excite molecules (~ 5,000 – 10,000 K)
- Need a **UV/optical "pump"** to excite levels, provided by background star
- Molecular material in front of source cannot be dense (< 100 cm^{-2})

  ⇒ used in Diffuse Clouds
- Diffuse clouds contain primarily diatomic species

  ⇒ UV radiation photo-dissociates molecules readily
- Almost always **2-3 atom species**

  - relatively simple spectra observed in **ABSORPTION**
- Also important in stellar photospheres of cool stars

  - molecules can survive radiation field



Spectroscopy: Primary Molecule Identification Method!

ELECTRONIC STATES

Photospheric Spectra (Stars)

Credit: L. Ziurys

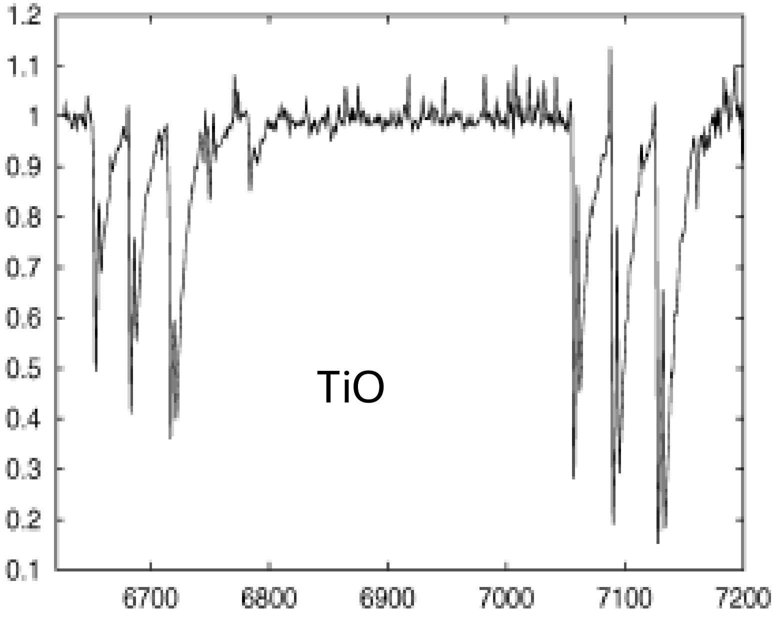


Figure 5. The 6630–7200 Å region of the JD 245 1221 optical spectrum of IRAS 08182−6000, showing the γ (1, 0), (2,1) and (0, 0) bands of TiO and some of the atomic emission lines recorded in Table 4.

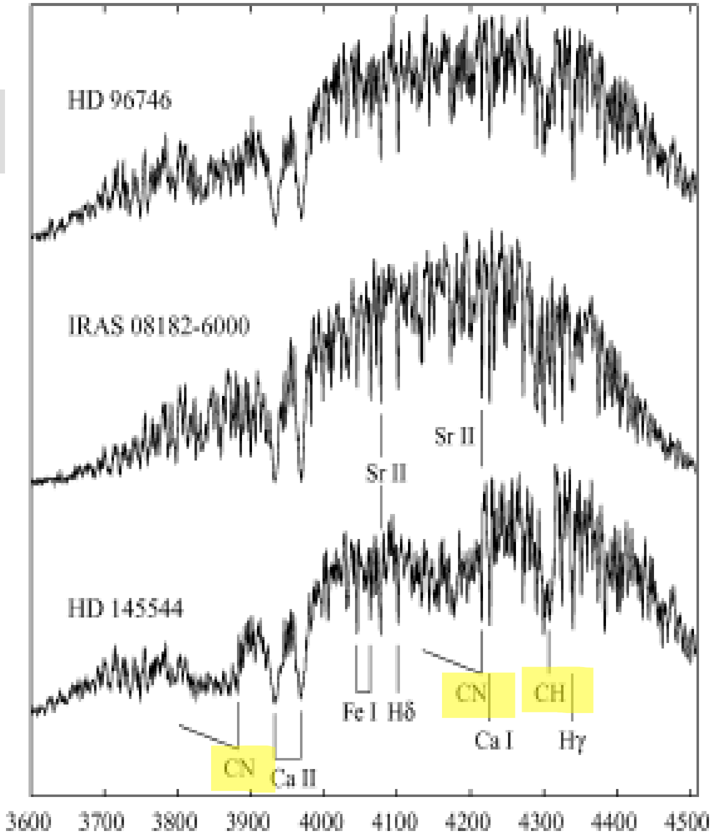


Figure 4. The spectrum of IRAS 08182−6000 (JD 244 9426) compared with those of HD 96746, G2Iab (above) and HD 145544, G2Ib-II (below).

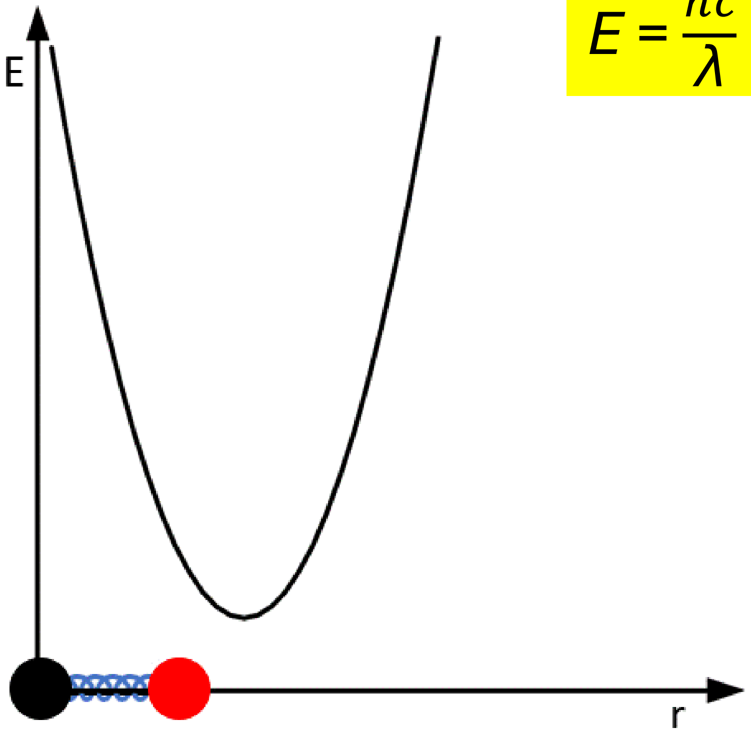
CN
&
CH

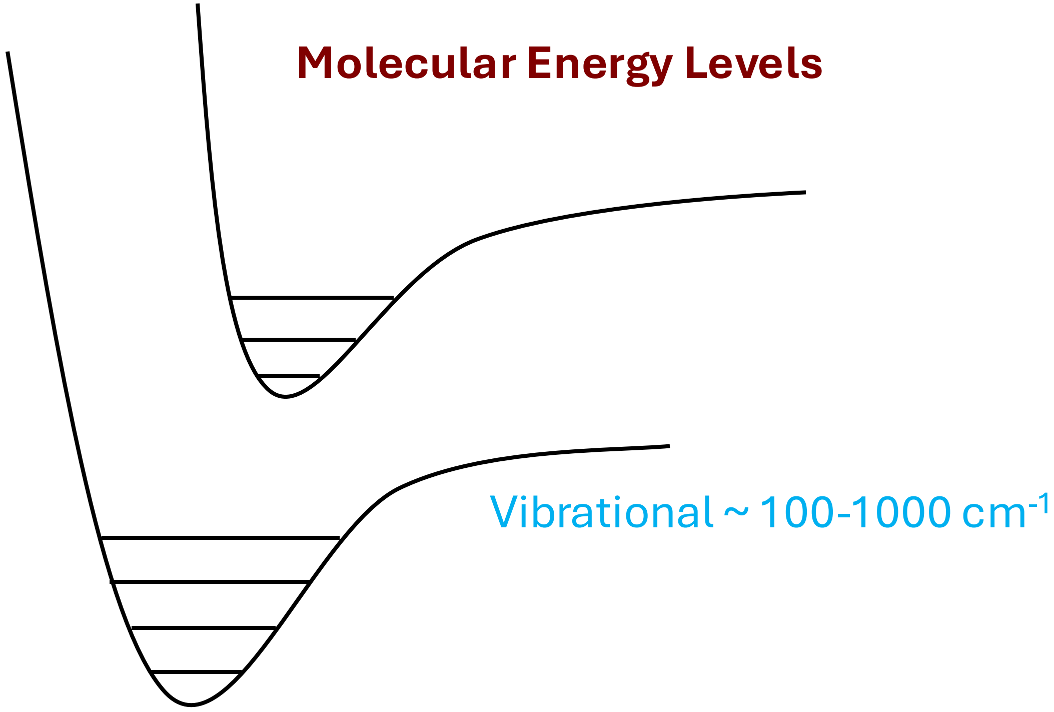
Spectroscopy: Primary Molecule Identification Method!

VIBRATIONAL STATES

- For a simple two-atom molecule, think back to your 'simple harmonic oscillator' whose energy can be quantized

$$E = \frac{hc}{\lambda} = hv$$





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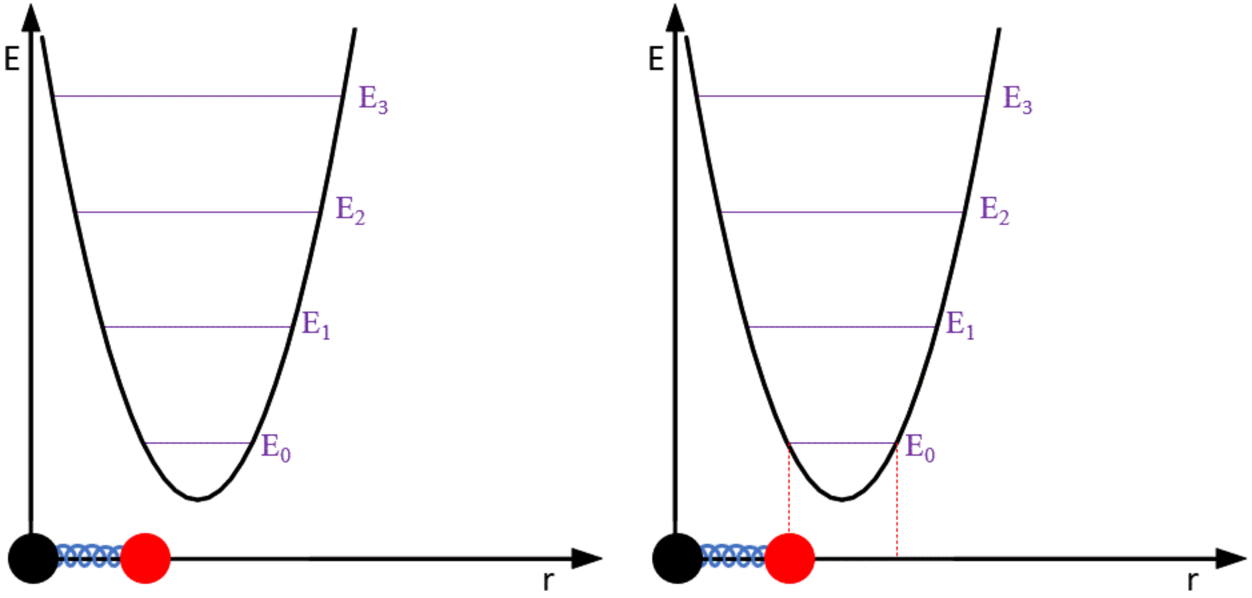
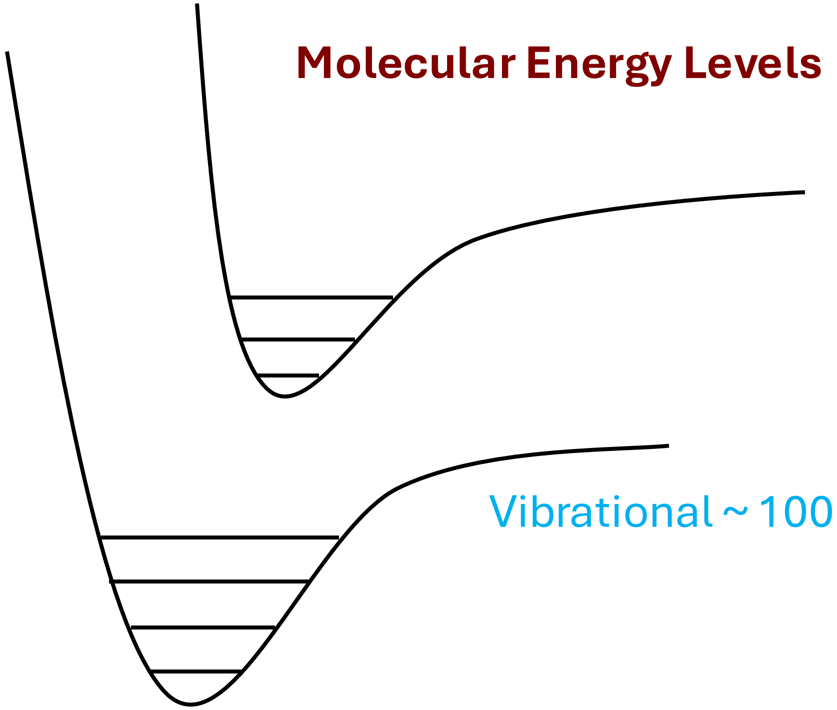


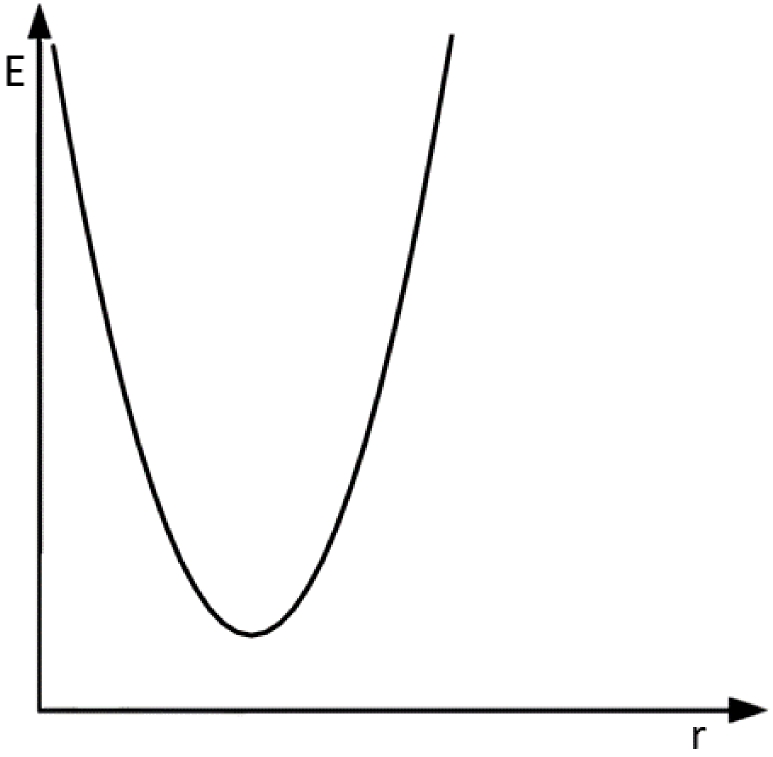


Vibrational ~ 100-1000 cm^{-1}

Spectroscopy: Primary Molecule Identification Method!

