

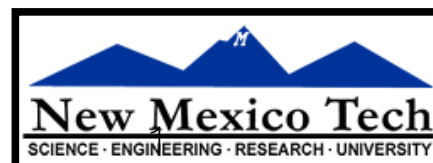


ASTROCHEMISTRY

Brett A. McGuire (NRAO)



Sixteenth Synthesis Imaging Workshop
16-23 May 2018



HISTORY AND CONTEXT

AS • TRO • CHEM • IS • TRY

/ astrō'keməstrē /

(*n*) the study of molecules in space - where they are, how they got there, and what they are doing

HISTORY AND CONTEXT



Big Bang
H, He

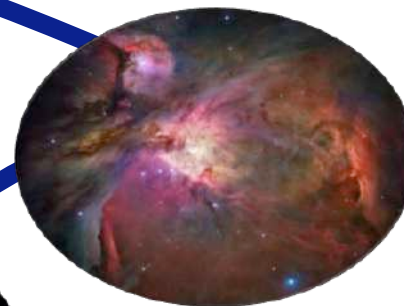
First Stars Born



First Stars Die
'Heavy' Element Synthesis



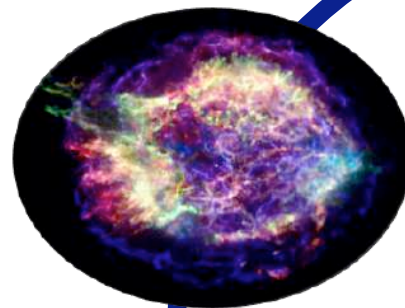
Stellar Nursery



New Stars



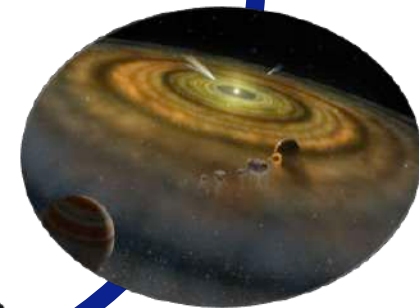
Fiery **C**ataclysm
(Whomp whomp)



Life! (Awww)



Planet Formation



Chemical Delivery



FUNDAMENTAL DRIVING QUESTION OF ASTROCHEMISTRY

How do you make a cat from H and He?

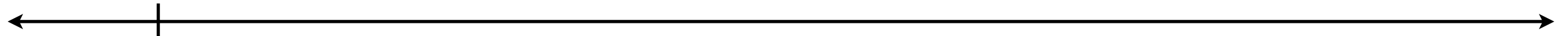
HISTORY AND CONTEXT

AS • TRO • CHEM • IS • TRY

/ astrō'keməstrē /

(*n*) the study of molecules in space - where they are, how they got there, and what they are doing

1937



First Molecule
(CH) Detected

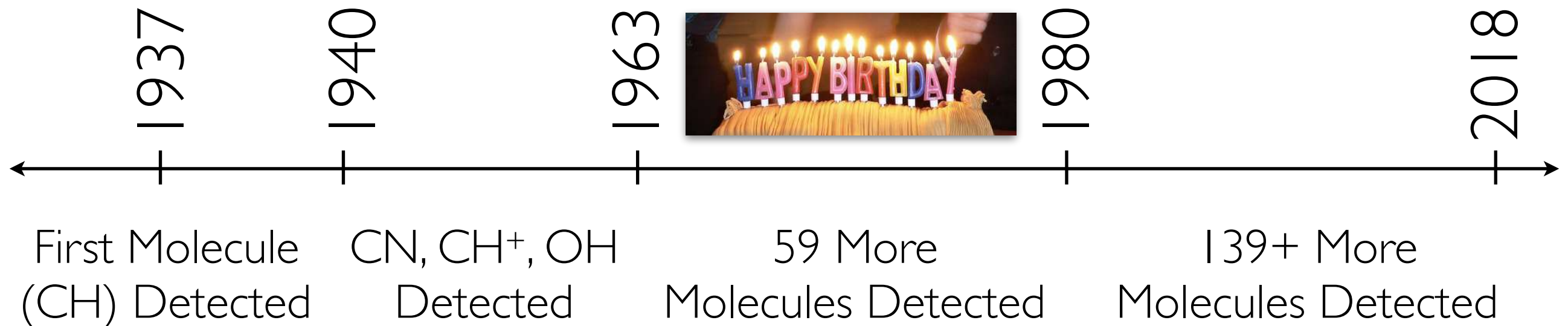


HISTORY AND CONTEXT

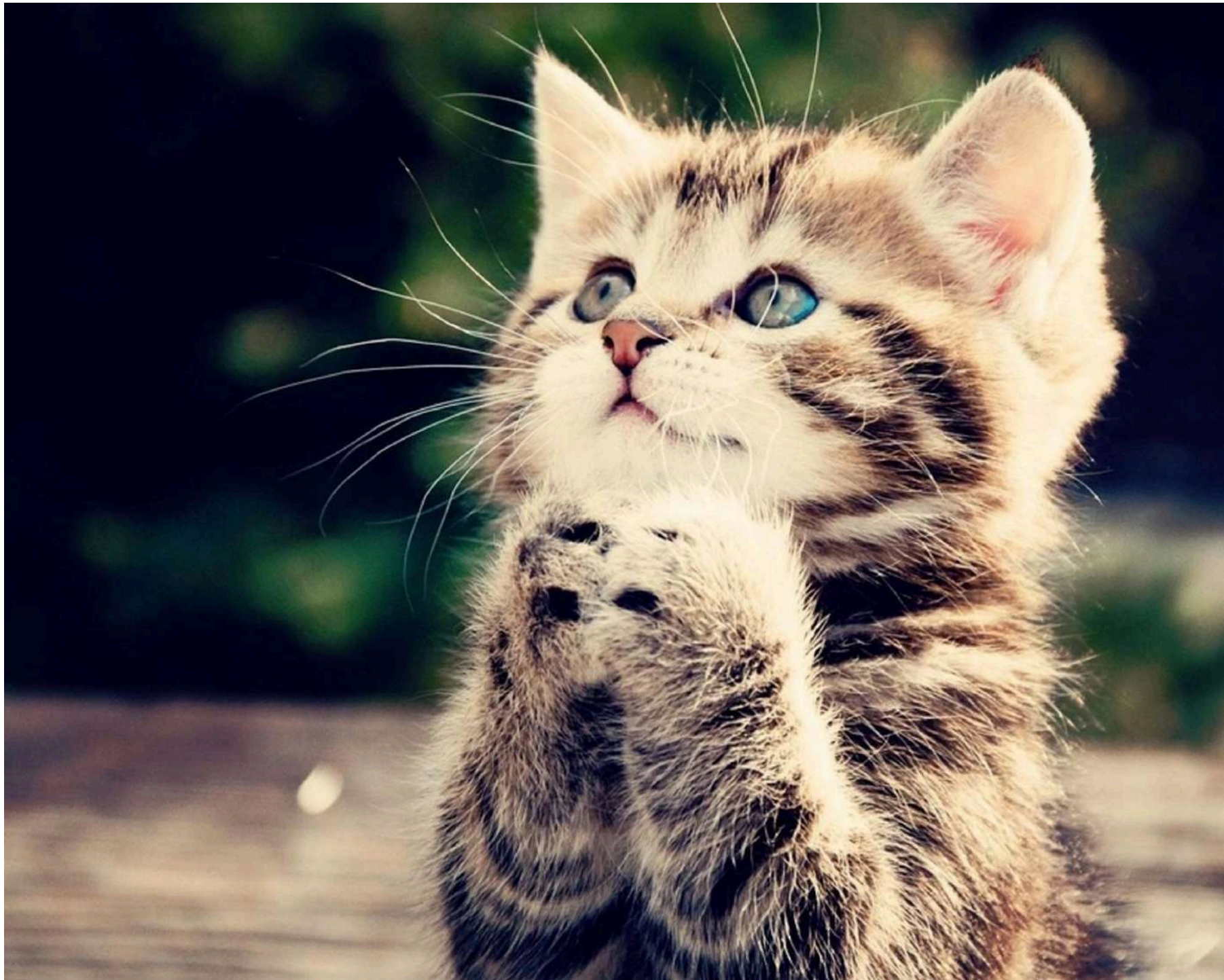
AS • TRO • CHEM • IS • TRY

/ astrō'keməstrē /

(*n*) the study of molecules in space - where they are, how they got there, and what they are doing

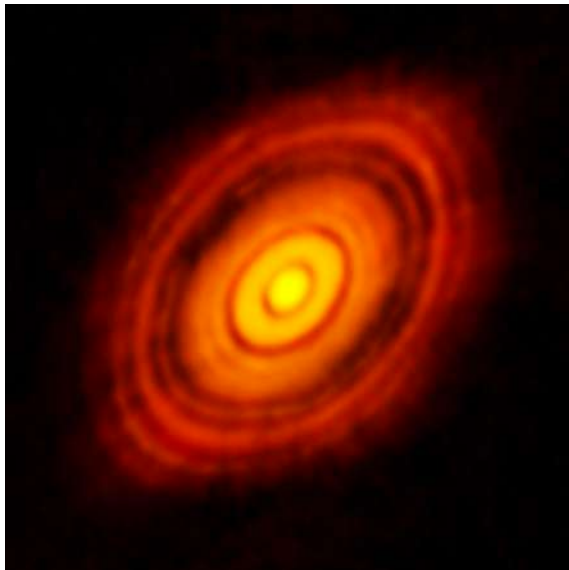


WHY DO I CARE?



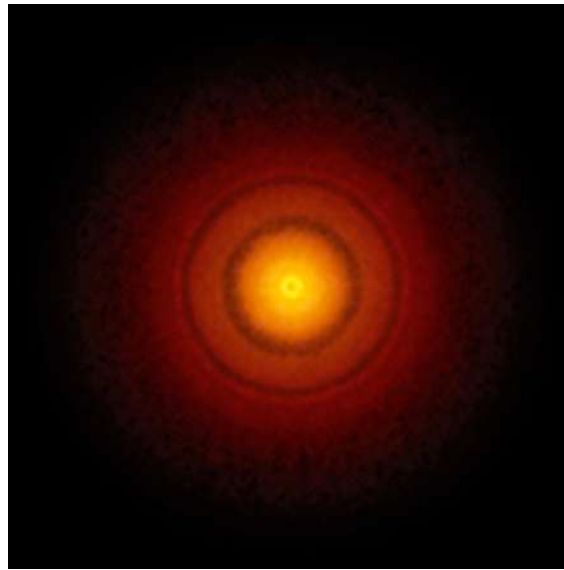
WHY SHOULD YOU CARE?

HL Tau



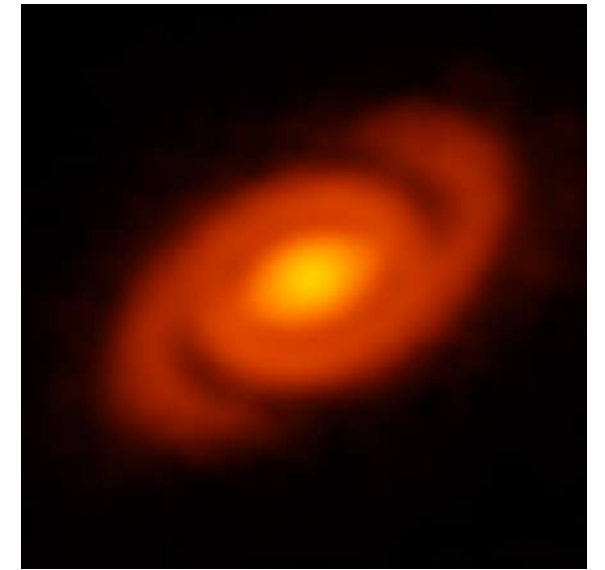
Brogan, ALMA et al.
(2015 *ApJL* 808, L3)

TW Hydrae



Andrews et al.
(2018 *ApJL* 820, L40)

Elias 2-27



Pérez et al.
(2016 *Science* 353, 6307)

Do these gaps correspond to snow lines?
How much H₂O is available for these planets?
What's the C/O ratio?
Can you tell me where a planet formed?
Did it move?

WHAT CAN ASTROCHEMISTRY DO FOR YOU?

We can tell you why that SiO emission in your source is probably a good tracer of a shock

We can tell you whether that comet you observed was probably formed in a very cold environment, and maybe even where in the disk

We can tell you whether that CH₃OH maser you're observing is collisionally or radiatively pumped

WHAT CAN ASTROCHEMISTRY DO FOR YOU?

Question

“Where can I find a table of molecules and what they trace?”