VIBRATIONAL STATES

- In the real world, eventually your 'spring snaps'
- The gap between higher excited states thus begins to narrow



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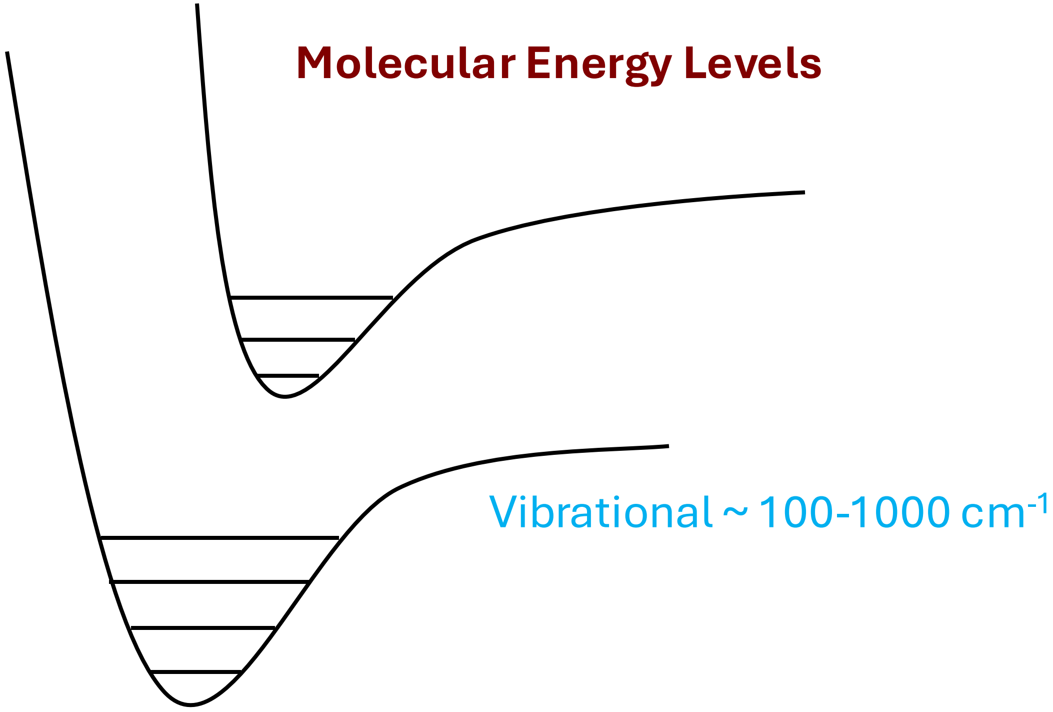
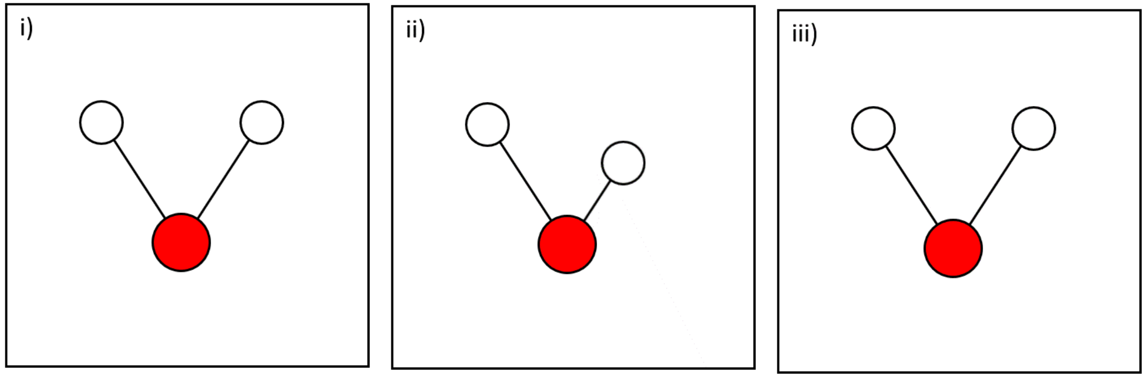


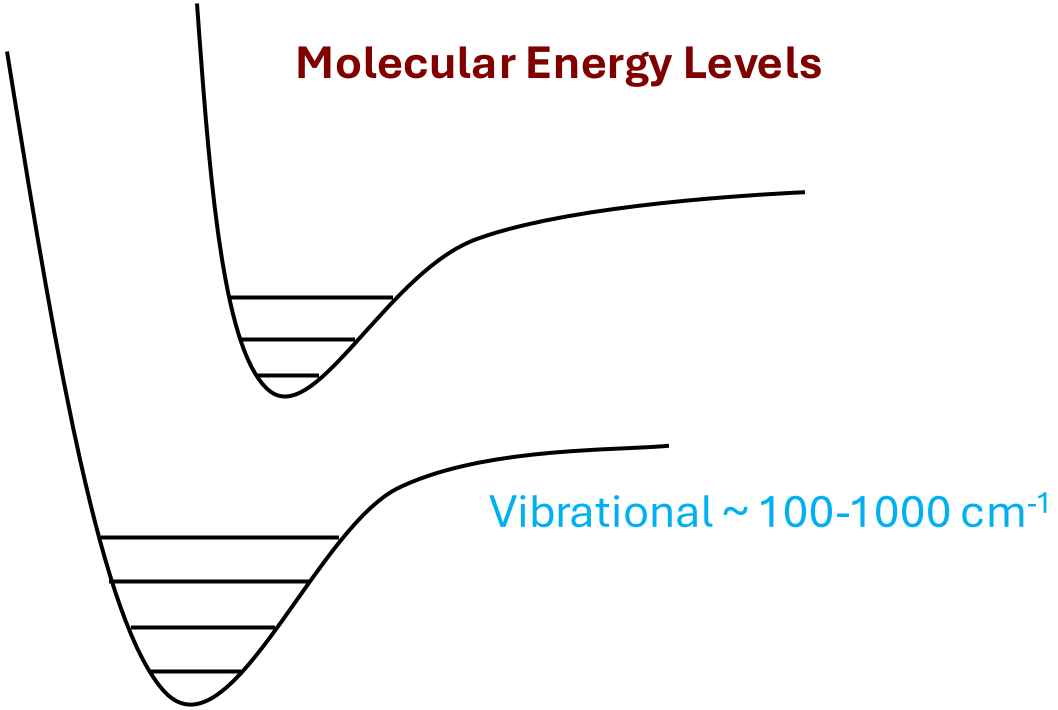
Spectroscopy: Primary Molecule Identification Method!

VIBRATIONAL STATES

- For molecules with several atoms, the type of possible vibrations increases, and more fundamental bands observed!
- The total number of possible vibrations for a molecule is equal to 3N-6 where N is the # of atoms in the molecule
  - E.g., water, H_2O, has 3!



i) symmetric stretch, (ii) asymmetric stretch and (iii) bending modes.



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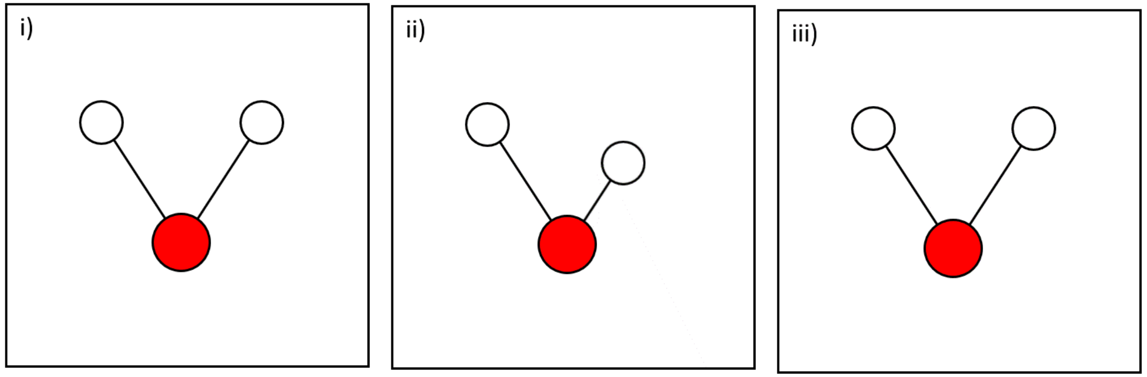

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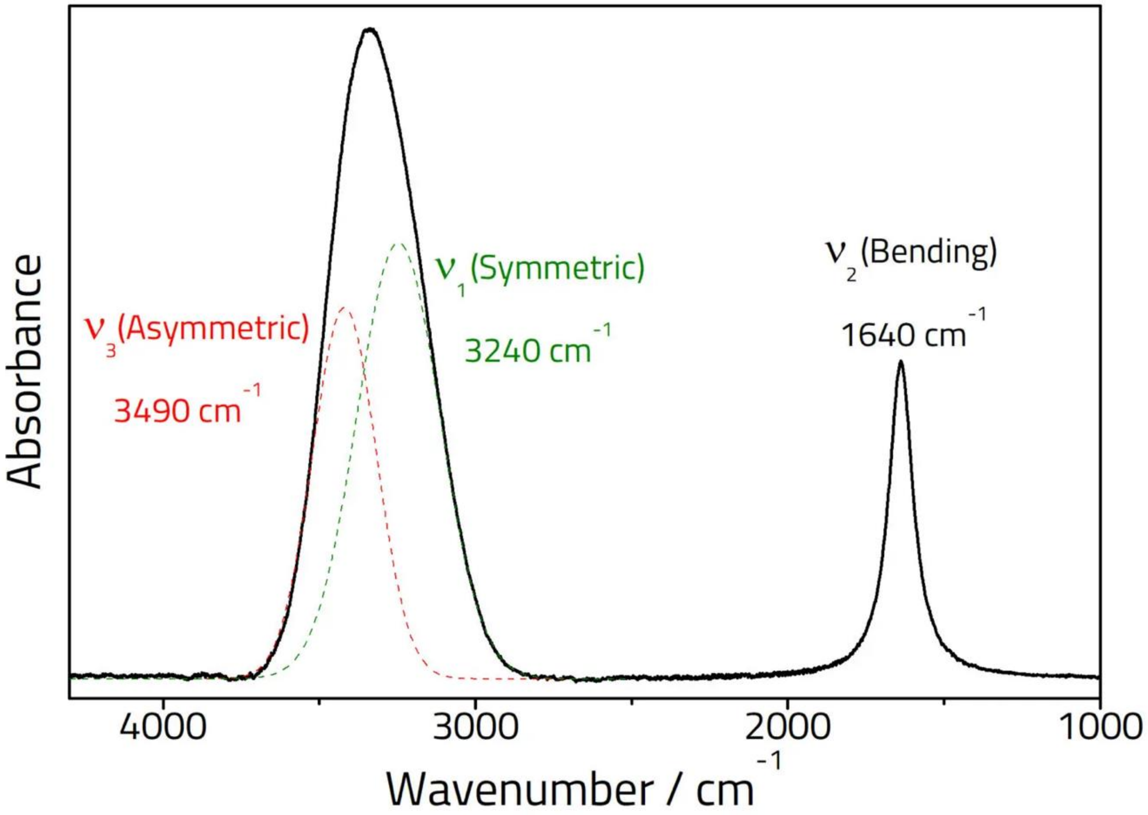

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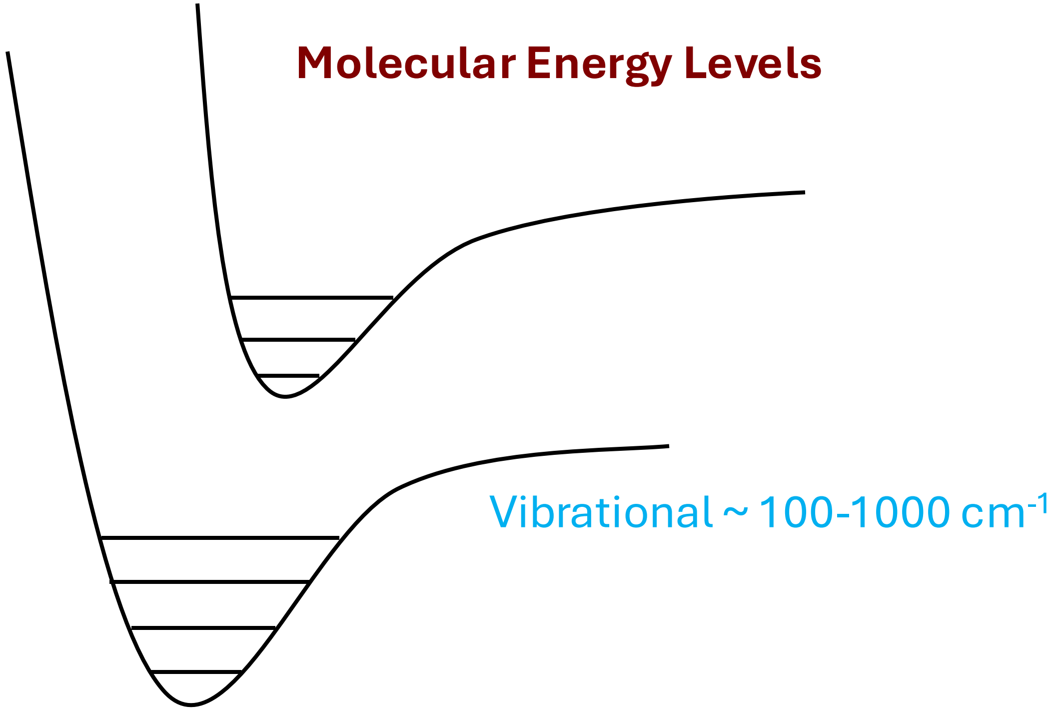
Spectroscopy: Primary Molecule Identification Method!