Answer

Hopefully nowhere

What astrochemistry can provide is the ability to draw contextualized conclusions on physical conditions and evolutionary history of an observed source based on the synthesis of laboratory, observational, and modeling studies



LABORATORY ASTROPHYSICS

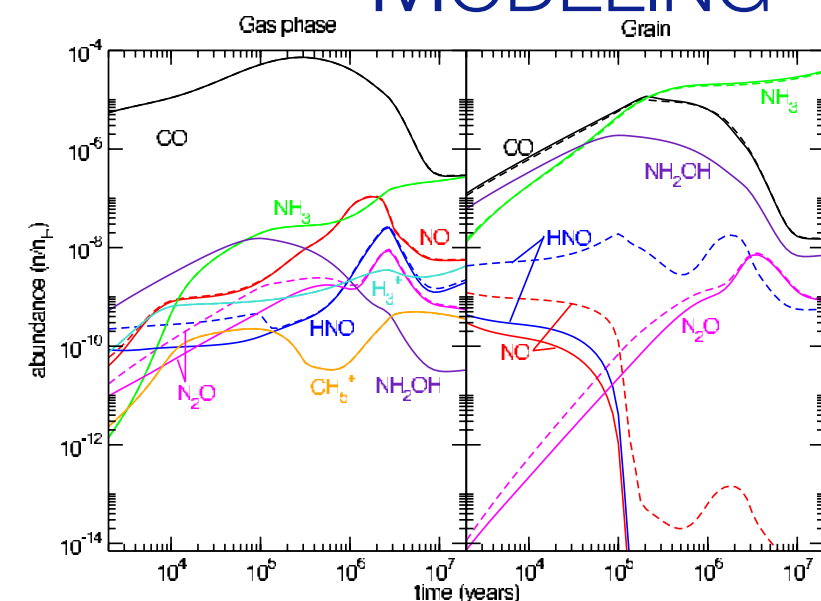


ASTROCHEMISTRY

Chemical Reactions, Kinetics, Thermodynamics

Species and Reactions of Interest

ASTROCHEMICAL MODELING



Temperatures, Abundances,
and Densities

Rotational, Vibrational,
and Electronic Spectra

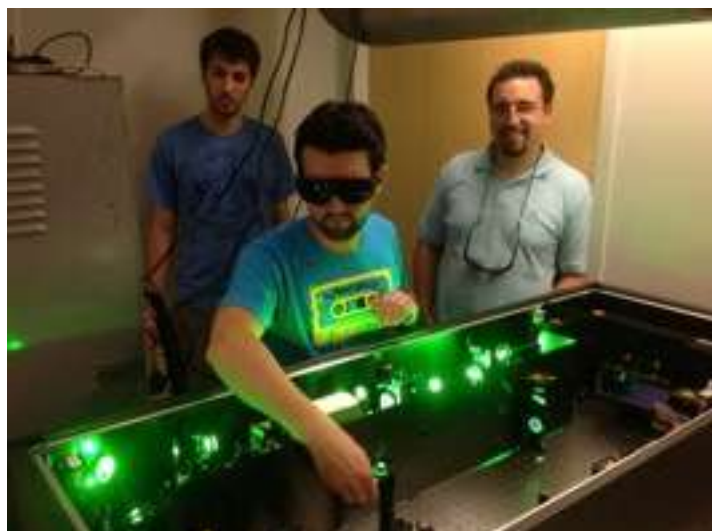
Environments and Species
of Interest

Chemical Inventories
Temperatures, Abundances,
and Densities

OBSERVATIONAL ASTRONOMY

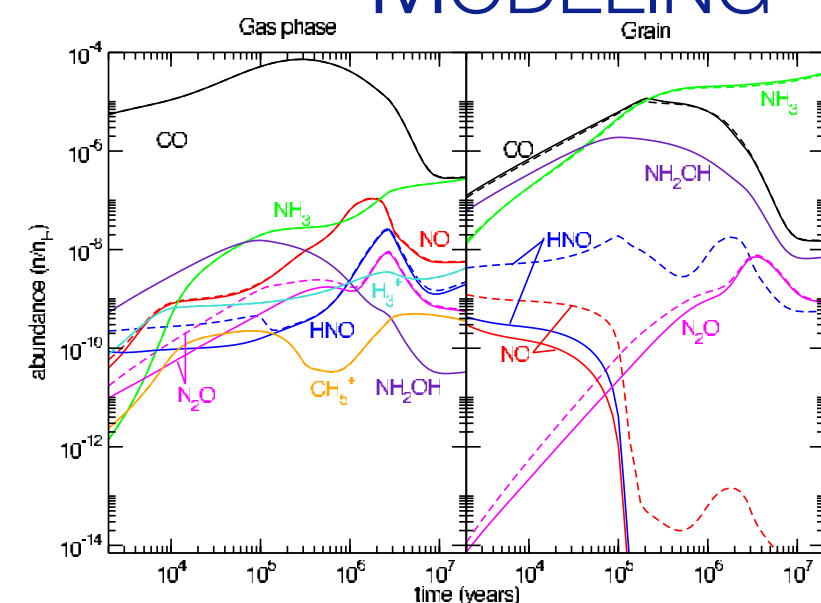


LABORATORY ASTROPHYSICS



ASTROCHEMISTRY

ASTROCHEMICAL MODELING

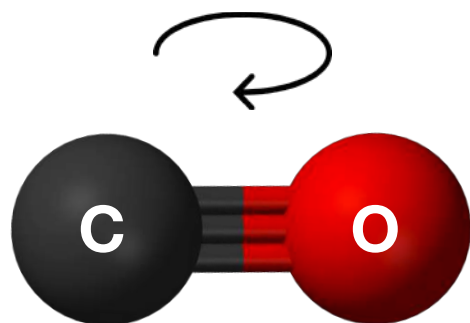


Rotational, Vibrational,
and Electronic Spectra

OBSERVATIONAL ASTRONOMY



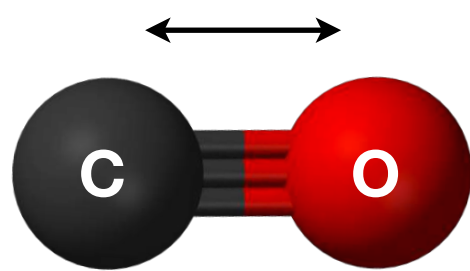
LABORATORY SPECTROSCOPY



Rotational 'Microwave' Spectroscopy

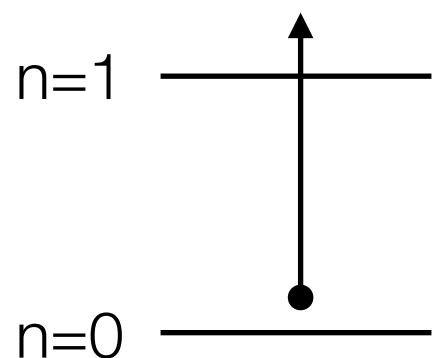
>90%

- <2000 GHz; Permanent Dipole Moment Req'd



(Ro-)Vibrational Spectroscopy

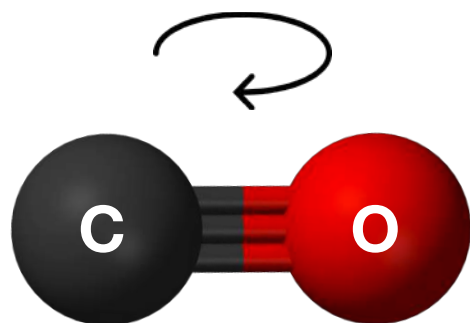
- (Far-)Infrared; Permanent Dipole Moment Not Req'd
- Each vibrational level also has rotational transitions



Electronic (Rovibronic) Spectroscopy

- UV-Visible; Permanent Dipole Moment Not Req'd
- Each electronic level also has vibrational and rotational transitions

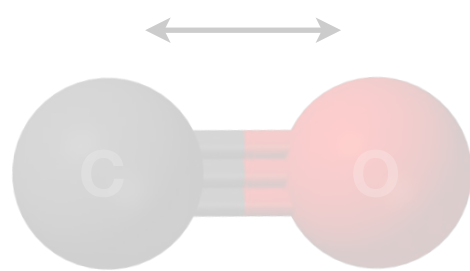
LABORATORY SPECTROSCOPY



Rotational 'Microwave' Spectroscopy

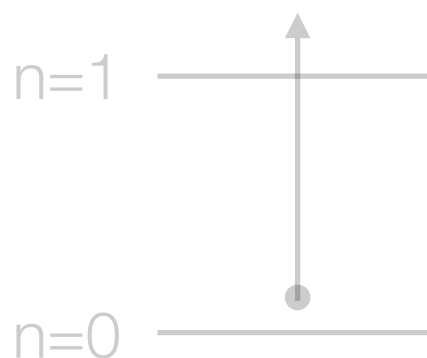
>90%

- <2000 GHz; Permanent Dipole Moment Req'd



(Ro-)Vibrational Spectroscopy

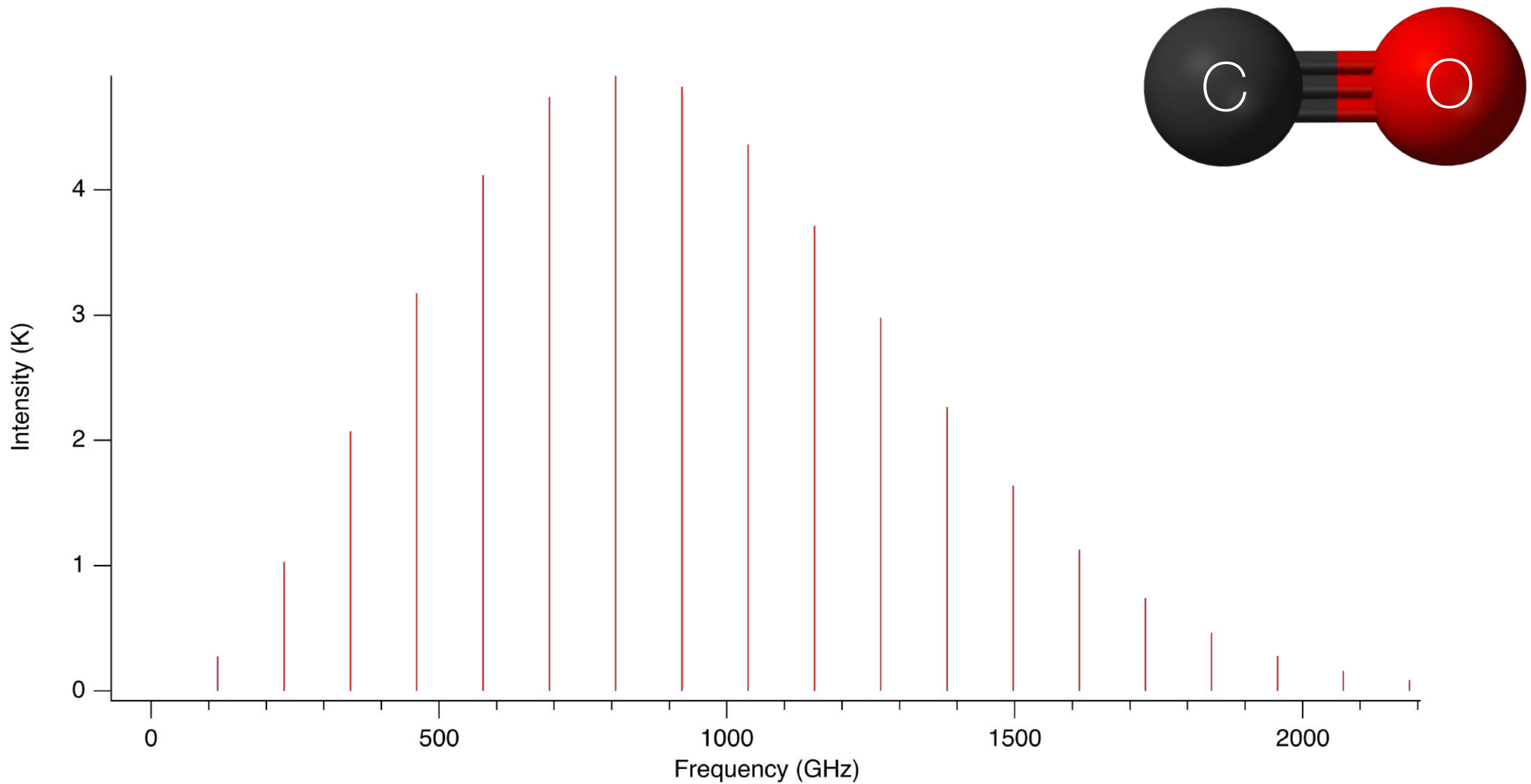
- (Far-)Infrared; Permanent Dipole Moment Not Req'd
- Each vibrational level also has rotational transitions



Electronic (Rovibronic) Spectroscopy

- UV-Visible; Permanent Dipole Moment Not Req'd
- Each electronic level also has vibrational and rotational transitions

ROTATIONAL SPECTROSCOPY



ROTATIONAL SPECTROSCOPY

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

↓

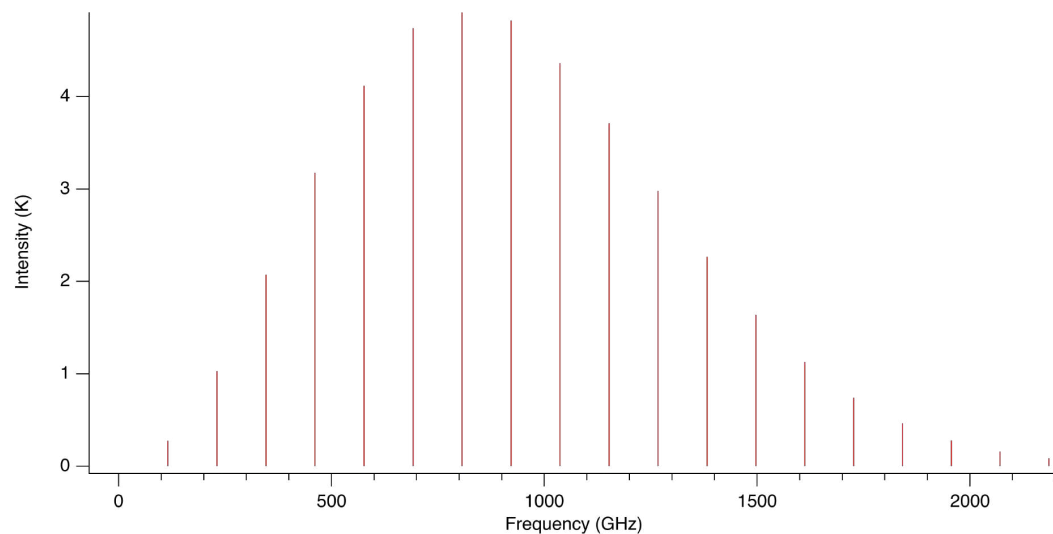
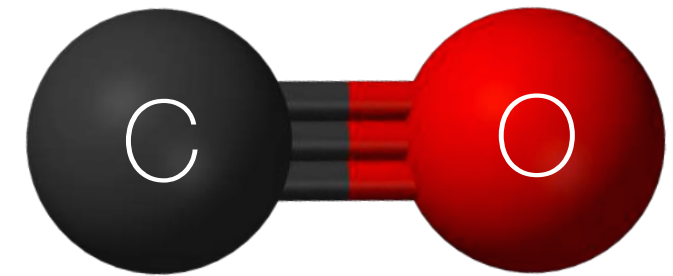
$$B = \frac{h}{8\pi^2 c I}$$

↓

$$I = \mu r^2$$

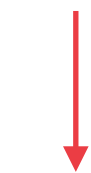
↓

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



ROTATIONAL SPECTROSCOPY

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



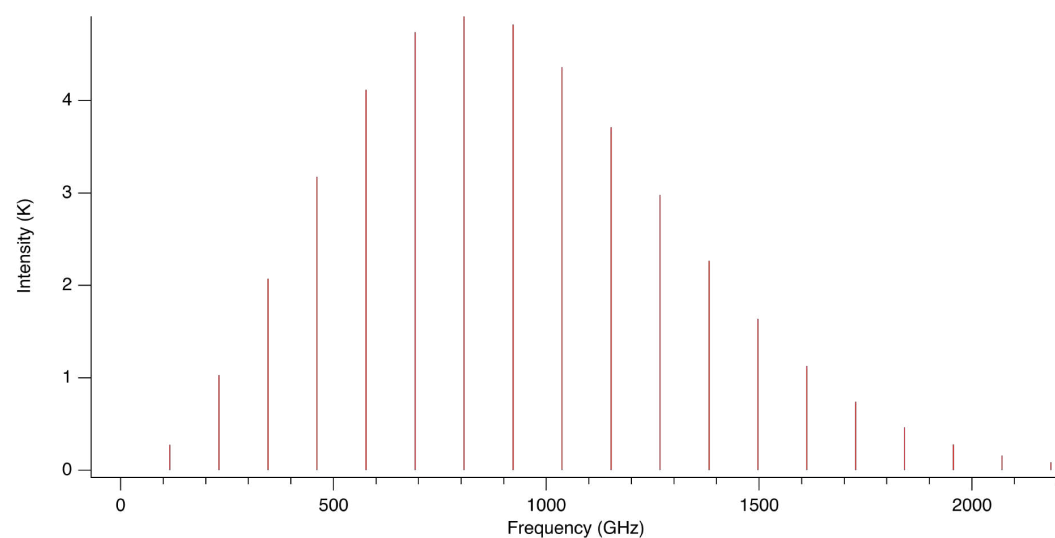
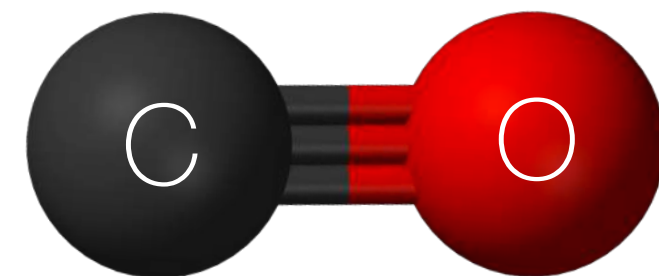
$$B = \frac{h}{8\pi^2 c I}$$



$$I = \mu r^2$$

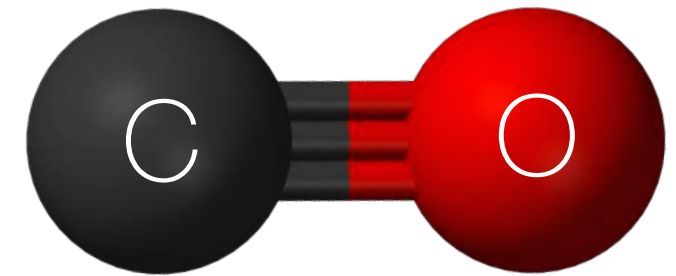


$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$



ROTATIONAL SPECTROSCOPY

To first order, the rotational frequencies of a molecule are determined exclusively by its structure.



To ∞ -order, no two molecules can share the same rotational spectrum. A rotational spectrum is a unique molecular fingerprint.