VIBRATIONAL STATES

- Need **energies** ~ 200 – 2000 cm^{-1} to excite molecules (300 - 3000 K)
- Need an **IR "pump"** to excite levels: background source
- Provided by **DUST from Circumstellar Envelopes**: strong IR emission background
- Young Protostar as background: **IR source**
- Density restrictions not as high as in optical region
- Used to study *chemical composition* of ***circumstellar shells*** close to stellar photosphere
- Molecules in denser material near **cloud cores**
- Spectra primarily observed **in absorption, except H_2**
- Useful for symmetric molecules
  - HCCH, H_3^+, CCC, H_2CCH_2

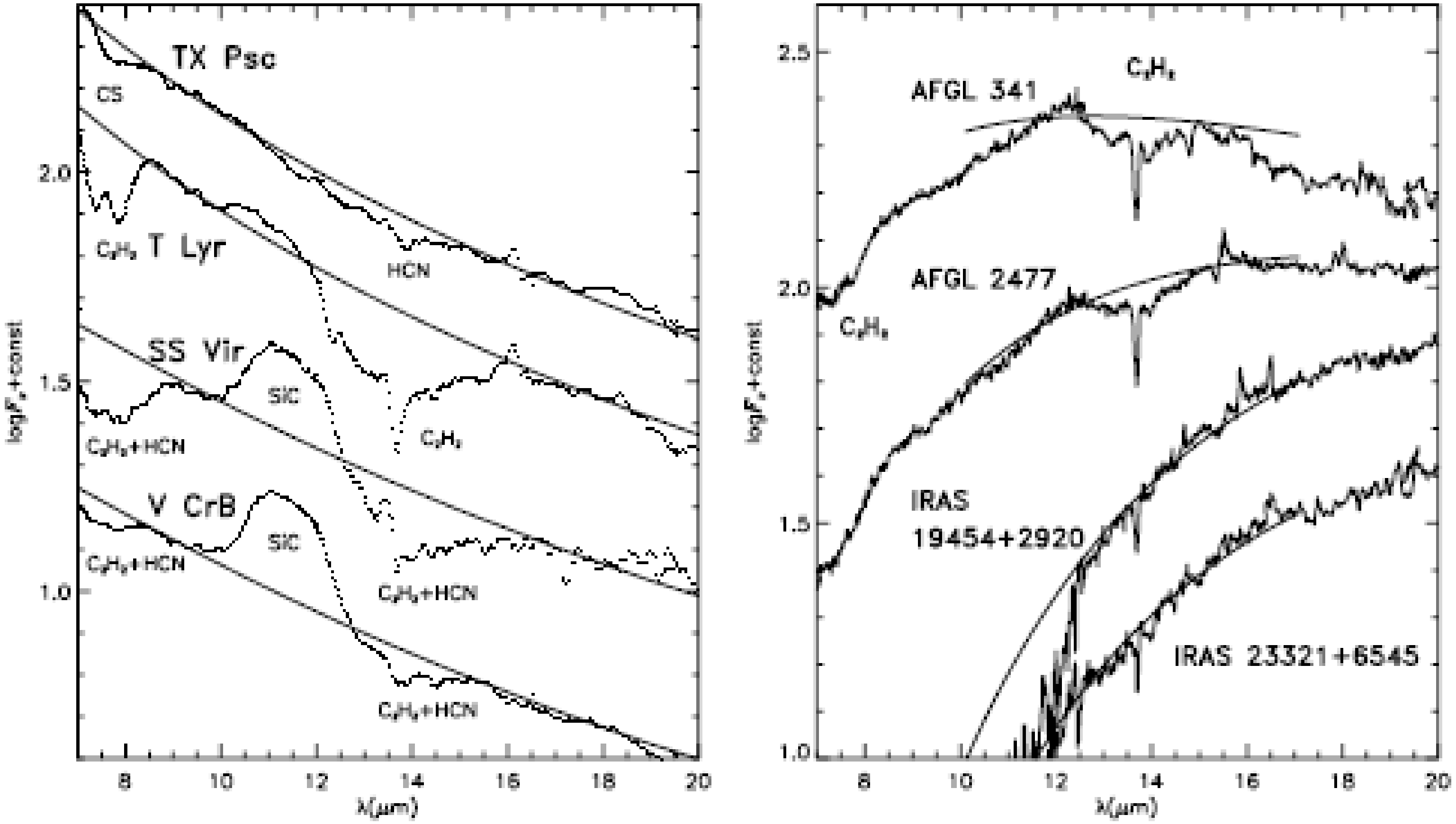
Credit: L. Ziurys



Spectroscopy: Primary Molecule Identification Method!

VIBRATIONAL STATES

C_2H_2 & HCN Vibrational Spectra around Evolved Stars



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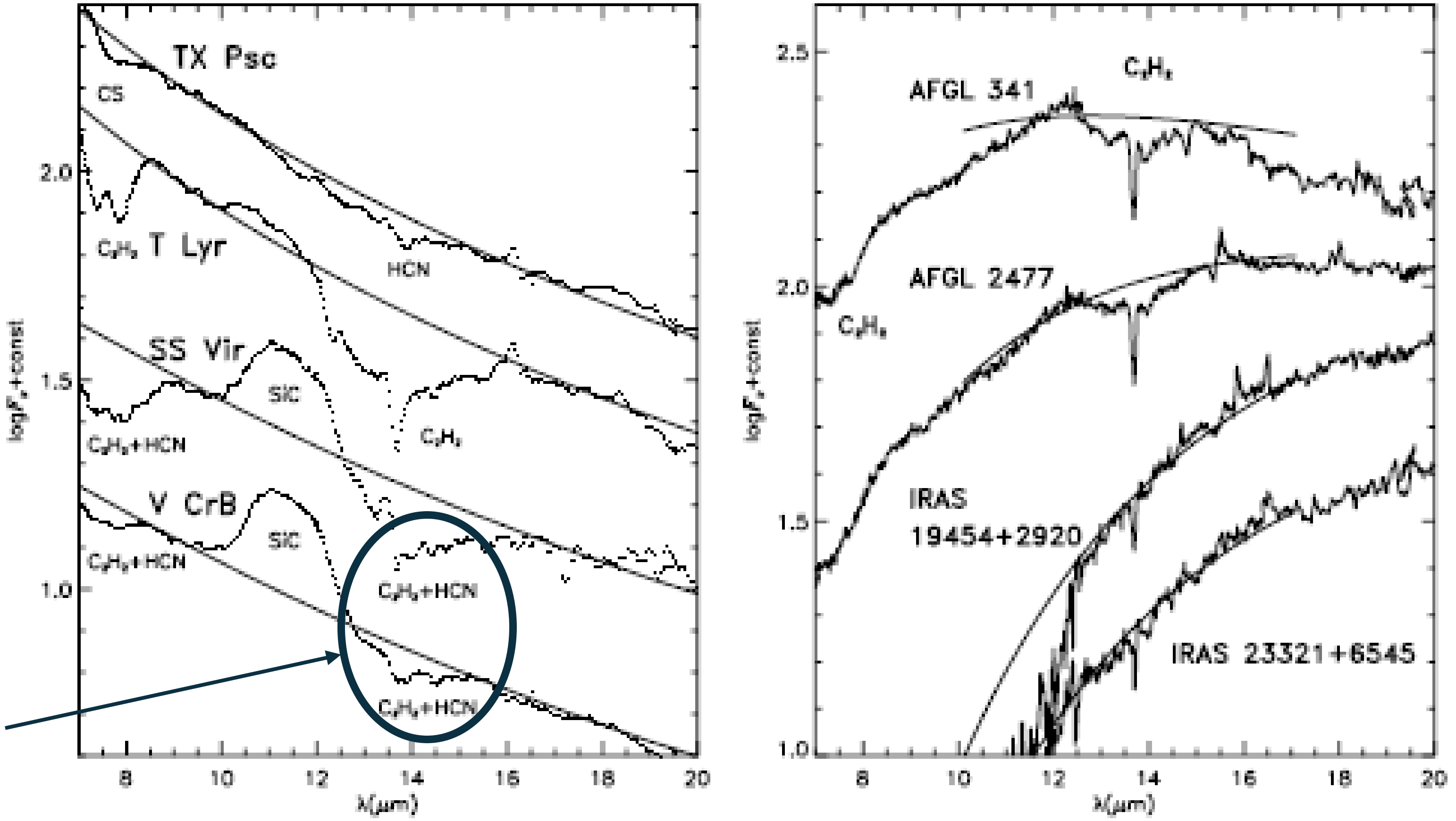
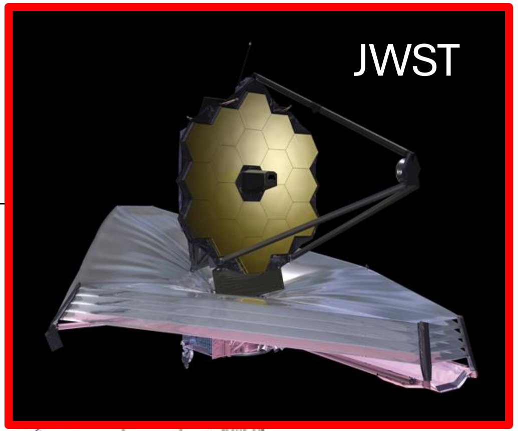


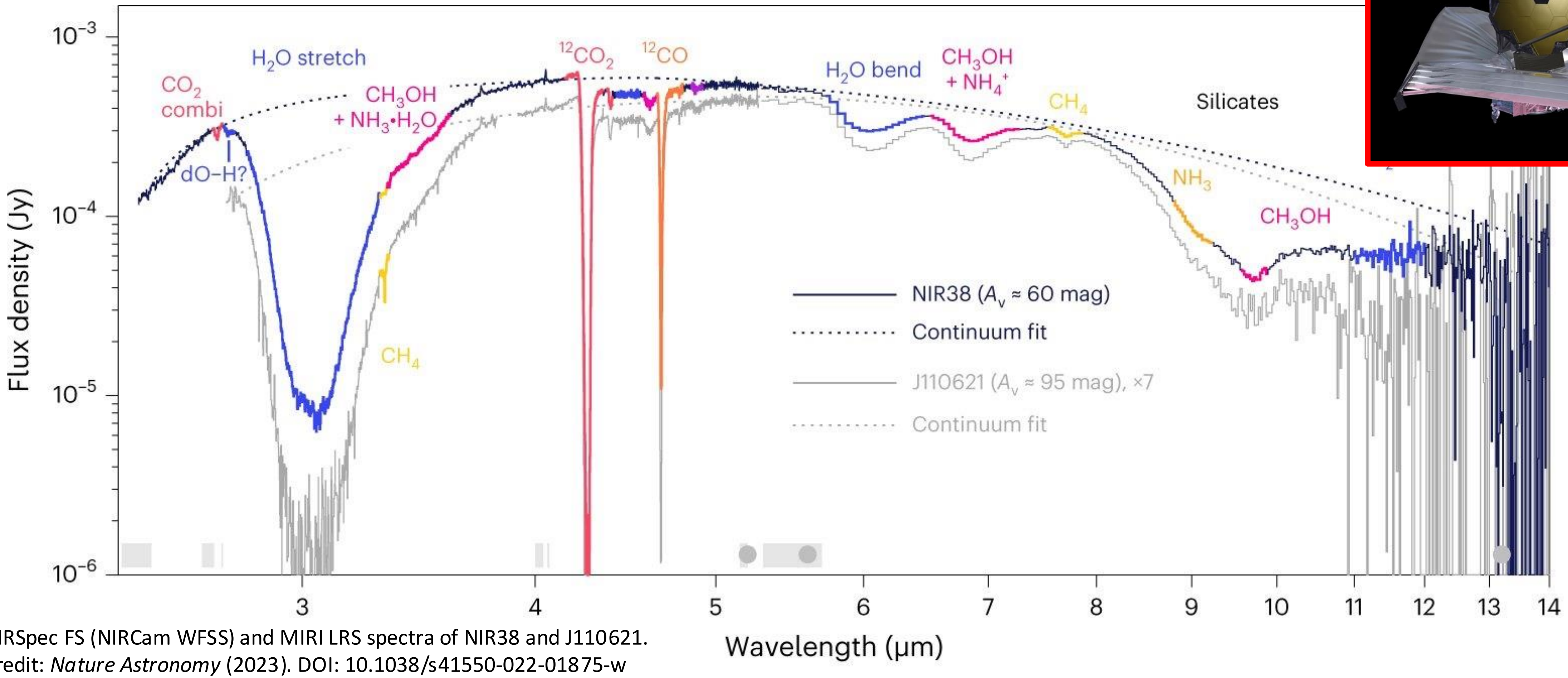
Often hard to distinguish individual modes!

Spectroscopy: Primary Molecule Identification Method!



VIBRATIONAL STATES

IR Spectra of Star-Forming Core



NIRSpec FS (NIRCam WFSS) and MIRI LRS spectra of NIR38 and J110621.
Credit: *Nature Astronomy* (2023). DOI: 10.1038/s41550-022-01875-w

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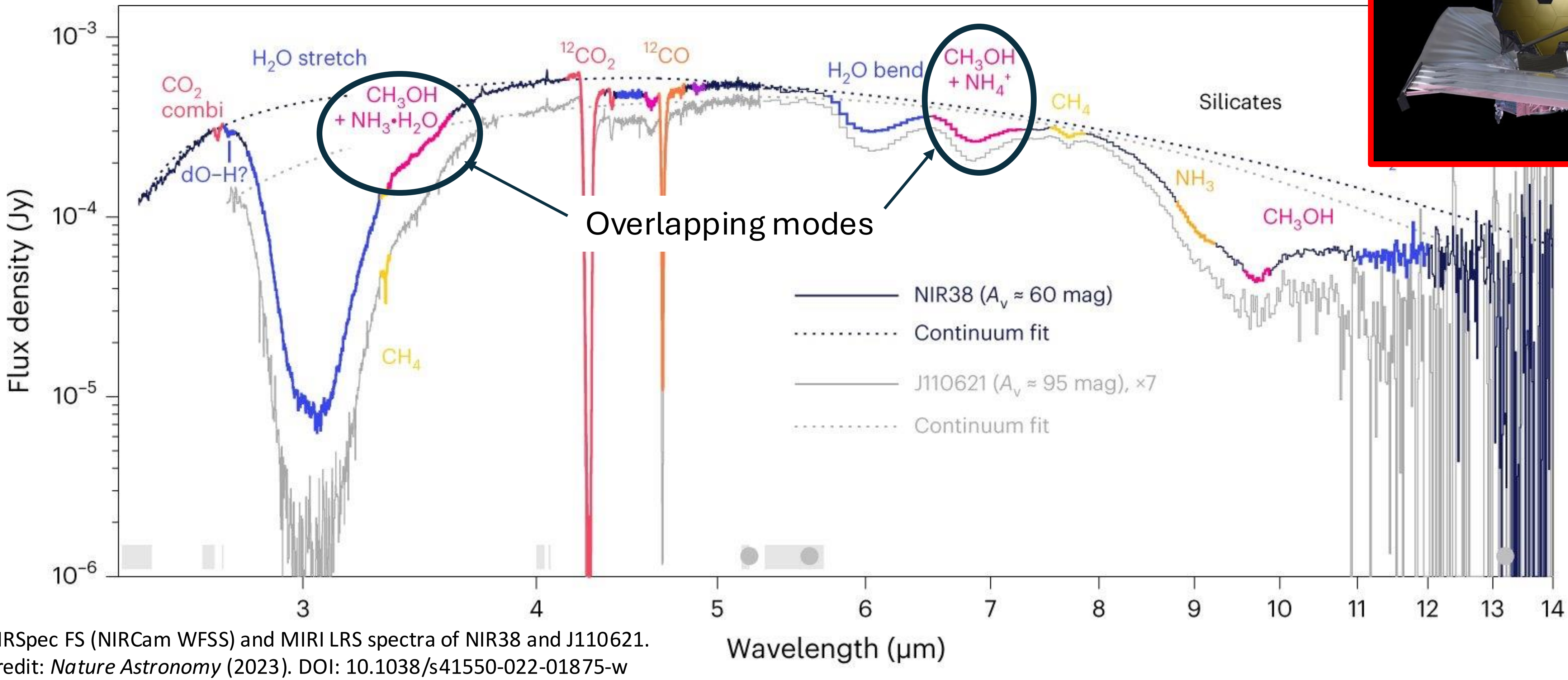

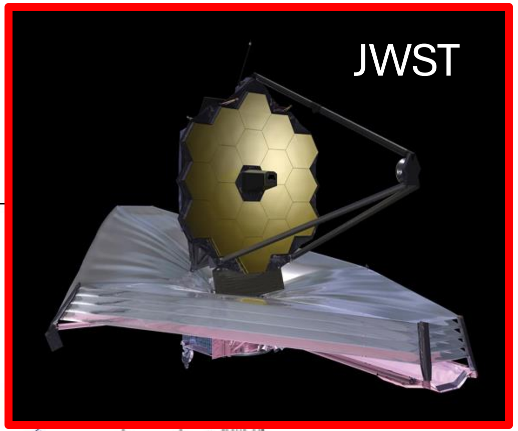

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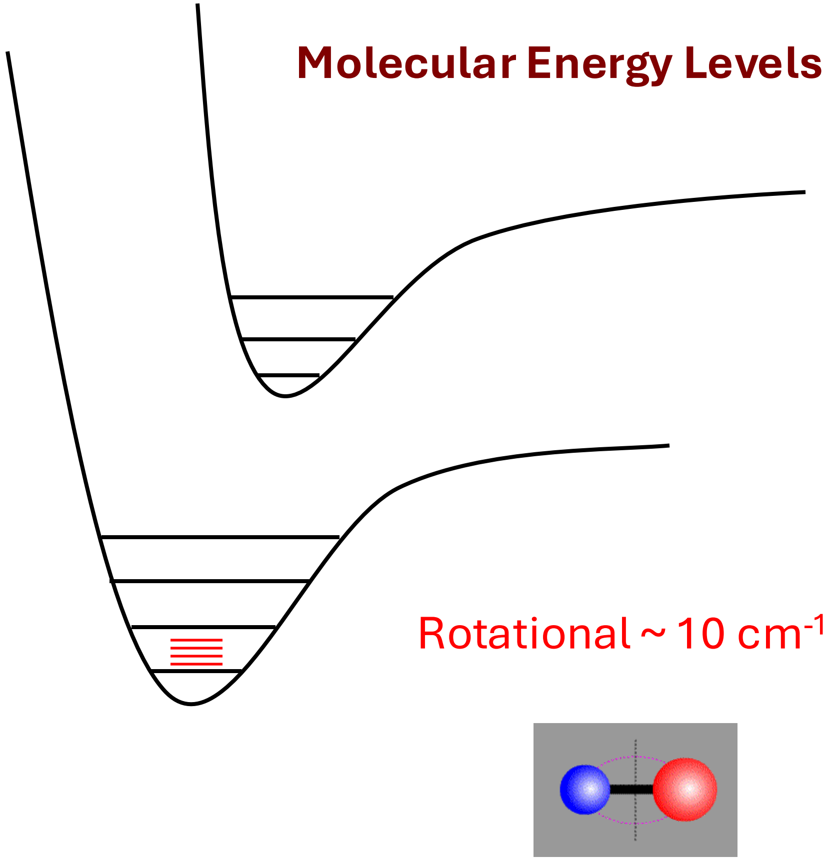
Spectroscopy: Primary Molecule Identification Method!

ROTATIONAL STATES

Credit: L. Ziurys

- Submillimeter and millimeter observations!
- Interstellar Molecular Gas is primarily **COLD**
  (T ~ 10 -100 K)
- **Rotational Levels** predominantly populated
  ⇒ two-body **collisions** with H_2
- No background source needed
- **Spontaneous Decay** results in **narrow emission lines**
- Rotational Spectrum is "Fingerprint" Pattern
- Unique to a Given Chemical Compound!
- Allows for ***unambiguous*** identification
- Rotational Transition Frequencies
  ⇒ **quantized** and proportional to
  moments of inertia



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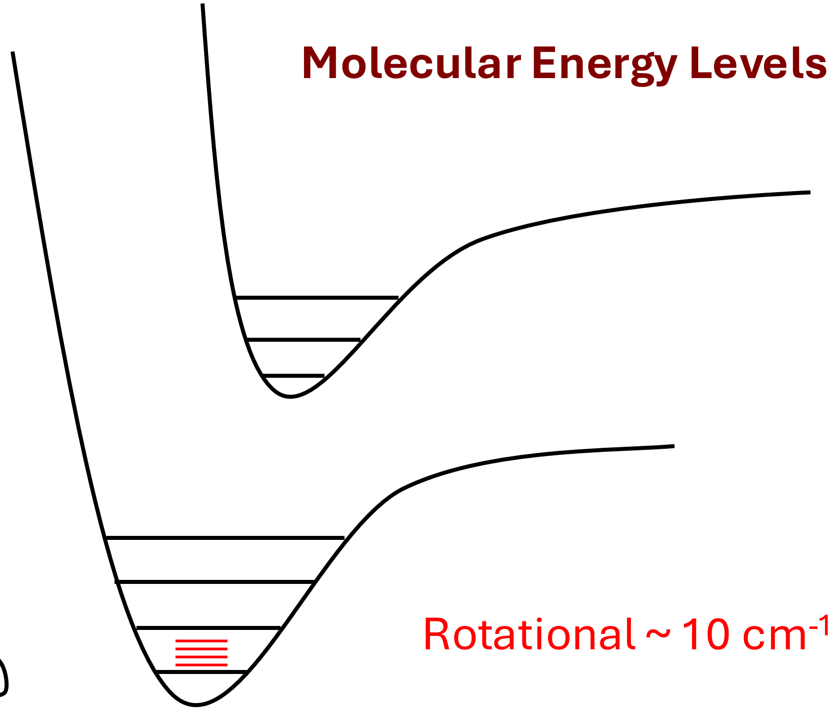
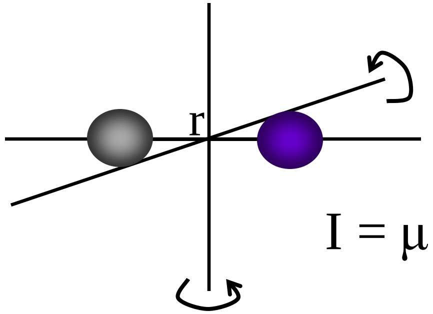
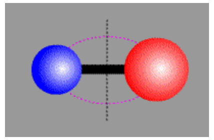




$I = \mu r^2$



Rotational Spectroscopy (from ERA):

Larmor's formula for a time-varying dipole can be applied to estimate the average power radiated by a rotating polar molecule. The **electric dipole moment** $\vec{p}$ of any charge distribution $\rho(\vec{x})$ is defined as the integral :

$$\vec{p} \equiv \int x\vec{\rho}\,(v)\,dv, \qquad (7.120)$$

Over the volume *v* containing the charges. The average charge distribution in the case of two point charges +q and -q with separation r_e,

$$|\vec{p}| = qr_e. \qquad (7.120)$$

A **polar molecule** with a nonzero electric dipole moment will have a **rotation frequency** based on the quantization of angular momentum,

$$\boxed{L = n\hbar.} \qquad (7.100)$$

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RULE: L is an integer multiple of $\hbar$. This applies to the angular momentum of a rotating molecule

Rotational Spectroscopy (from ERA):

For a **diatomic molecule** with two atoms of masses m_A and m_B and whose centers are separated by equilibrium distance r_e

$$r_e = r_A + r_B \quad \text{and} \quad r_A m_A = r_B m_B. \qquad (7.101)$$

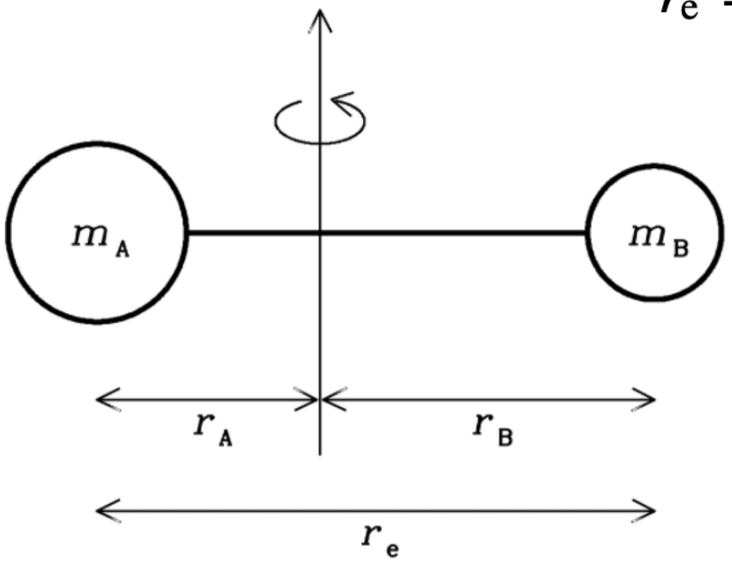


Fig. 7.12 (ERA)

In this case, we define the angular momentum in terms of the moment of inertia, *I*, and angular frequency, ω,

$$L = I\omega, \qquad (7.102)$$

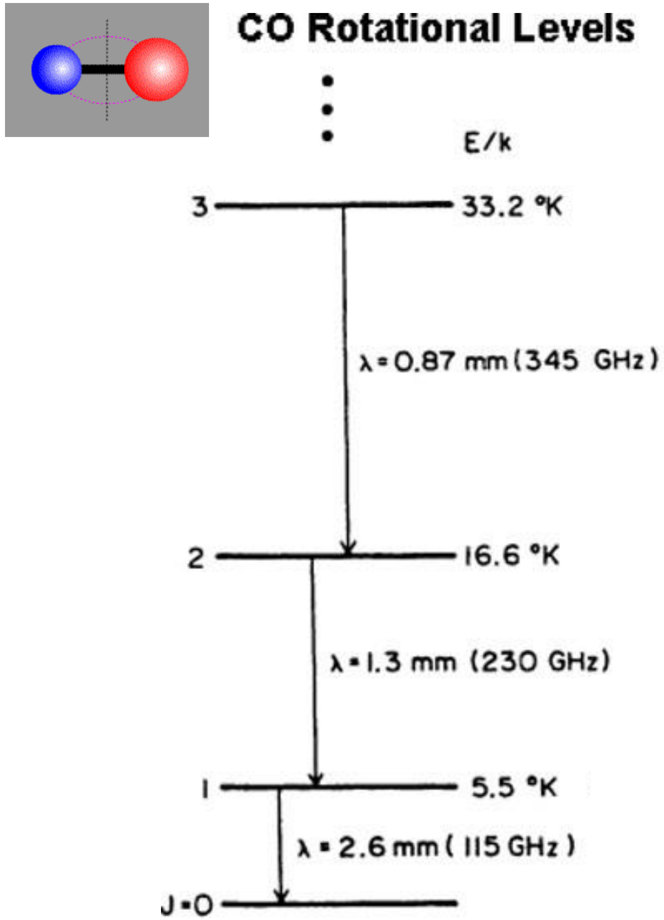
The moment of inertia is dependent on the **reduced mass** and the equilibrium distance squared so that,

$$\boxed{L = m r_e^2 \omega,} \qquad (7.104)$$

* Or more typically the symbol 'μ' is used →

$$\boxed{m \equiv \left(\frac{m_A m_B}{m_A + m_B}\right)} \qquad (7.105)$$

Rotational Spectroscopy (from ERA):