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

↓

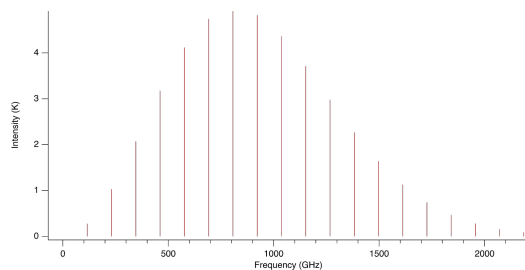
$$B = \frac{h}{8\pi^2 c I}$$

↓

$$I = \mu r^2$$

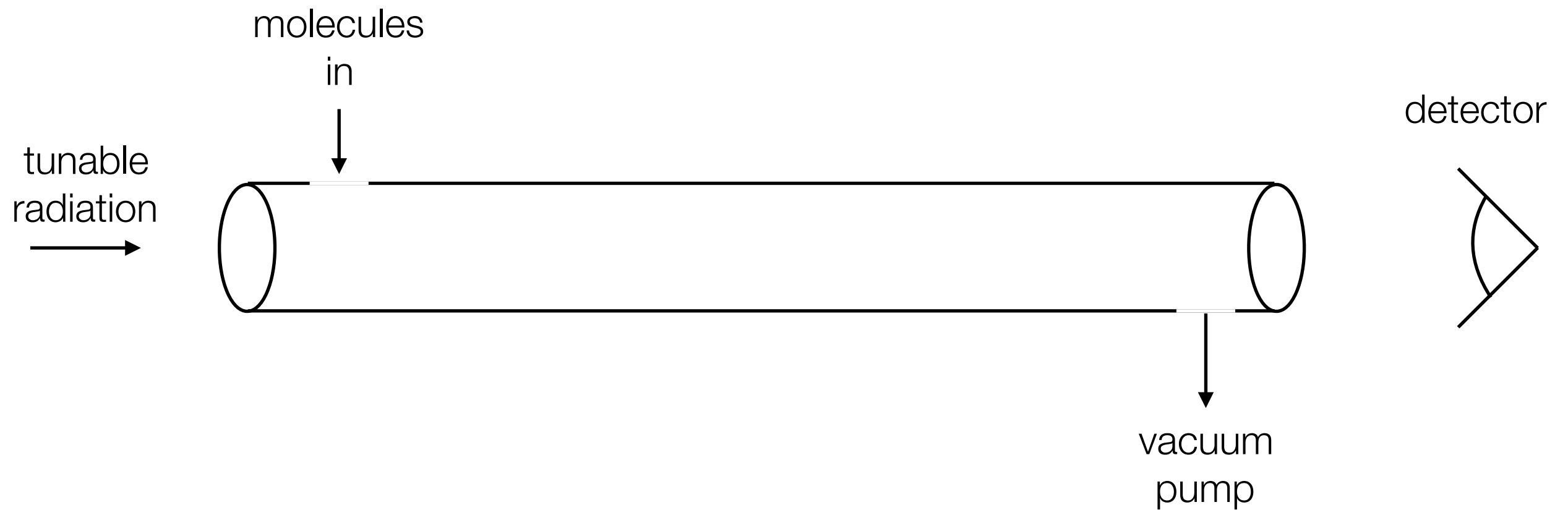
↓

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



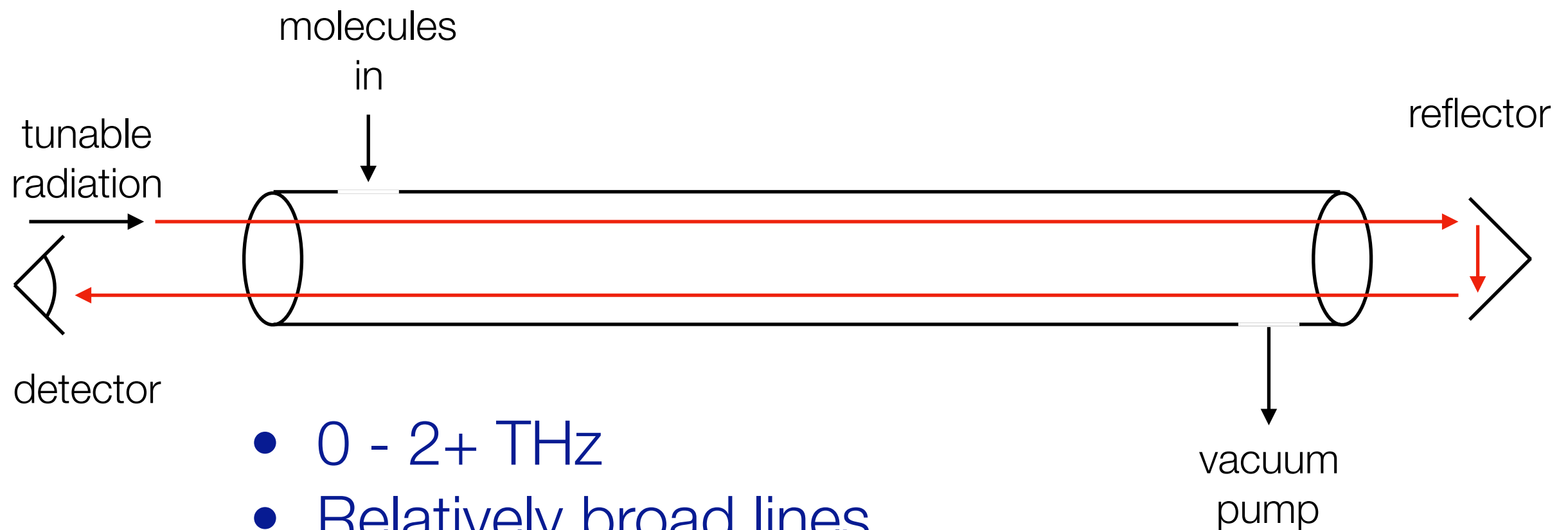
ROTATIONAL SPECTROSCOPY

Direct Absorption



ROTATIONAL SPECTROSCOPY

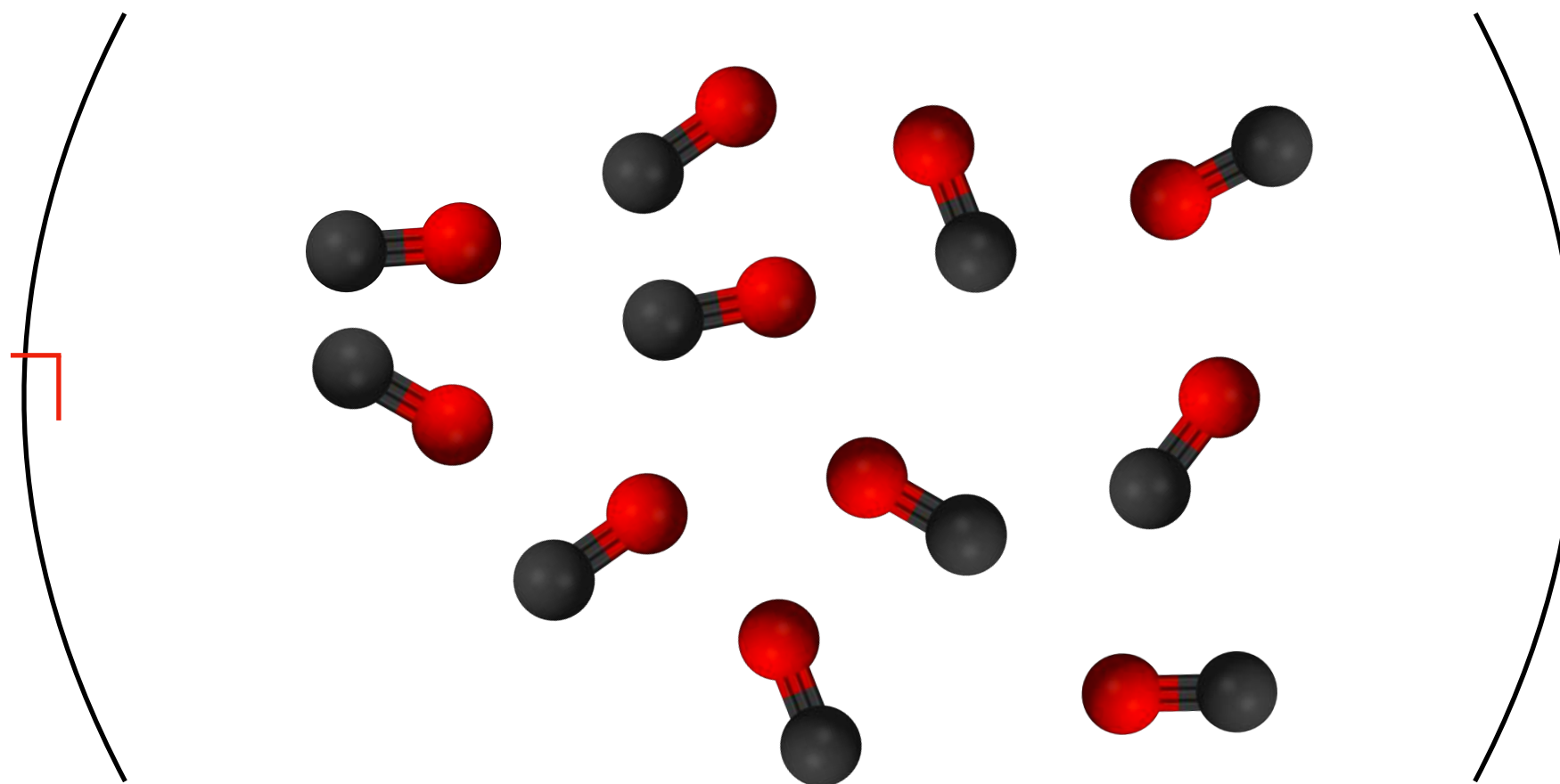
Direct Absorption



- 0 - 2+ THz
- Relatively broad lines
- 10-25 kHz accuracy
- Modest sensitivity
- Slow

ROTATIONAL SPECTROSCOPY

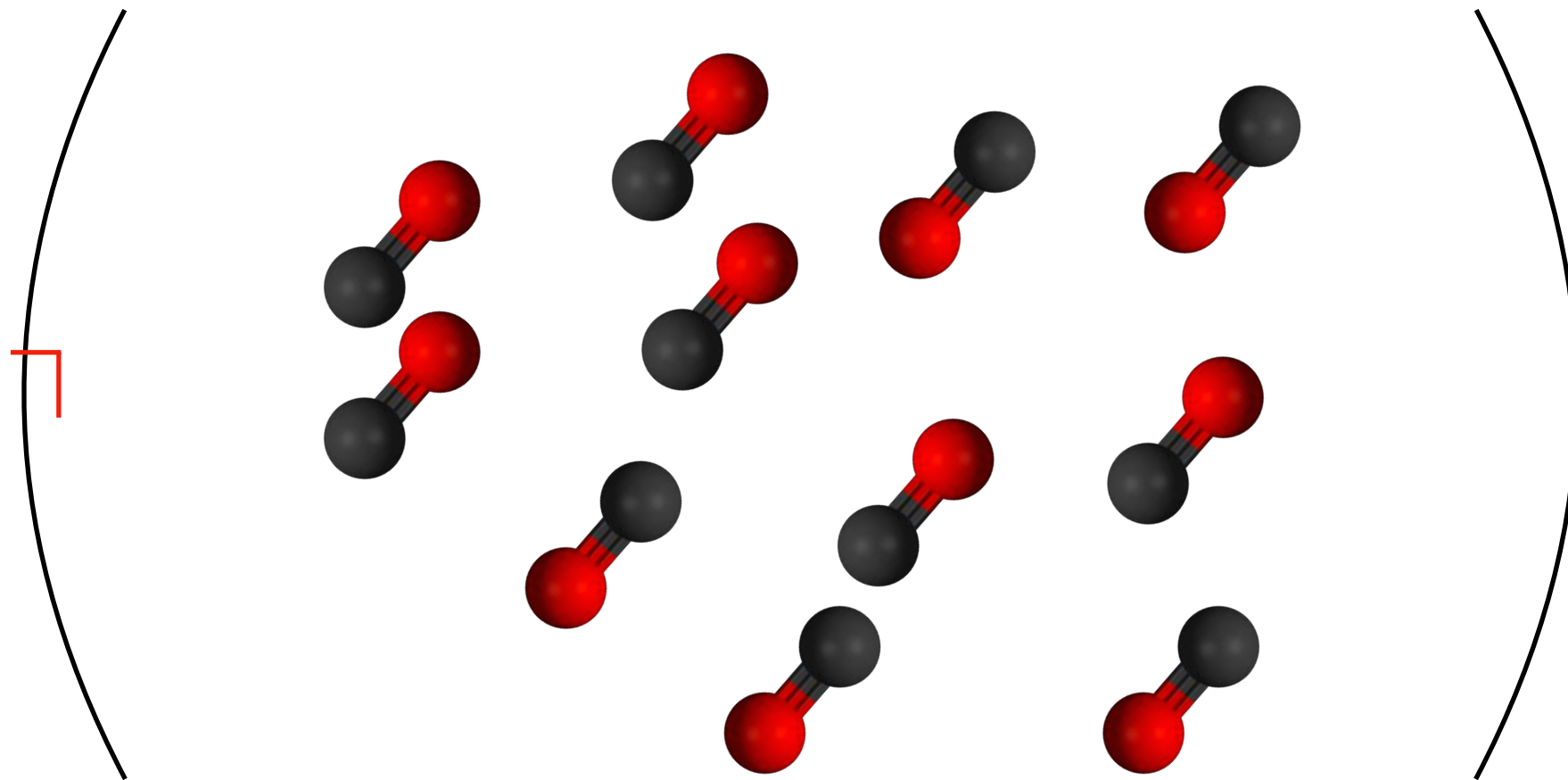
Cavity FTMW



It's an FFT. Our power is distributed over one mode, and amplified in cavity.

ROTATIONAL SPECTROSCOPY

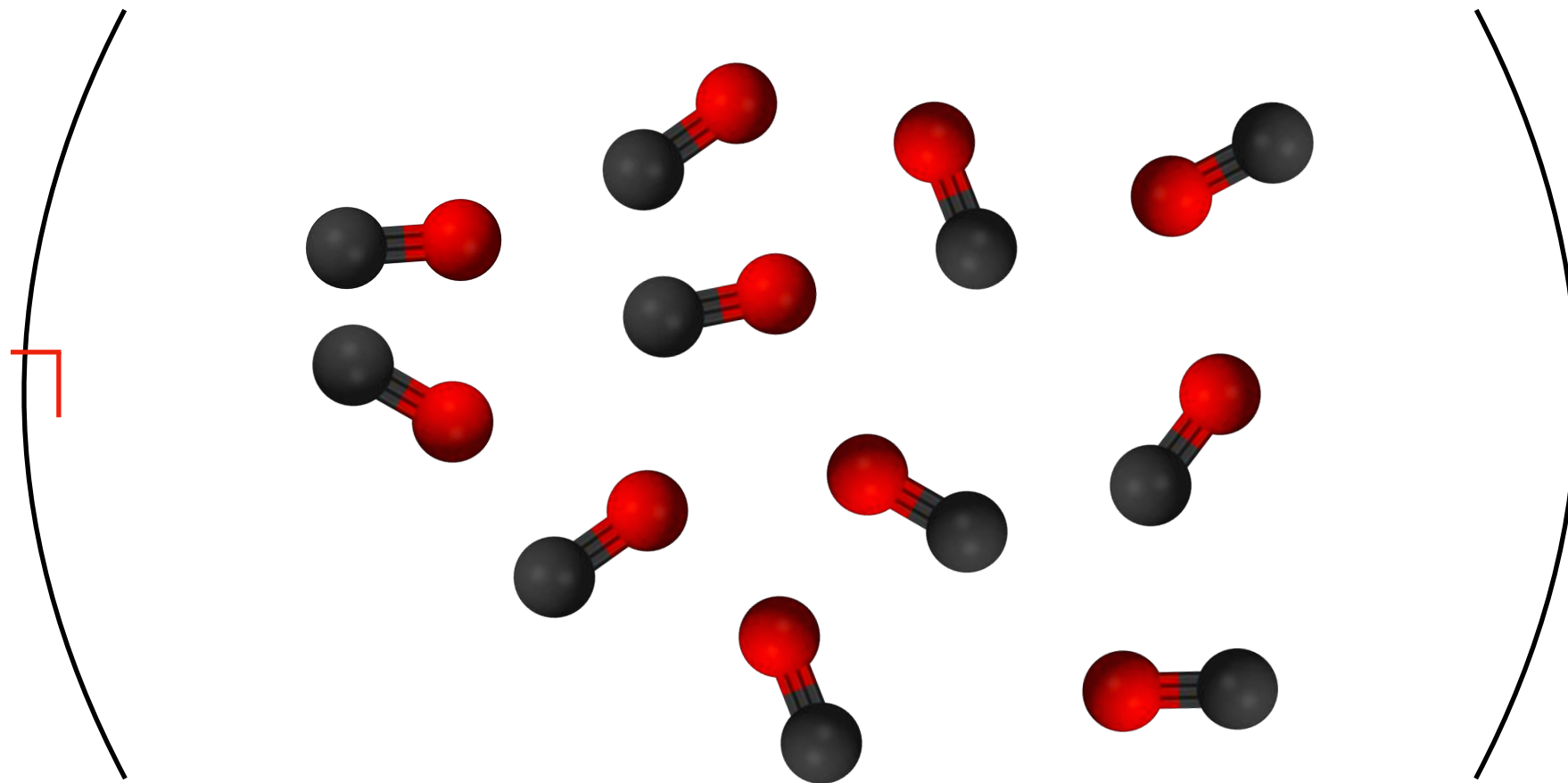
Cavity FTMW



It's an FFT. Our power is distributed over one mode, and amplified in cavity.

ROTATIONAL SPECTROSCOPY

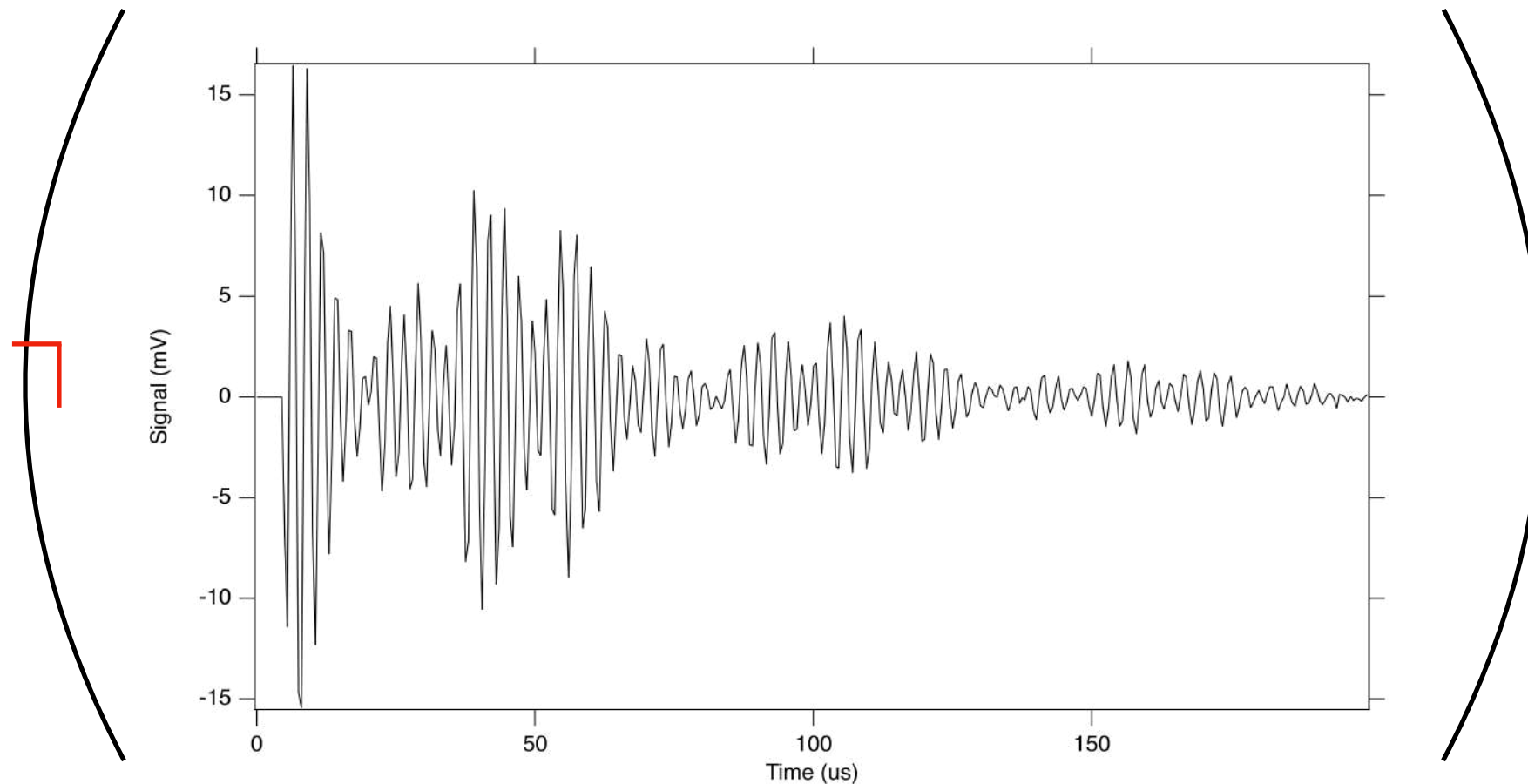
Cavity FTMW



It's an FFT. Our power is distributed over one mode, and amplified in cavity.