Wilson et al., 1970

The rotational kinetic energy associated with the angular momentum is,

$$E_{\text{rot}} = \frac{I\omega^2}{2} = \frac{L^2}{2I}. \qquad (7.106)$$

Which of course also becomes quantized!

$$E_{\text{rot}} = \left(\frac{\hbar^2}{2I}\right) J\,(J+1), \qquad J = 0, 1, 2, \ldots. \qquad (7.107)$$

This quantization of rotational energy implies that changes in rotational energy are quantized, and the states permitted are restricted by quantum-mechanical **selection rules**, which in this simple case is,

$$\Delta J = \pm 1. \qquad (7.108)$$

The frequency of the photon can be written,

$$\nu = \frac{\Delta E_{\text{rot}}}{h} = \frac{\hbar J}{2\pi I}, \qquad J = 1,\ 2, \ldots, \qquad (7.109)$$

$$\nu = \frac{hJ}{4\pi^2 m r_e^2}, \qquad J = 1, 2, \ldots. \qquad (7.110)$$

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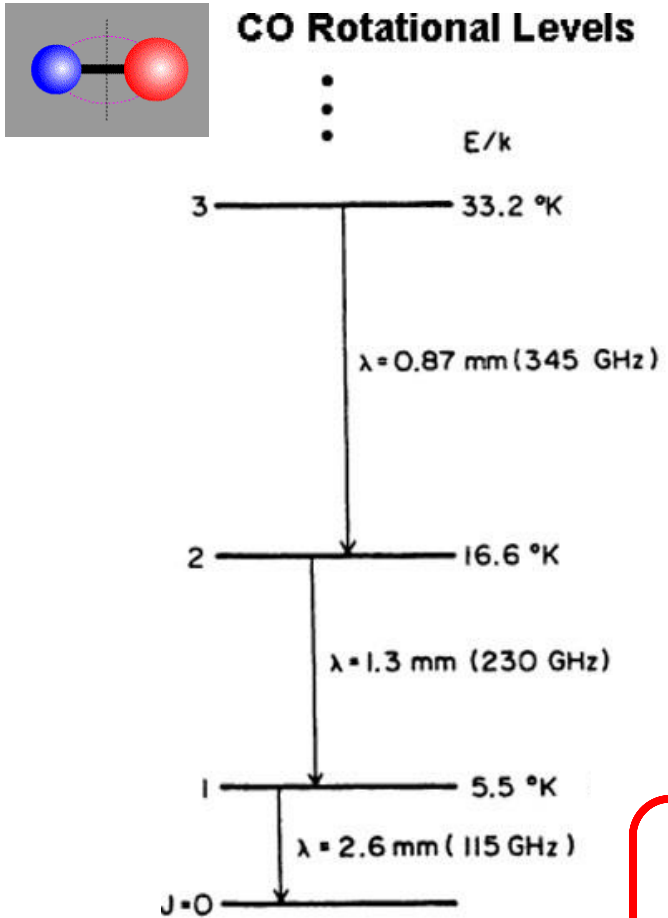

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Use to calculate your rotational frequency → (structured like a ladder)

$$\boxed{\nu = \frac{hJ}{4\pi^2 m r_e^2}, \qquad J = 1, 2, \ldots.} \qquad (7.110)$$

Rotational Spectroscopy

* Important caveat! Most molecules are not simple diatomic…

Easier to define **Rotational Constants, e.g.,**

$$B = \frac{h}{8\pi^2 c I_B}$$

Rotational Constants	Type of Rotor	Example Molecules
$I_A = 0;\ I_B = I_C$	Linear Rotor	CO, OCS, N_2O
$I_A < I_B = I_C$	Prolate symmetric top	CH_3CN
$I_A = I_B < I_C$	Oblate symmetric top	BF3, $H3^+$, CH_3^+, NH_3
$I_A = I_B = I_C$	Spherical top	CH_4, SF_6
$I_A < I_B < I_C$	Asymmetric top	H_2O, CD_2H^+, CH_3OH, CH_3OCH_3, $HCOOCH_3$

Scibelli Thesis

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$I_A < I_B < I_C$	Asymmetric top	H_2O, CD_2H^+, CH_3OH, CH_3OCH_3, $HCOOCH_3$

Scibelli Thesis

'Ray's parameter is a measure of asymmetry where **κ** = -1 and **κ** = +1 are the prolate and oblate symmetric tops, respectively:

$$\kappa = \frac{(B - A + (B - C))}{(A - C)},$$

And, depending on the asymmetric projection of the molecule, another variable, *K*, is introduced that denotes the projection of *J* along either the a- or c-axis

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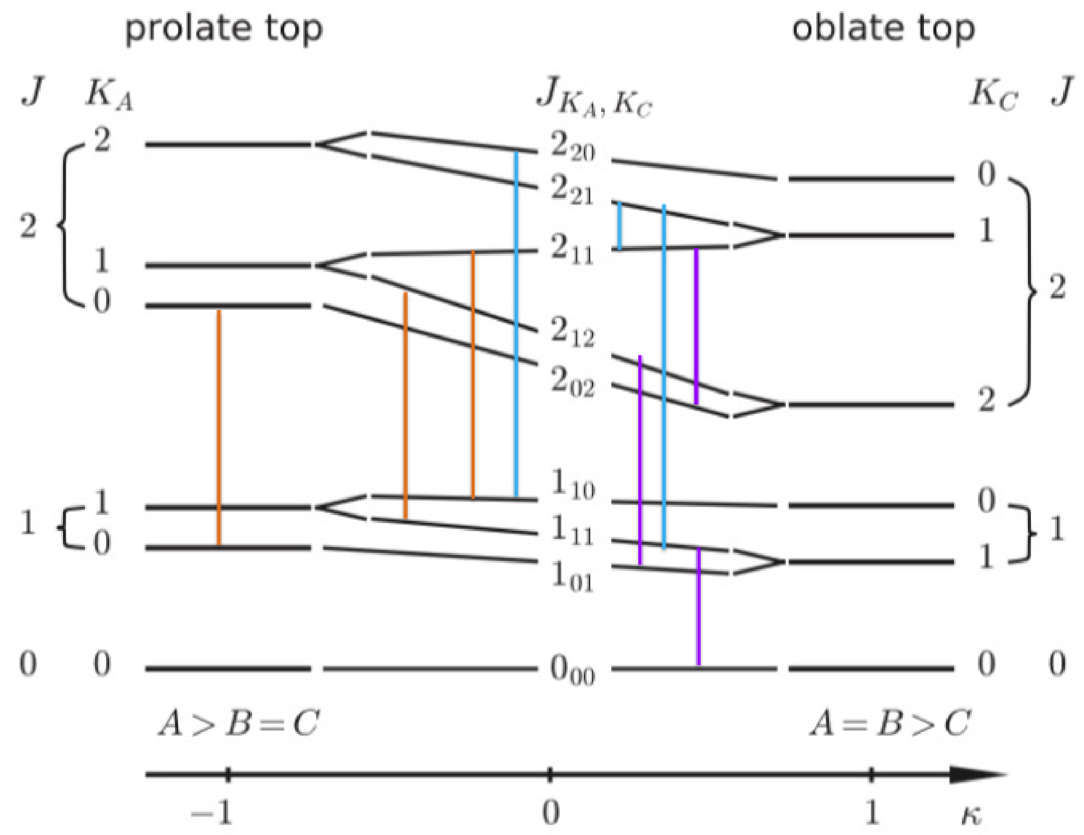

Selection rules for a-type transitions: ΔJ = 0, ±1, ΔK_a = 0, ± 2, … ΔK_c = ± 1, ± 3, …

Selection rules for b-type transitions: ΔJ = 0, ±1, ΔK_a = ± 1, ± 3, … ΔK_c = ± 1, ± 3, …

Selection rules for c-type transitions: ΔJ = 0, ±1, ΔK_a = ± 1, ± 3, … ΔK_c = 0, ± 2, …

Main takeaway:

This is why you'll see molecular transitions written out with different notations! … It gets complicated!

o-NH_3 (3,3)   (23.870 GHz)   →

CH_3OH $1_{0,1} - 0_{0,0}$ A (48.37GHz)

CH_3CHO $5_{0,5} - 4_{0,4}$ A (95.963 GHz)

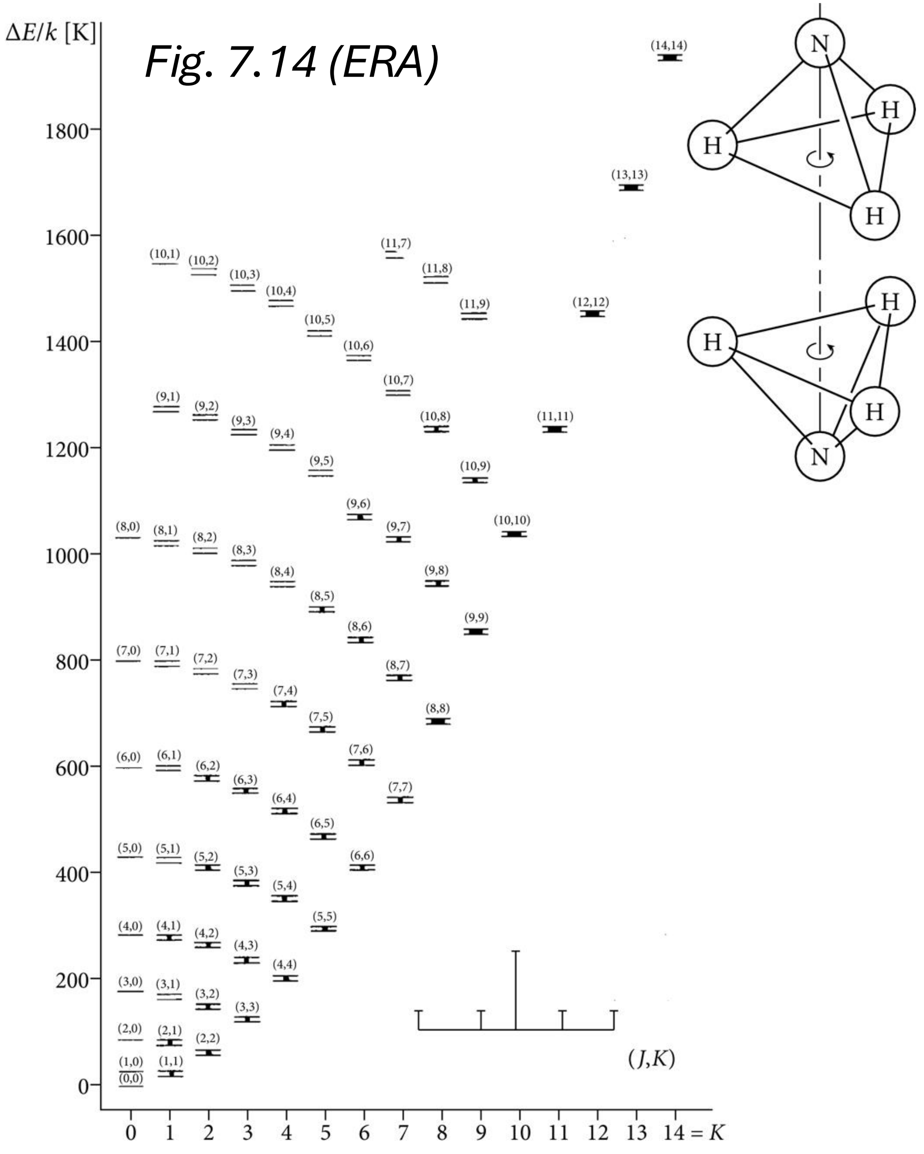

Fig. 7.14 (ERA)

GREEN BANK OBSERVATORY
National Radio Astronomy Observatory

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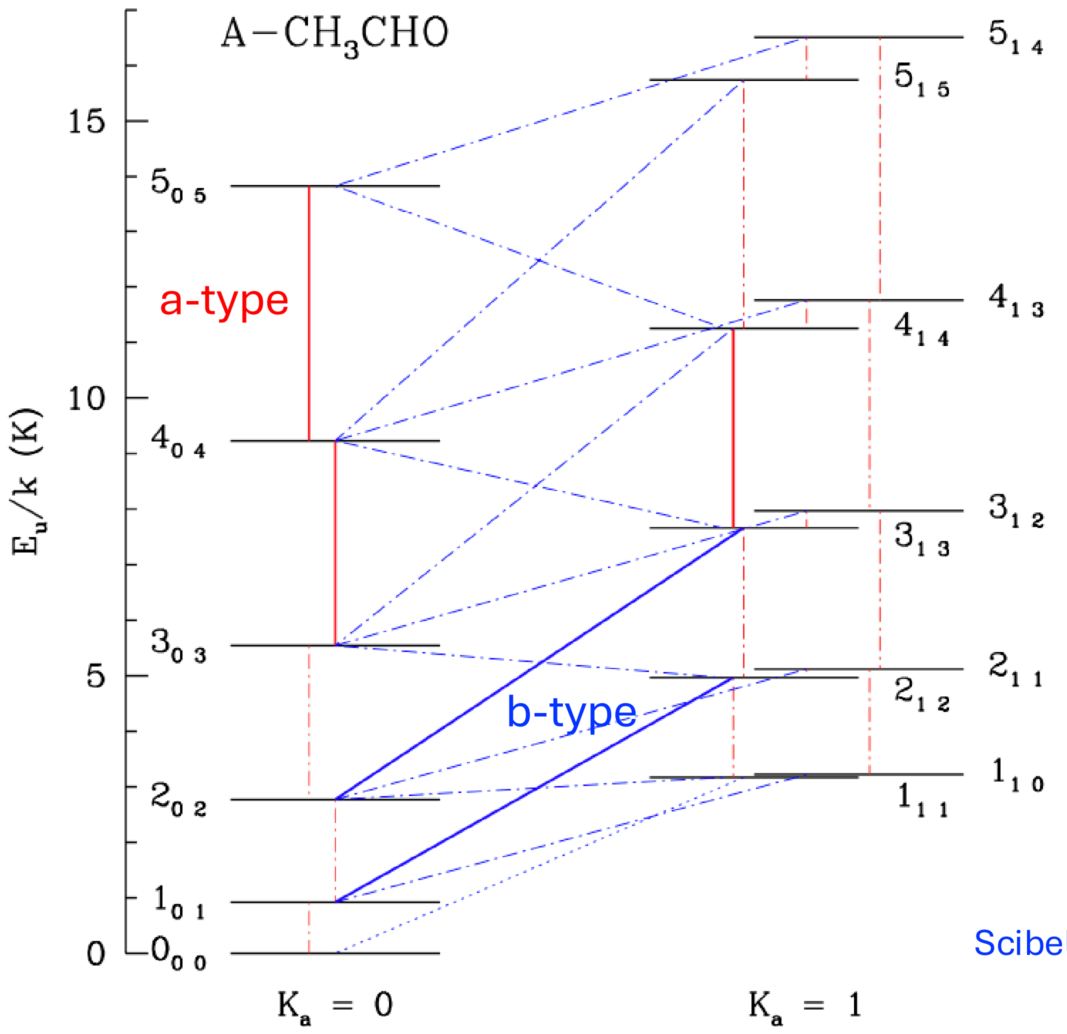
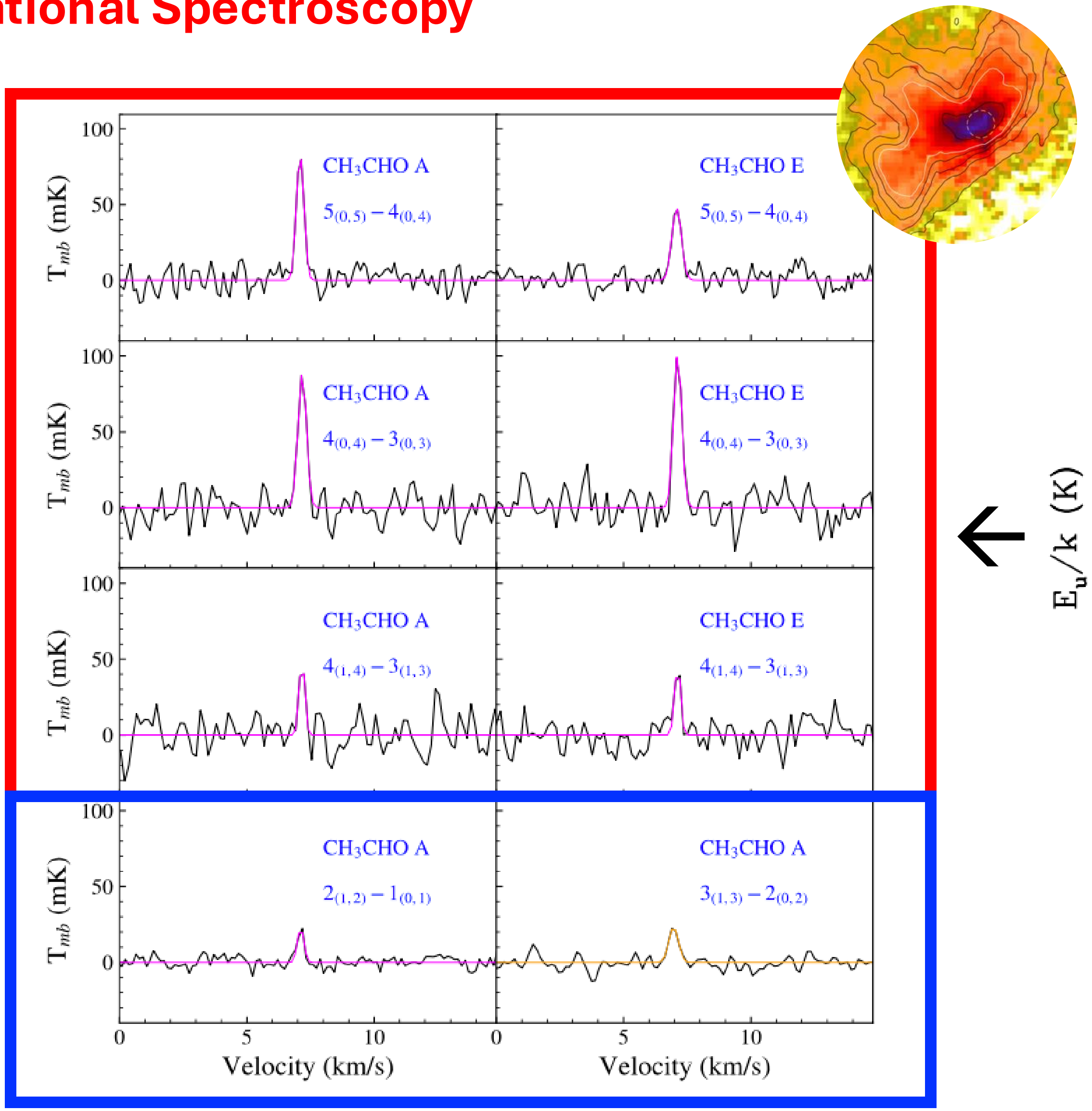
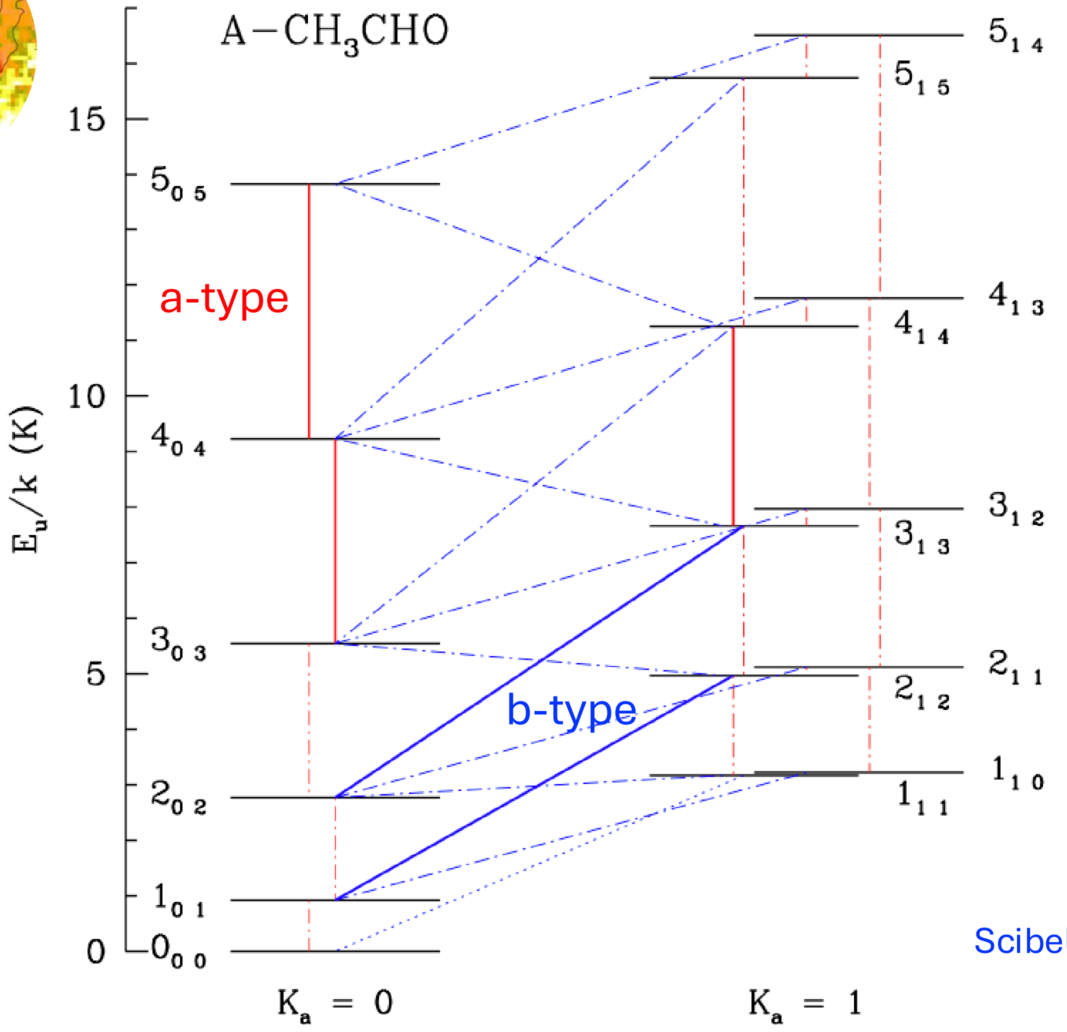


Scibelli et al., 2021

Rotational Spectroscopy





Scibelli et al., 2021

Rotational Spectroscopy:

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

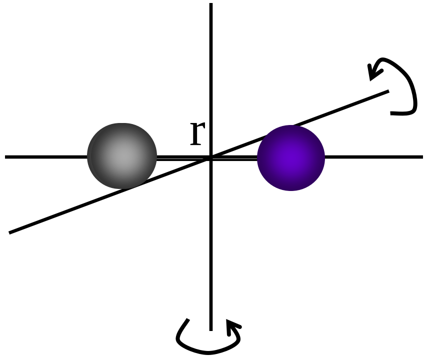
Frequency

$$B = \frac{h}{8\pi^2 c I}$$

Rotational Constant

$$I = \mu r^2$$

Moment of Inertia



$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

Reduced Mass

Credit: B. McGuire

Rotational Spectroscopy:

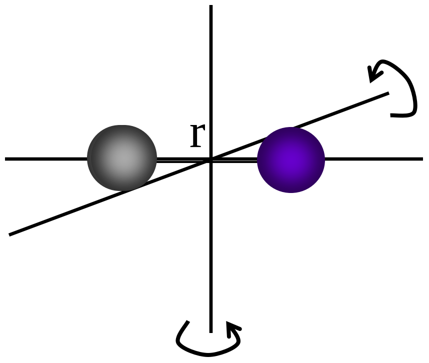
$$\nu = 2B(J+1)$$

Frequency

$$B = \frac{h}{8\pi^2 cI}$$

Rotational Constant

Increasing the size/mass of a molecule shifts transitions to lower frequencies!