ROTATIONAL SPECTROSCOPY

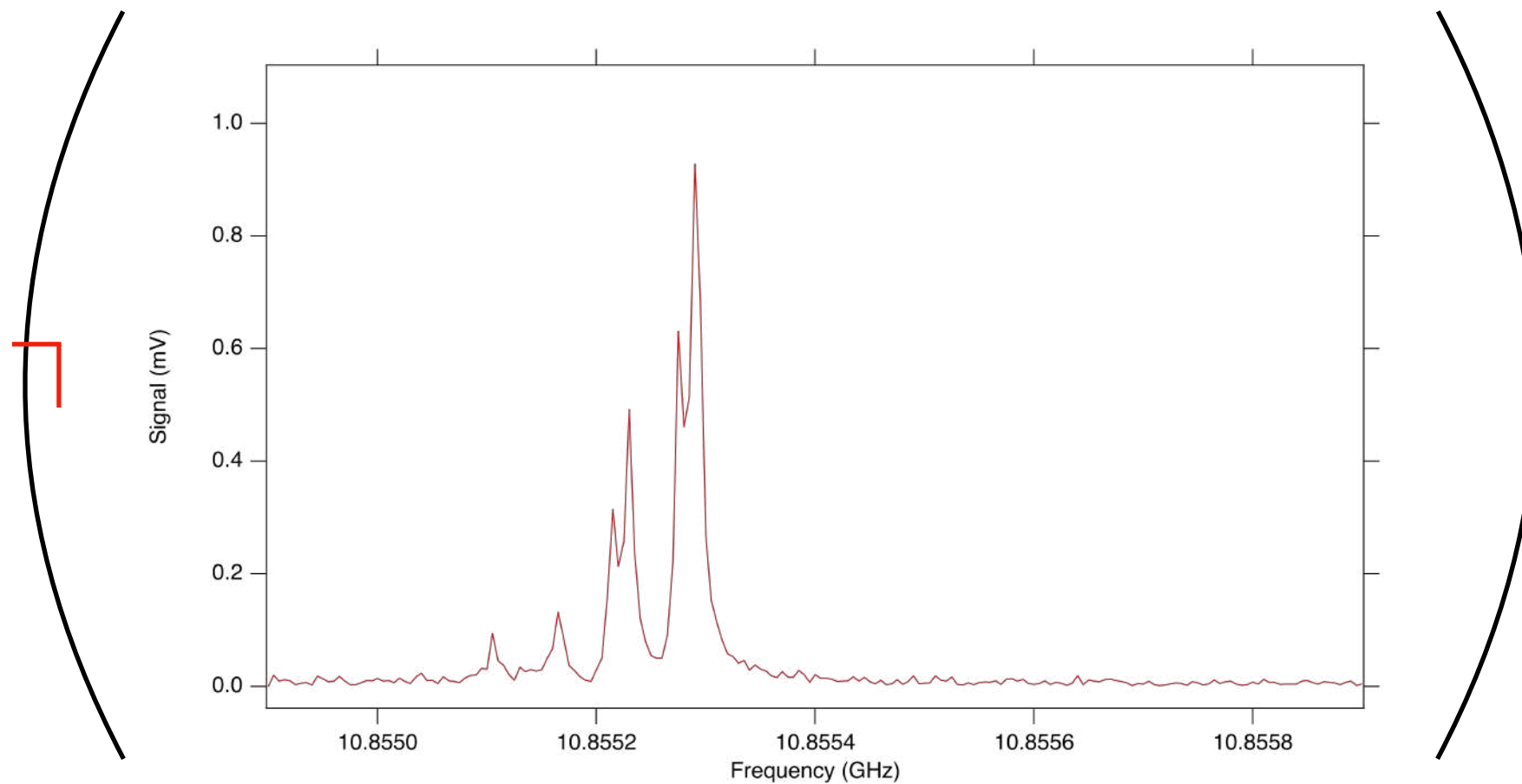
Cavity FTMW



It's an FFT. Our power is distributed over one mode, and amplified in cavity.

ROTATIONAL SPECTROSCOPY

Cavity FTMW



ROTATIONAL SPECTROSCOPY

Cavity FTMW

- 0 - 45 GHz
- Extremely narrow lines
- <1 kHz accuracy
- Very high sensitivity
- Slow

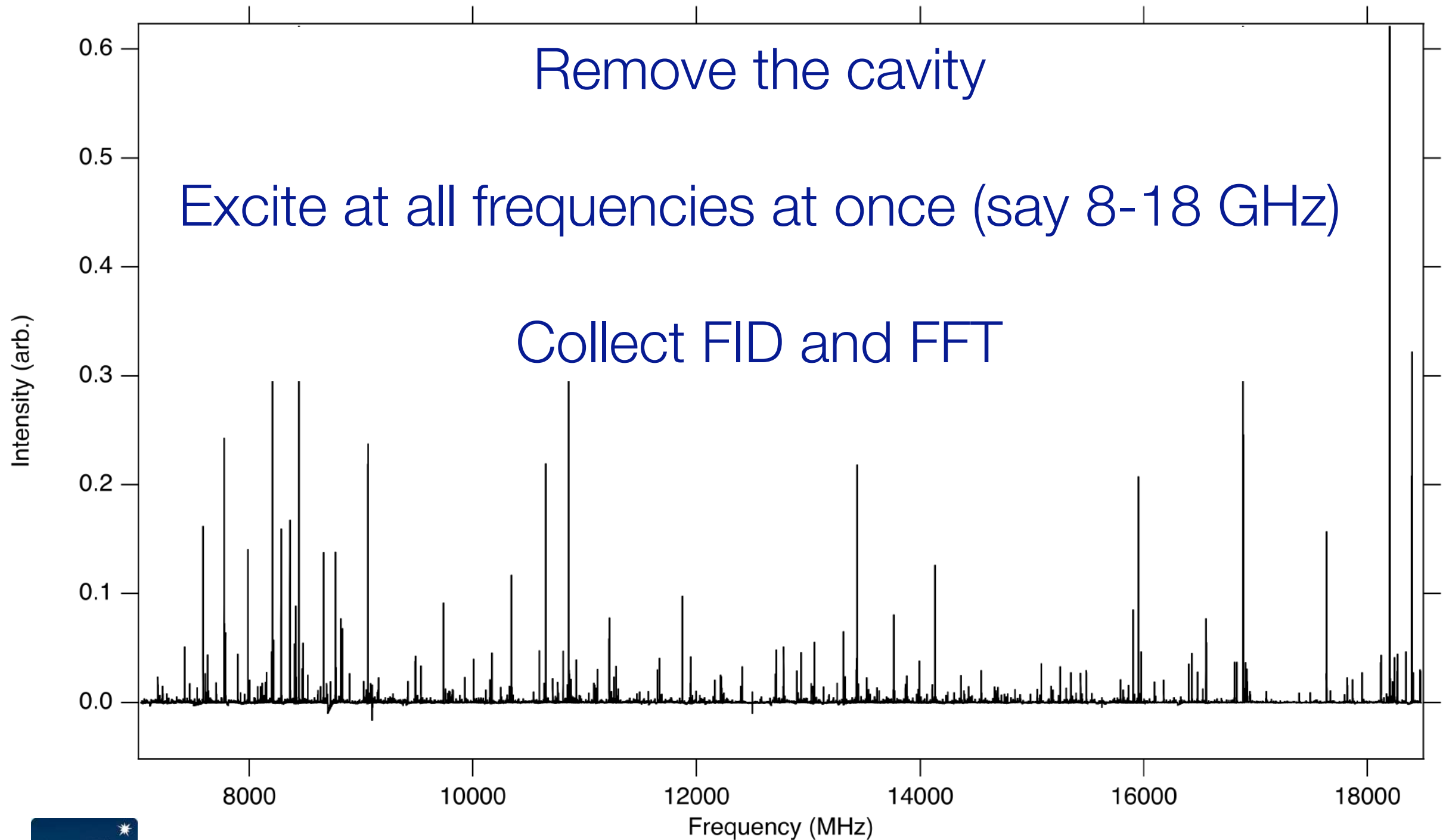
ROTATIONAL SPECTROSCOPY

CP-FTMW

Remove the cavity

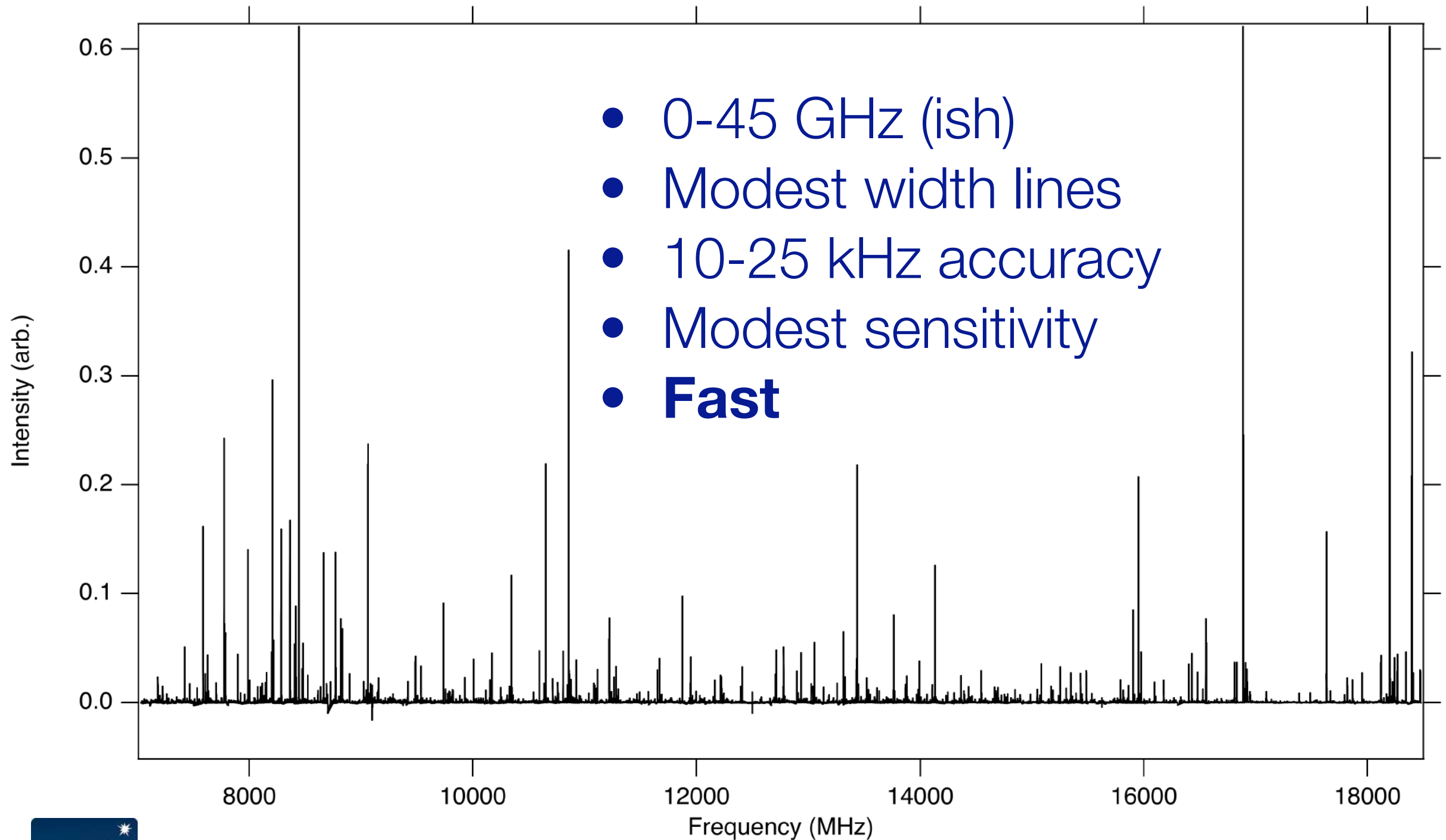
Excite at all frequencies at once (say 8-18 GHz)