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Reduced Mass

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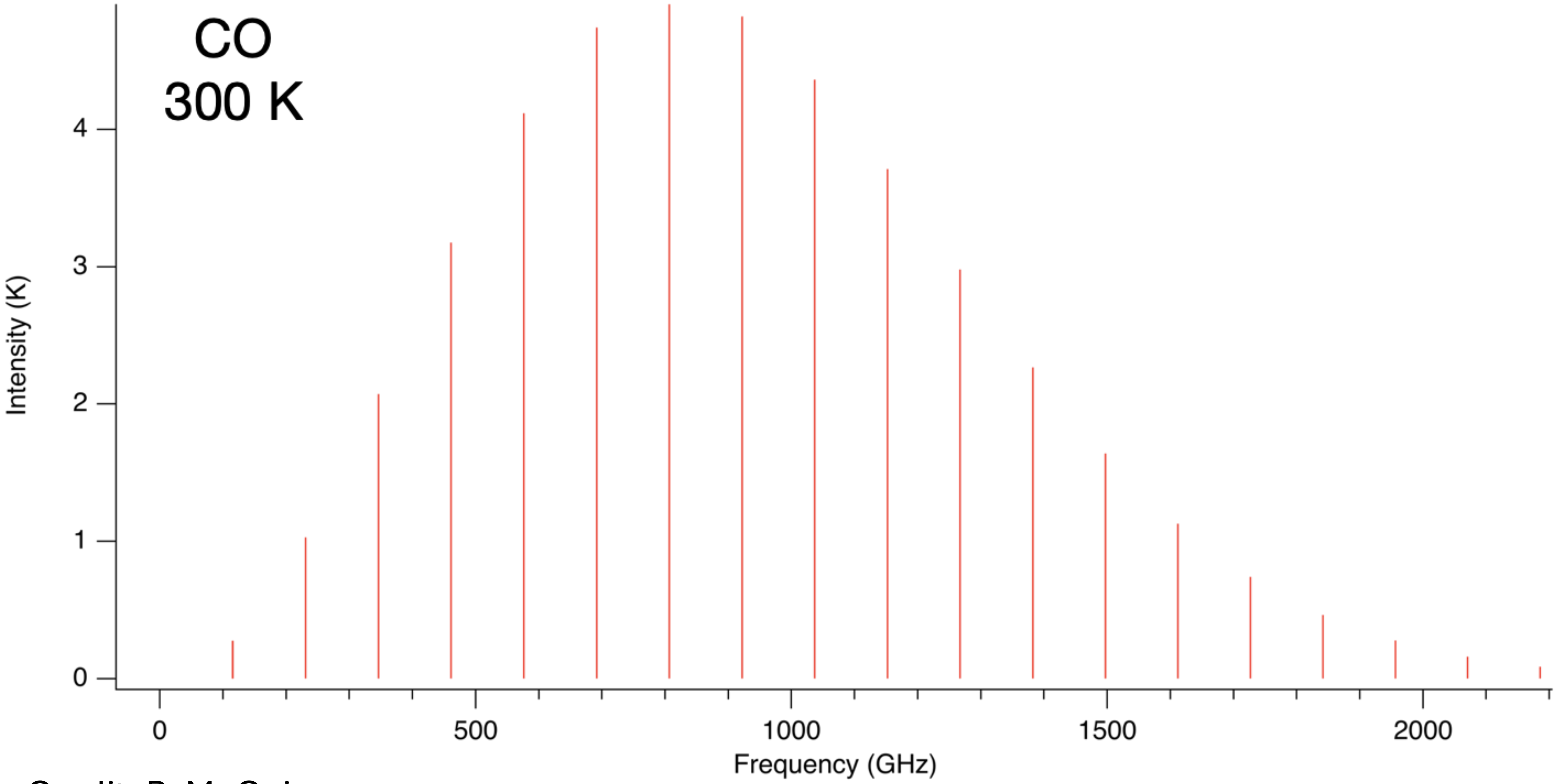
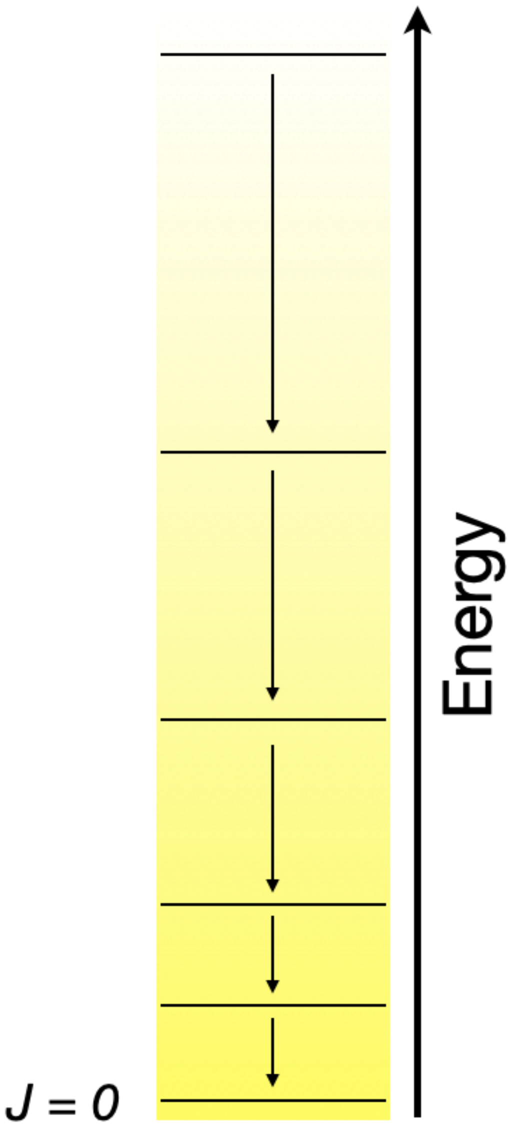
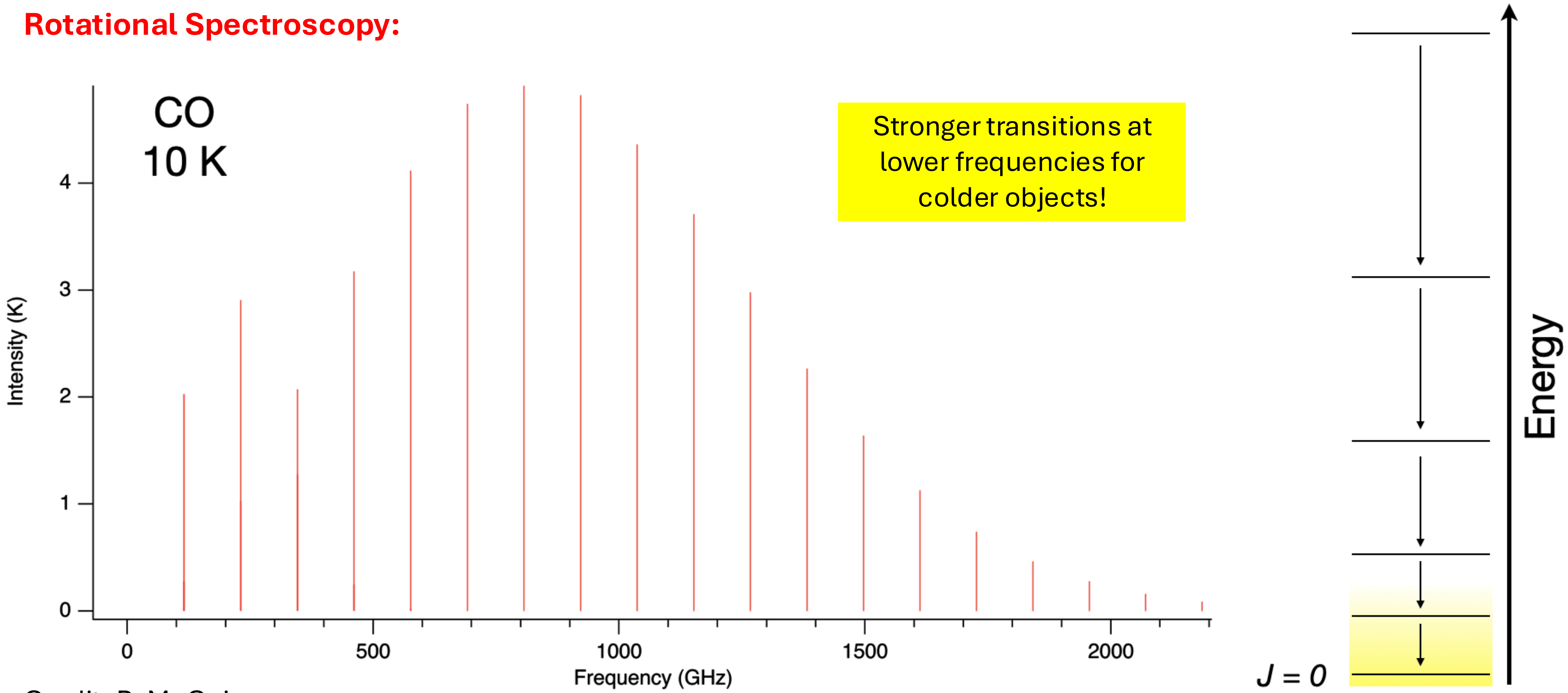




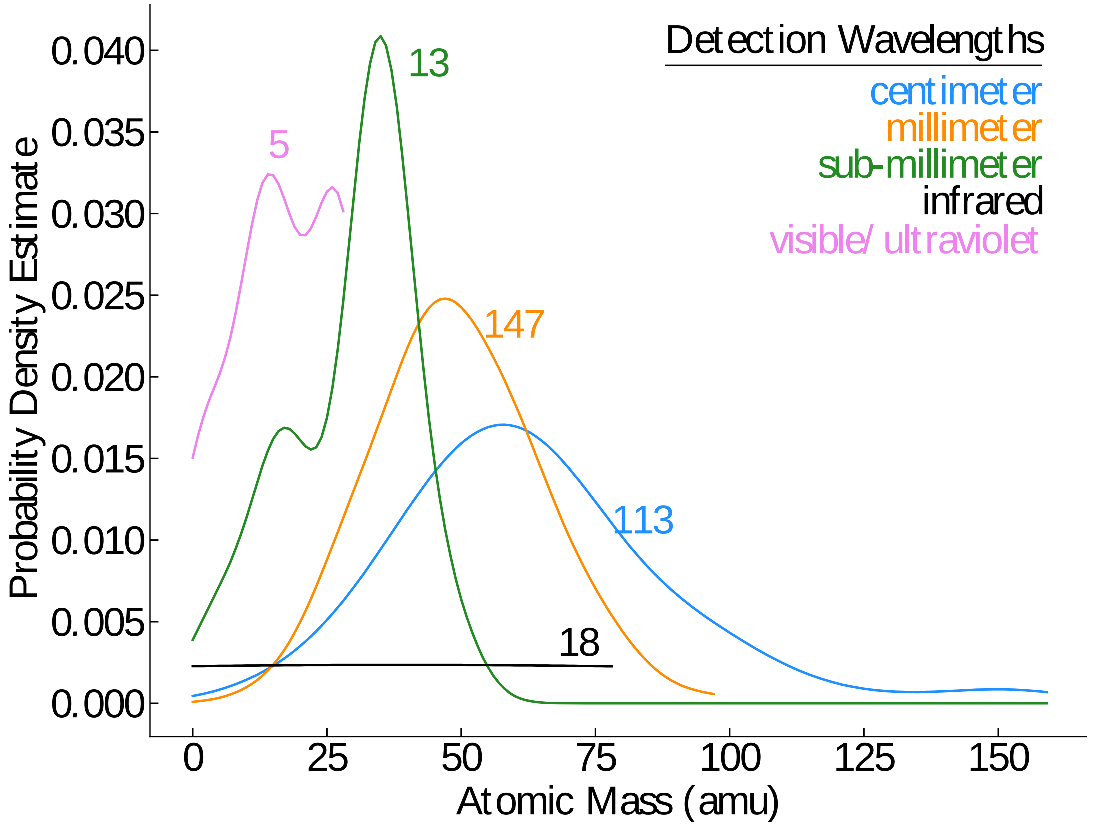
Credit: B. McGuire

Rotational Spectroscopy:



Credit: B. McGuire

Rotational Lines at Radio Wavelengths: The Best Probe of *Complex* Molecules



McGuire 2022

The **heavier a molecule/ more complex**, the more likely it is to be first detected at longer wavelengths.

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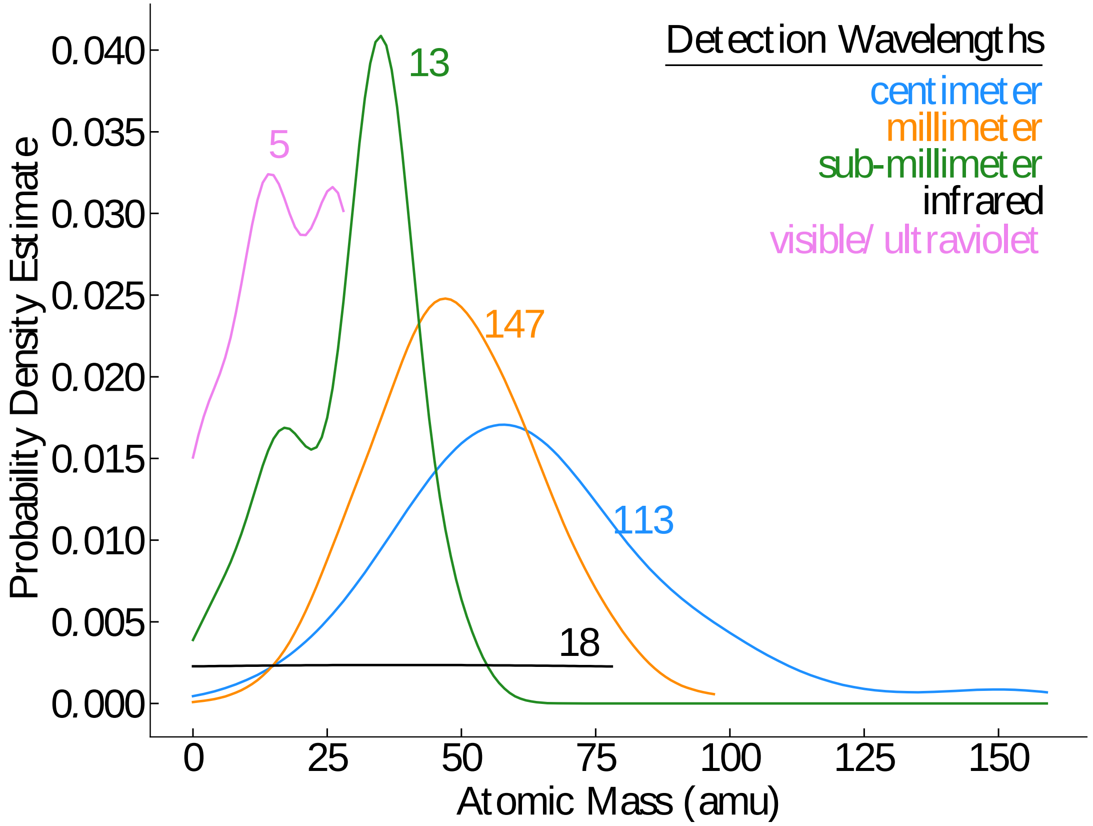
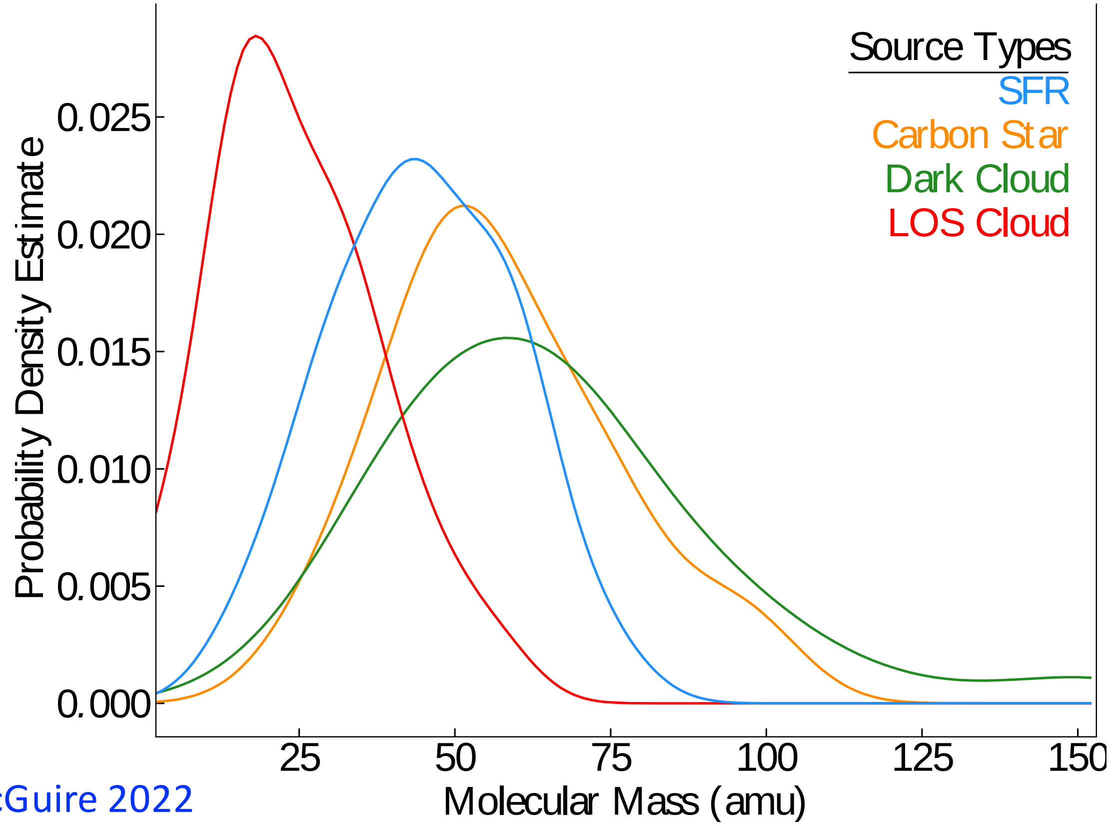