Collect FID and FFT



ROTATIONAL SPECTROSCOPY

CP-FTMW



DELIVERABLE PROCESS

Measure $10^1 - 10^4$ lines

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



Determine the rotational constants to high accuracy



Use those constants to predict other unmeasured lines and
construct a 'complete' spectrum

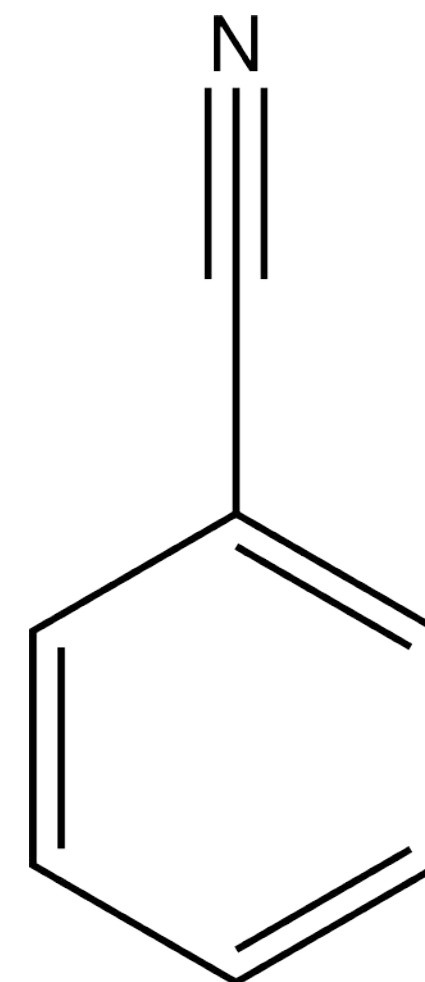


Publish

ROTATIONAL SPECTROSCOPY DATABASES

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

Constant	Ref. (24)	This work ^{1,2}	Global ^{1,3}
A (MHz)	5655.2654(72)	5655.26522(59)	5655.26519(59)
B (MHz)	1546.875864(66)	1546.875836(63)	1546.875822(54)
C (MHz)	1214.40399(10)	1214.404061(48)	1214.404047(40)
Δ_J (kHz)	0.0456(15)	0.045629(284)	0.04555(235)
Δ_{JK} (kHz)	0.9381(56)	0.93328(241)	0.93304(234)
Δ_K (kHz)	0.50(38)	0.272(64)	0.272(64)
δ_J (kHz)	0.01095(41)	0.011106(163)	0.011094(157)
δ_K (kHz)	0.628(53)	0.6136(73)	0.6141(72)
$\chi_{aa}(\text{N})$ (MHz)	-4.23738(36)	-4.23797(89)	-4.23749(45)
$\chi_{bb}(\text{N})$ (MHz)	2.2886(11)	2.28907(118)	2.28871(65)
Number of Measurements	78	146	175
σ (MHz)	0.00524	0.00130	0.00123
weighted average	0.709	0.622	0.628



ROTATIONAL SPECTROSCOPY DATABASES

Splatalogue

[Basic](#)
[Advanced](#)

[Motivation](#)
[Notes on Observing Frequencies](#)
[Notes on Quantum Numbers](#)

[Applications \(SLAP Interface\)](#)
[NRAO Homepage](#)
[NAASC/ALMA Homepage](#)

[ALMA Science Portal](#)
[Helpdesk](#)
[Splatalogue Quick Start Guide \(PDF\)](#)
[Splatalogue Changelog](#)

03006 13C17O - Carbon Monoxide
03007 H13CO+ - Formylium
03008 HC17O+ - Formylium
03009 HCO+ - Formylium

Enter Molecular Formula (Case sensitive) to Calculate Mass

Calculate Mass

Data Versions +/-
Version 3 (7/1/2016) ▾

Specify Ranges +/-

Specify a Frequency Range:
From 12340 To 12370
+ Frequency - Frequency
☒ MHz ☐ GHz

Specify an Energy Range:
From to
☐ E_L (cm⁻¹) ☐ E_U (cm⁻¹)
☐ E_L (K) ☐ E_U (K)

Line Intensity Lower Limits +/-

Search Results

Found 145 lines from 12340 - 12370 MHz, showing 1 - 145
Click on the chemical formula below for more information about that species

	Species	Chemical Name	Freq in MHz (Err)	Meas Freq in MHz (Err)	Resolved QNs	CDMS/JPL Intensity	Lovas/AST Intensity	E _L (cm ⁻¹)	Linelist
1	CH₃NH₂	Methylamine	12340.01200 (0.008)		6(1)E2-1- 5(2)E2-1, F= 7 - 6	0.00000		33.22400	SLAIM
2	H₂NCH₂COOH - II v=1	Glycine	12340.13420 (3.0698)		24(7,17)-24(7,18), F=24-24	-8.98960		1570.12040	JPL
3	C¹³CC₄H	1,3,5-Hexatriynyl		12340.32800 (0.01)	J=9/2-7/2, Ω=3/2, F ₁ = 5- 4, F=11/2-9/2, l=f	-5.67320		0.54970	CDMS
4	CH₃NH₂	Methylamine	12340.37000 (0.008)		6(1)E2-1- 5(2)E2-1	0.00000		33.22400	SLAIM
5	C¹³CC₄H	1,3,5-Hexatriynyl		12340.40300 (0.01)	J=9/2-7/2, Ω=3/2, F ₁ = 5- 4, F=9/2-7/2, l=f	-5.76210		0.54970	CDMS
6	CH₃NH₂	Methylamine	12340.43060 (0.0056)		J = 6 - 5, K = 1 - 2, E ₂ , l = -1	-7.59660		33.22350	JPL
7	CH₃CH₂CH₂CN-gauche	Butyronitrile	12340.43840 (0.0446)		42(6,37)-43(4,40)	-9.35220		281.10860	JPL
8	NH₃ v=0	Ammonia	12340.44520 (0.2898)		22(17)0a-22(17)0s	-11.85300		3895.89460	JPL
9	CH₃COOH v=1	Acetic Acid	12341.07000 (0.005)		6(6, 0)- 6(5, 1) +- v=1	0.00000		92.36000	SLAIM
10	CH₃NH₂	Methylamine	12341.25100 (0.008)		6(1)E2-1- 5(2)E2-1, F= 6 - 5	0.00000		33.22400	SLAIM

ALMA OT

Transition Filter

*
e.g. CO*2-1* or *oxide*

☒ Include description

Frequency Filters

ALMA Band

1 2 3 4 5 6 7 8 9 10

Sky Frequency (GHz)

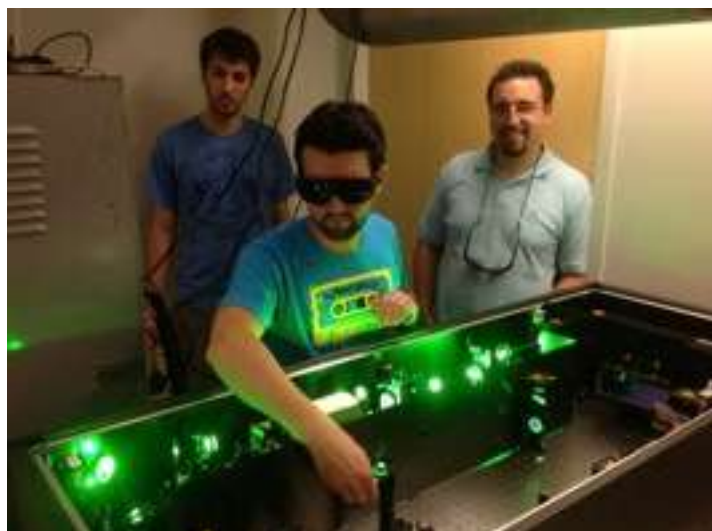
Min 31.3 Max 950

Transitions matching your filter settings:
(double-click column header for primary sort, single-click subsequent columns for secondary sorting. Single clicks will reverse sort order of already selected columns.)

Transition	Description	Rest Freq...	Sky Frequency	Upper-state ...	Lovas Inte...	Sij μ ²	Cata...
I-C5H J=35/2-33/2, Ω=3/2, F=17-16, l=f	2,4-Pentadiynylidyne	84.108238 ...	84.108319 ...	71.861 K	4.7	401.709 D ²	Offline
I-C5H J=35/2-33/2, Ω=3/2, F=18-17, l=f	2,4-Pentadiynylidyne	84.108398 ...	84.108480 ...	71.861 K	4.7	425.314 D ²	Offline
I-C5H J=35/2-33/2, Ω=3/2, F=17-16, l=e	2,4-Pentadiynylidyne	84.110087 ...	84.110168 ...	71.862 K		401.692 D ²	Offline
I-C5H J=35/2-33/2, Ω=3/2, F=18-17, l=e	2,4-Pentadiynylidyne	84.110244 ...	84.110325 ...	71.862 K		425.395 D ²	Offline
C4H v7 = 1 J=17/2-15/2, Ω=1/2, l=f	1,3-Butadiynyl radical	84.123003 ...	84.123085 ...	211.671 K	2.1	12.771 D ²	Offline
CH3CH2CN v=0 11(0,11)-10(1,10)	Ethyl Cyanide	84.151838 ...	84.151919 ...	28.102 K	0.1	10.328 D ²	Offline
CH3OH v t=1 11(10,1)-11(11,0)	Methanol	84.158571 ...	84.158652 ...	1066.119 K		1.459 D ²	Offline
U-84163	UNIDENTIFIED	84.163000 ...	84.163081 ...		0.06		Offline
30SiO v=1 2-1	Silicon Monoxide	84.164253 ...	84.164334 ...	1753.828 K		19.441 D ²	Offline
c-H13CCCH 2(1,2)-1(0,1)	Cyclopropenylidene	84.185621 ...	84.185703 ...	6.331 K	0.13	17.24 D ²	Offline
U-84215	UNIDENTIFIED	84.215000 ...	84.215081 ...		0.08		Offline
CH3CN v8=1 J = 36-36, K = 3-1	Methyl Cyanide	84.271390 ...	84.271472 ...	1139.034 K		0.122 D ²	Offline
SO2 v=0 32(5,27)-31(6,26)	Sulfur dioxide	84.320876 ...	84.320958 ...	549.36 K	0.1	13.463 D ²	Offline

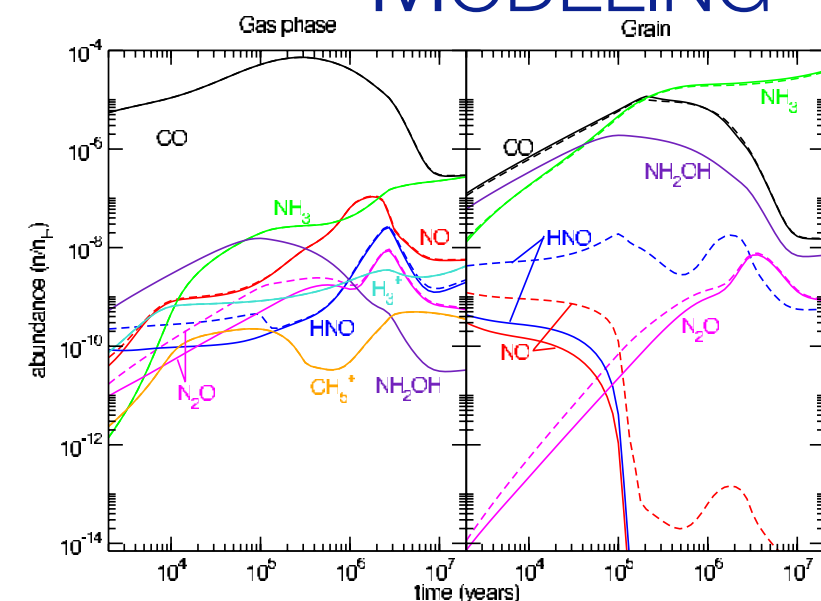


LABORATORY ASTROPHYSICS



ASTROCHEMISTRY

ASTROCHEMICAL MODELING



Temperatures, Abundances,
and Densities

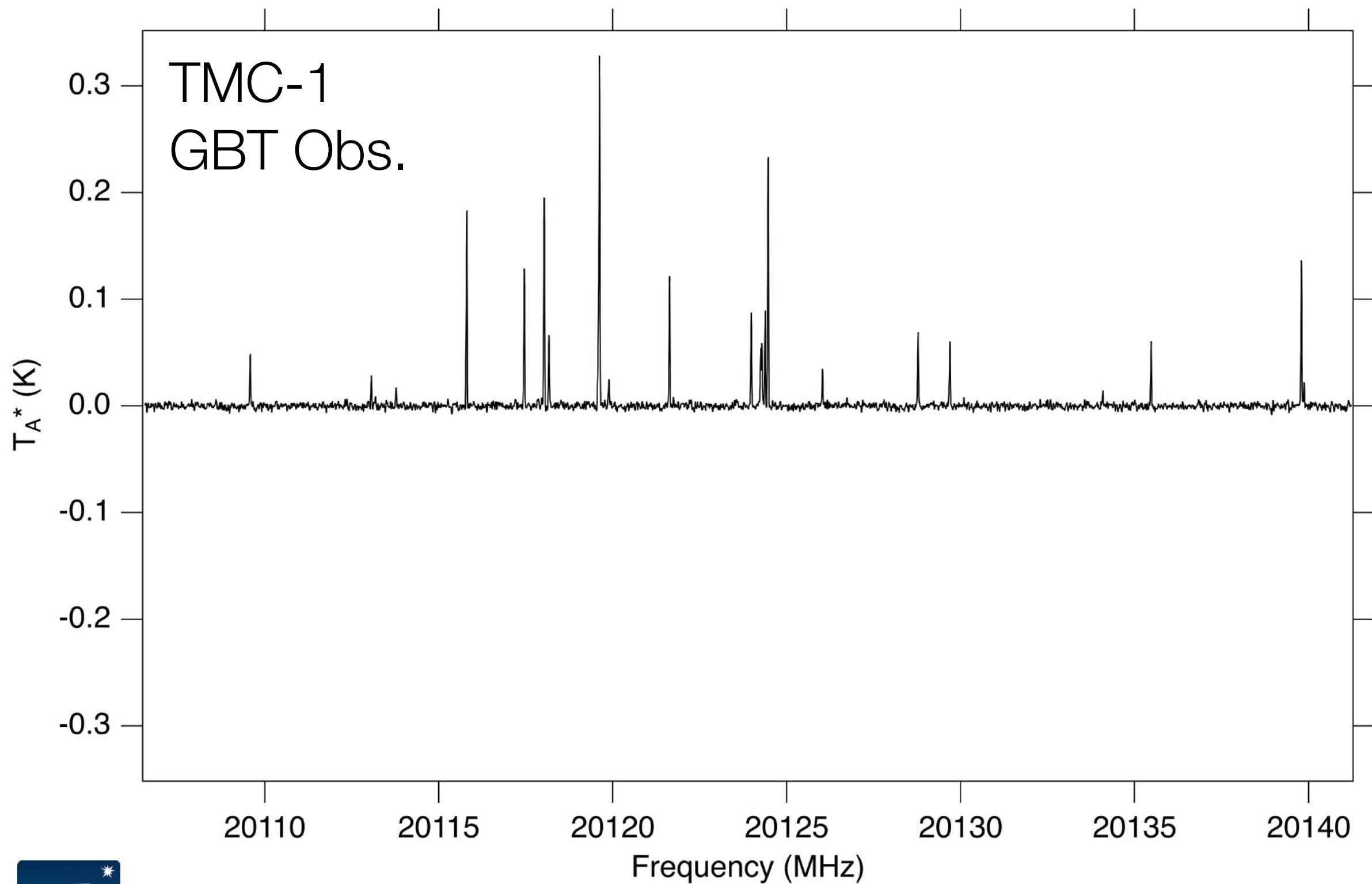
Rotational, Vibrational,
and Electronic Spectra

Chemical Inventories
Temperatures, Abundances,
and Densities

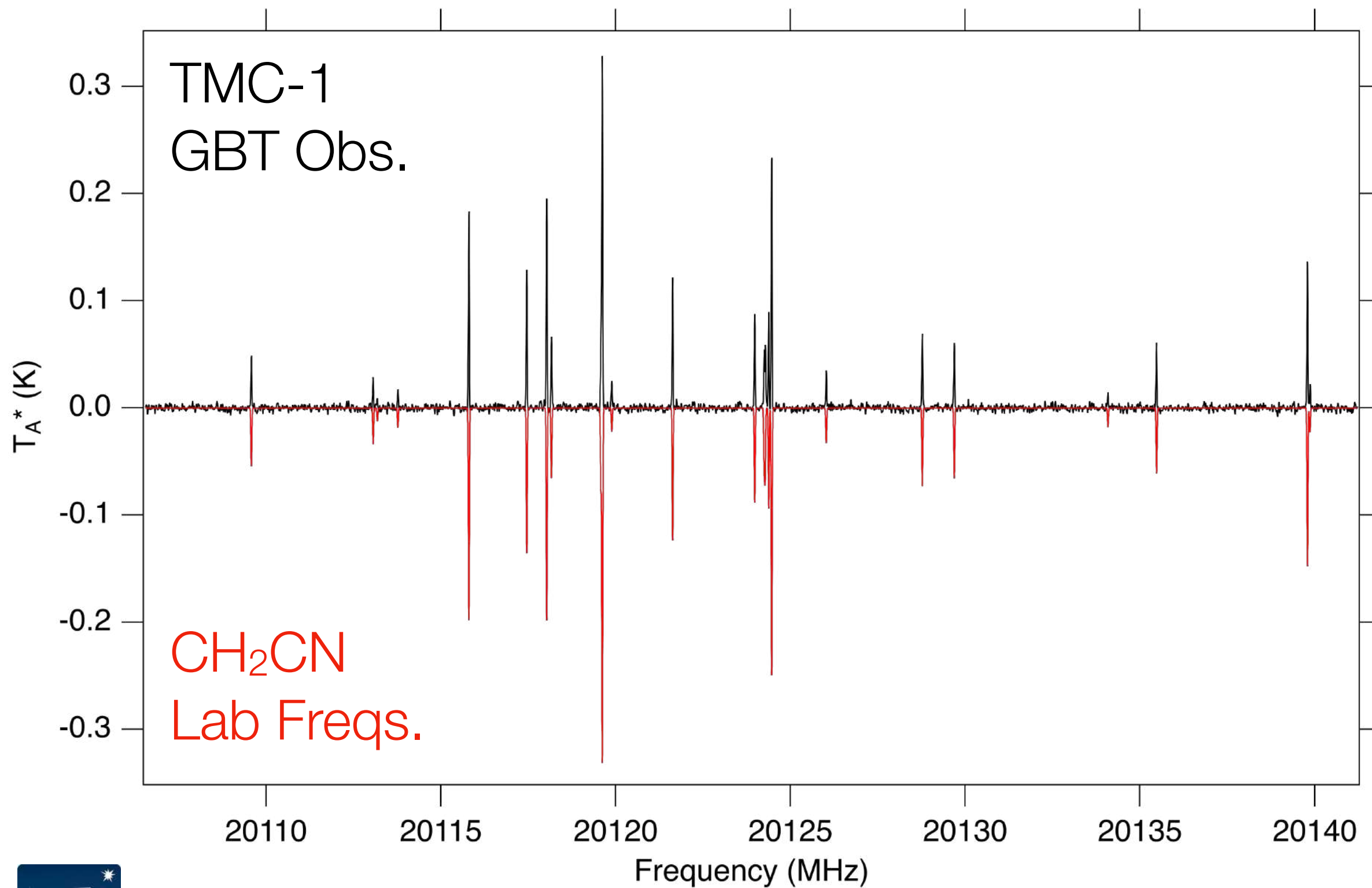
OBSERVATIONAL ASTRONOMY



INTERSTELLAR DETECTIONS



INTERSTELLAR DETECTIONS

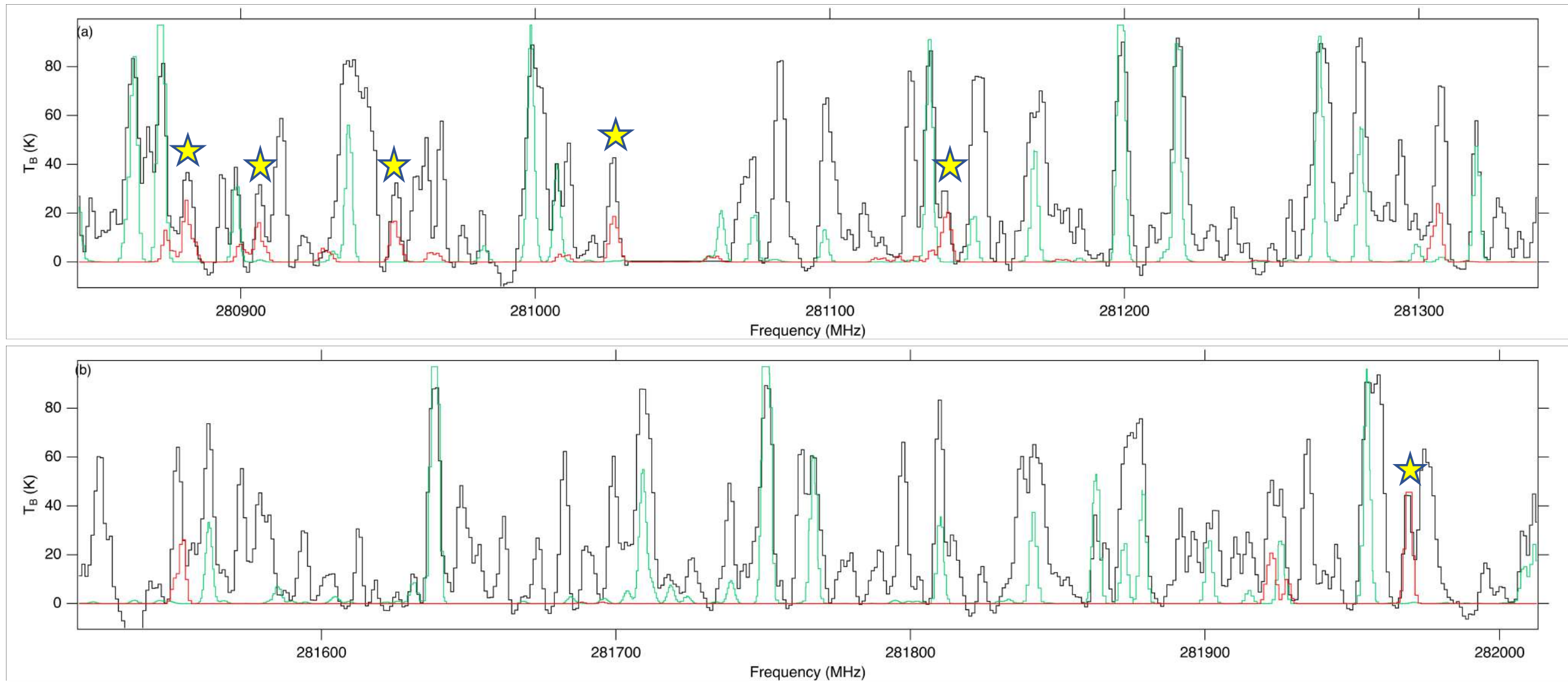


INTERSTELLAR DETECTIONS

NGC 6334I
(ALMA Obs)

Common Species
(Lab Freqs.)

methoxymethanol
(Lab Freqs.)



McGuire et al. 2017 *ApJL* 851, L46



WHAT HAS BEEN GLOSSED OVER/IGNORED?

How do we predict the relative intensities of the lines in observations?