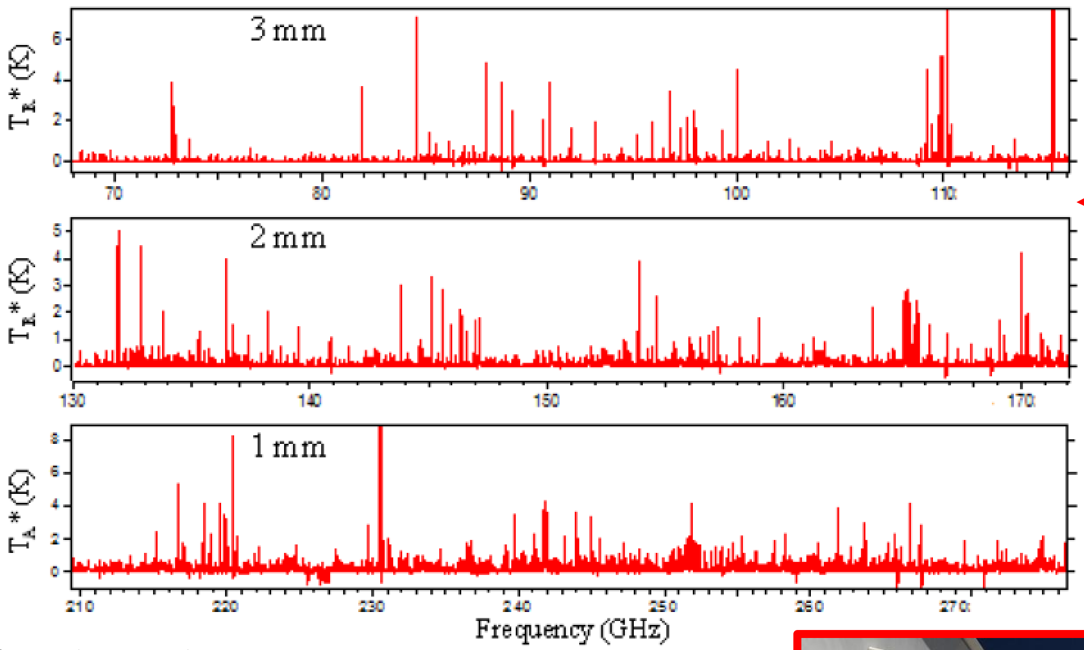


McGuire 2022

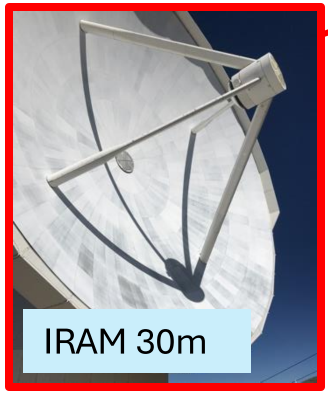
The **heavier a molecule/ more complex**, the more likely it is to be first detected at longer wavelengths.

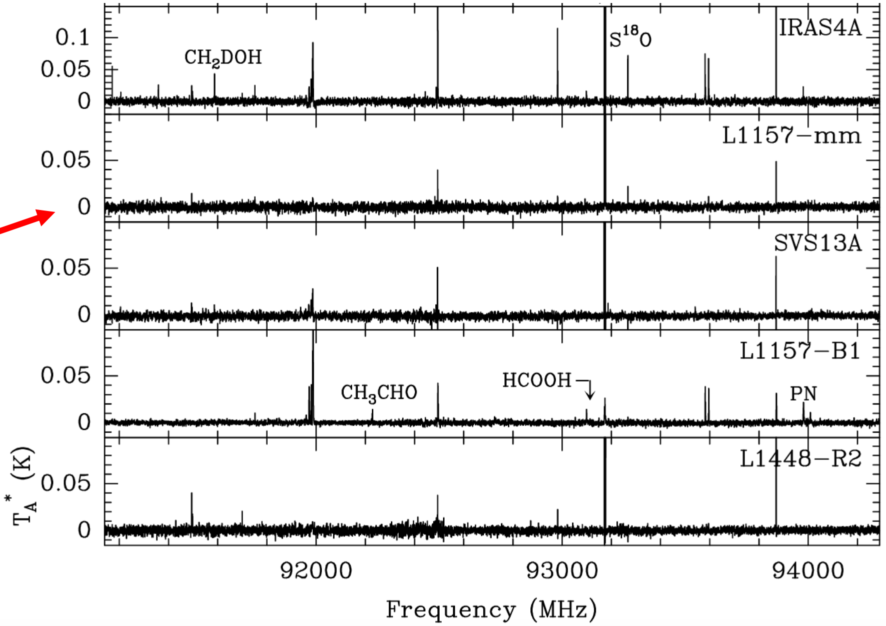
The **heavier a molecule/more complex**, the more likely it is to be first detected in a **dark cloud** or carbon star.

Rotational Lines at Radio Wavelengths: The Best Probe of *Complex* Molecules



Credit: L. Ziurys





Lefloch 2018

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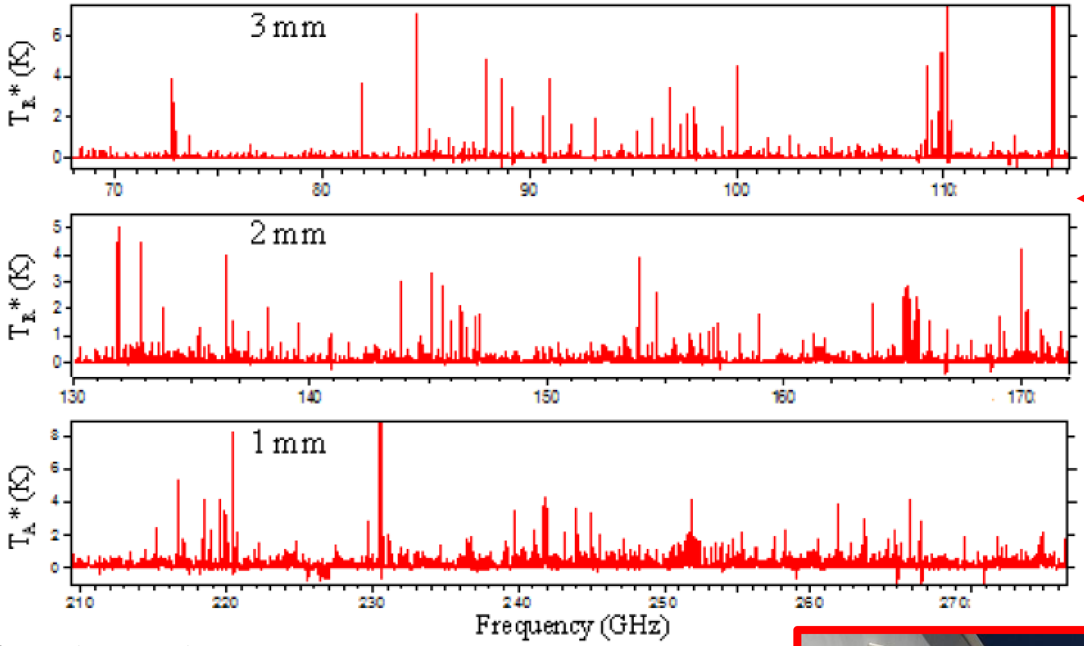

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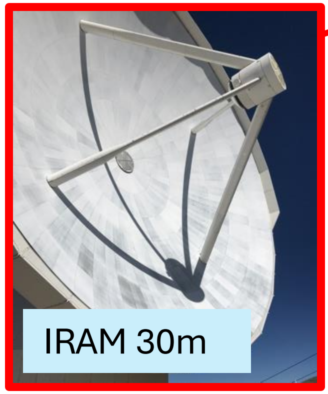
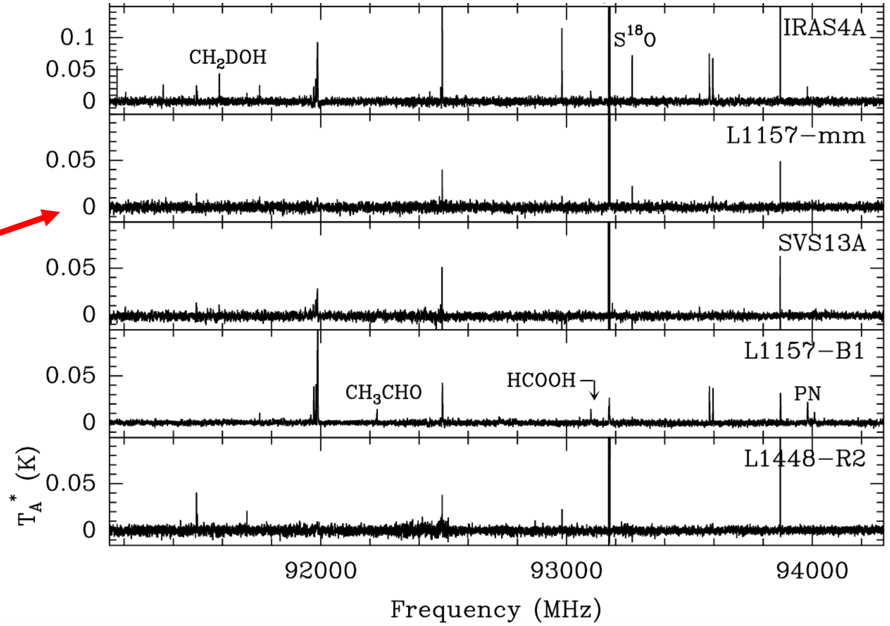
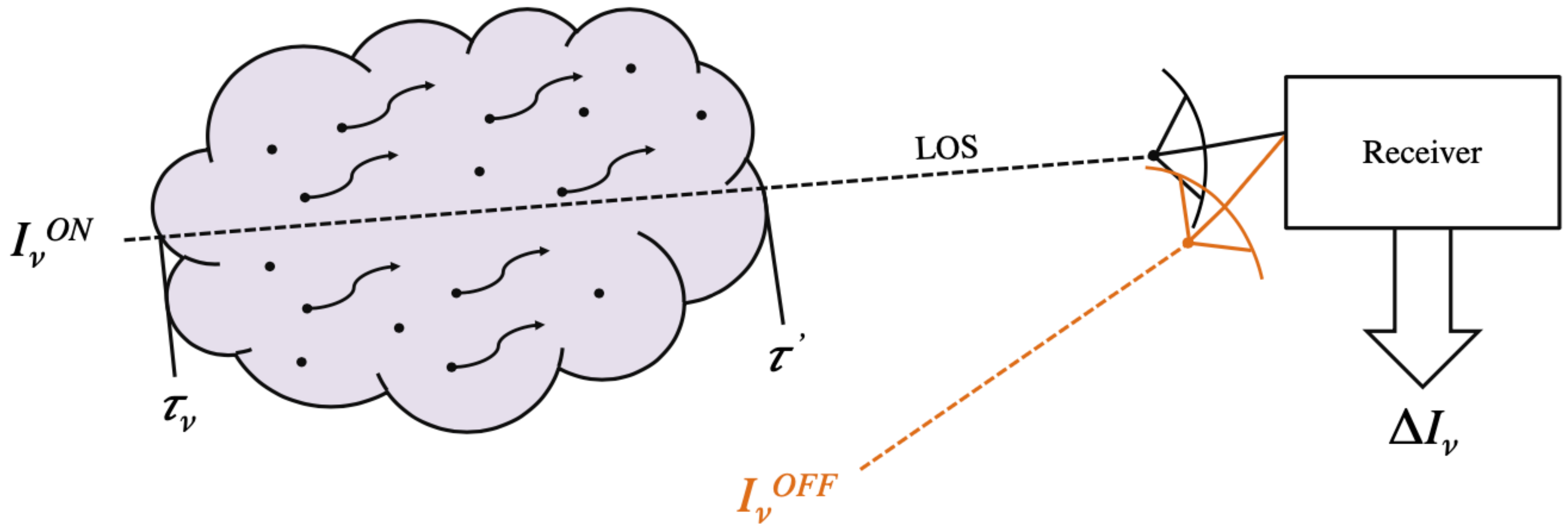




So, how do we know what molecules to look for, and in what ISM conditions? And how do we extract useful parameters out for our science? …

Line Radiative Transfer (ERA 7.3, 7.4, +7.7)



So, how do we know what molecules to look for, and in what ISM conditions? And how do we extract useful parameters out for our science? …