Intrinsic Line Strength
Excitation Temperature (T_{ex})
Background Continuum
Beam Size vs Source Size
Linewidth
Excitation Conditions (Radiation/Density)
Optical Depth

INTERSTELLAR DETECTIONS

2 Atoms		3 Atoms		4 Atoms		5 Atoms		6 Atoms		7 Atoms		8 Atoms		9 Atoms	
H ₂	SiS	C ₃	SiCN	c-C ₃ H	H ₂ CS	C ₅		C ₅ H		C ₆ H		CH ₃ C ₃ N		CH ₃ C ₄ H	
AlF	CS	C ₂ H	AlNC	/-C ₃ H	H ₃ O ⁺	C ₄ H		/-H ₂ C ₄		CH ₂ CHCN		HC(O)OCH ₃		CH ₃ CH ₂ CN	
AlCl	HF	C ₂ O	SiNC	C ₃ N	c-SiC ₃	C ₄ Si		C ₃ H ₄		CH ₃ C ₂ H		CH ₃ COOH		(CH ₃) ₂ O	
C ₂	HD	C ₂ S	HCP	C ₃ O	CH ₃	/-C ₃ H ₂		CH ₃ CN		HC ₅ N		C ₇ H		CH ₃ CH ₂ OH	
CH	FeO	CH ₂	CCP	C ₃ S	C ₃ N ⁻	c-C ₃ H ₂		CH ₃ NC		CH ₃ CHO		C ₆ H ₂		HC ₇ N	
CH ⁺	O ₂	HCN	AlOH	C ₂ H ₂	PH ₃	H ₂ CCN		CH ₃ OH		CH ₃ NH ₂		CH ₂ OHCHO		C ₈ H	
CN	CF ⁺	HCO	H ₂ O ⁺	NH ₃	HCNO	CH ₄		CH ₃ SH		c-C ₂ H ₄ O		/-HC ₆ H		CH ₃ C(O)NH ₂	
CO	SiH	HCO ⁺	H ₂ Cl ⁺	HCCN	HOCN	HC ₃ N		HC ₃ NH ⁺		H ₂ CCHOH		CH ₂ CHCHO		C ₈ H ⁻	
CO ⁺	PO	HCS ⁺	KCN	HCNH ⁺	HSCN	HC ₂ NC		HC ₂ CHO		C ₆ H ⁻		CH ₂ CCHCN		C ₃ H ₆	
CP	AlO	HOC ⁺	FeCN	HNCO	H ₂ O ₂	HCOOH		NH ₂ CHO		CH ₃ NCO		H ₂ NCH ₂ CN		CH ₃ CH ₂ SH	
SiC	OH ⁺	H ₂ O	HO ₂	HNCS	C ₃ H ⁺	H ₂ CNH		C ₅ N		HC ₅ O		CH ₃ CHNH		CH ₃ NHCHO	
HCl	CN ⁻	H ₂ S	TiO ₂	HOCO ⁺	HMgNC	H ₂ C ₂ O		/-HC ₄ H				CH ₃ SiH ₃			
KCl	SH ⁺	HNC	C ₂ N	H ₂ CO	HCCO	H ₂ NCN		/-HC ₄ N							
NH	SH	HNO	Si ₂ C	H ₂ CN		HNC ₃		c-H ₂ C ₃ O							
NO	HCl ⁺	MgCN	HS ₂			SiH ₄		H ₂ CCNH							
NS	TiO	MgNC	NCO			H ₂ COH ⁺		C ₅ N ⁻							
NaCl	ArH ⁺	N ₂ H ⁺	HSC			C ₄ H ⁻		HNCHCN							
OH	N ₂	N ₂ O	HCS			HC(O)CN		SiH ₃ CN							
PN	NO ⁺	NaCN				HNCNH									
SO	NS ⁺	OCS				CH ₃ O									
SO ⁺		SO ₂				NH ₄ ⁺									
SiN		c-SiC ₂				H ₂ NCO ⁺									
SiO		CO ₂				NCCNH ⁺									
		NH ₂				CH ₃ Cl									
		H ₃ ⁺				H ₂ NCO ⁺									

202 Individual
Species

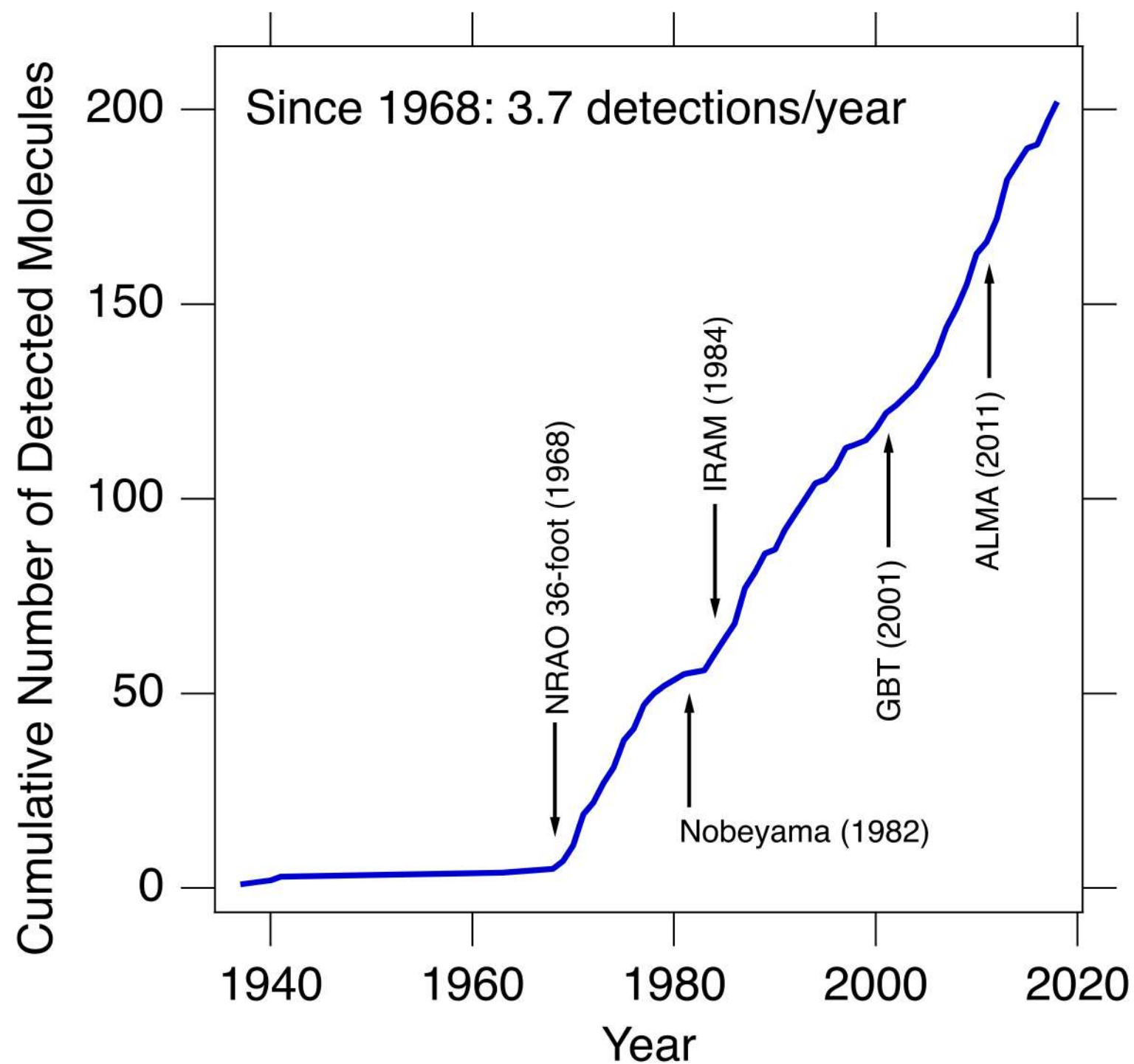


INTERSTELLAR DETECTIONS

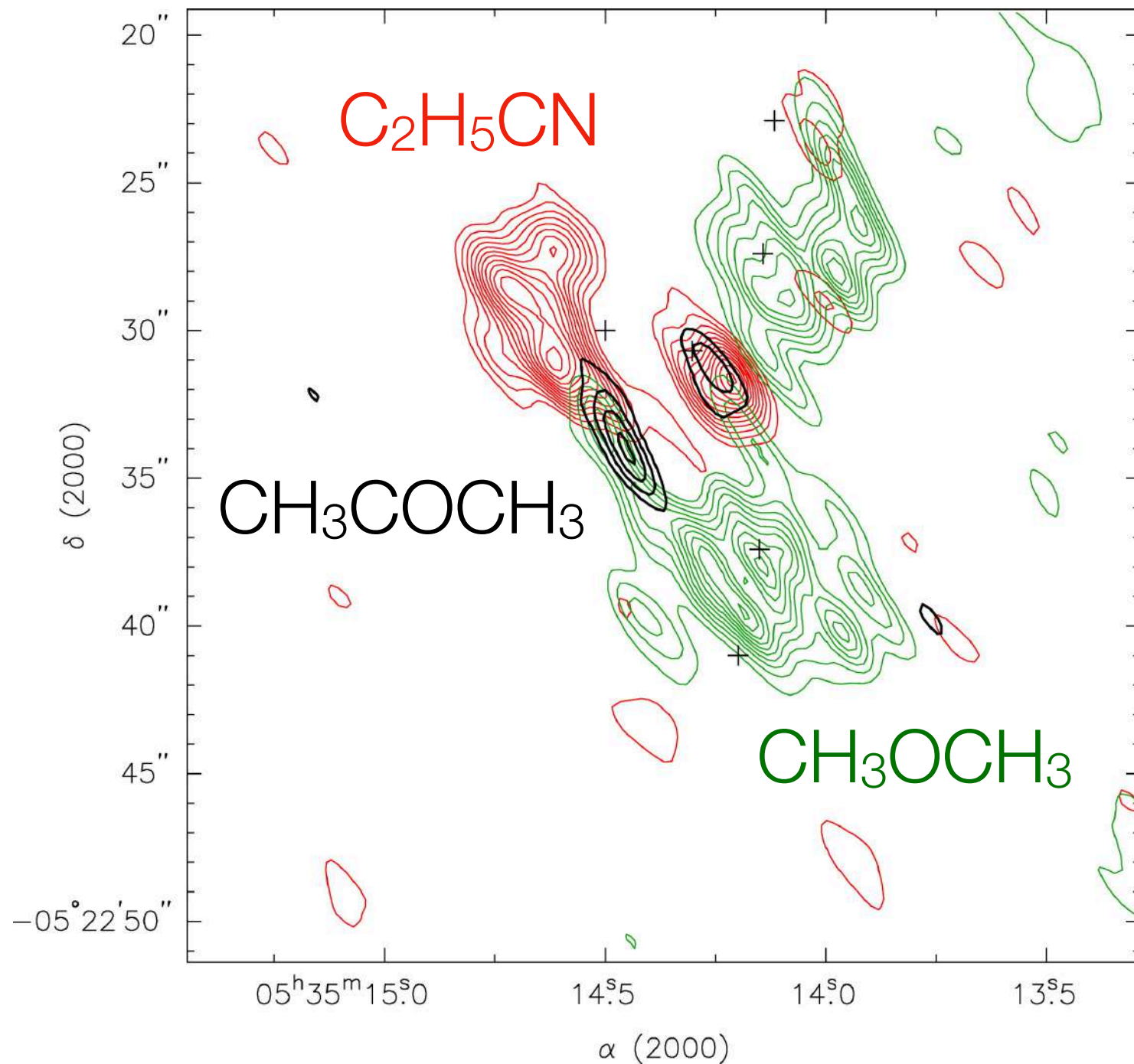
I	1 141																		2			
	H 1.00794 Hydrogen																		He 4.002602 Helium			
II	3		4																			
	Li 6.941 Lithium		Be 9.012182 Beryllium																			
III	11 2		12 3																			
	Na 22.98976928 Sodium		Mg 24.3050 Magnesium																			
IV	19 2		20	21	22 2		23	24	25	26 1		27	28	29	30	31	32	33	34	35	36	
	K 39.0983 Potassium		Ca 40.078 Calcium	Sc 44.955912 Scandium	Ti 47.867 Titanium		V 50.9415 Vanadium	Cr 51.9961 Chromium	Mn 54.938045 Manganese	Fe 55.845 Iron		Co 58.933195 Cobalt	Ni 58.6934 Nickel	Cu 63.546 Copper	Zn 65.38 Zinc	Ga 69.723 Gallium	Ge 72.64 Germanium	As 74.92160 Arsenic	Se 78.96 Selenium	Br 79.904 Bromine	Kr 83.798 Krypton	
V	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54				
	Rb 85.4678 Rubidium	Sr 87.62 Strontium	Y 88.90585 Yttrium	Zr 91.224 Zirconium	Nb 92.90638 Niobium	Mo 95.96 Molybdenum	Tc [98] Technetium	Ru 101.07 Ruthenium	Rh 102.90550 Rhodium	Pd 106.42 Palladium	Ag 107.8682 Silver	Cd 112.411 Cadmium	In 114.818 Indium	Sn 118.710 Tin	Sb 121.760 Antimony	Te 127.60 Tellurium	I 126.90447 Iodine	Xe 131.293 Xenon				
VI	55	56	LA		72	73	74	75	76	77	78	79	80	81	82	83	84	85	86			
	Cs 132.9054519 Cesium	Ba 137.327 Barium			Hf 178.49 Hafnium	Ta 180.94788 Tantalum	W 183.84 Tungsten	Re 186.207 Rhenium	Os 190.23 Osmium	Ir 192.217 Iridium	Pt 195.084 Platinum	Au 196.966569 Gold	Hg 200.59 Mercury	Tl 204.3833 Thallium	Pb 207.2 Lead	Bi 208.98040 Bismuth	Po [209] Polonium	At [210] Astatine	Rn [222] Radon			
VII	87	88	AC		104	105	106	107	108	109	110	111	112	113	114	115	116	117	118			
	Fr [223] Francium	Ra [226] Radium			Rf [267] Rutherfordium	Db [268] Dubnium	Sg [271] Seaborgium	Bh [272] Bohrium	Hs [270] Hassium	Mt [276] Meitnerium	Ds [281] Darmstadtium	Rg [280] Roentgenium	Cn [285] Copernicium	Nh [284] Nihonium	Fl [289] Flerovium	Mc [288] Moscovium	Lv [293] Livermorium	Ts [294] Tennessine	Og [294] Oganesson			
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18			



INTERSTELLAR DETECTIONS

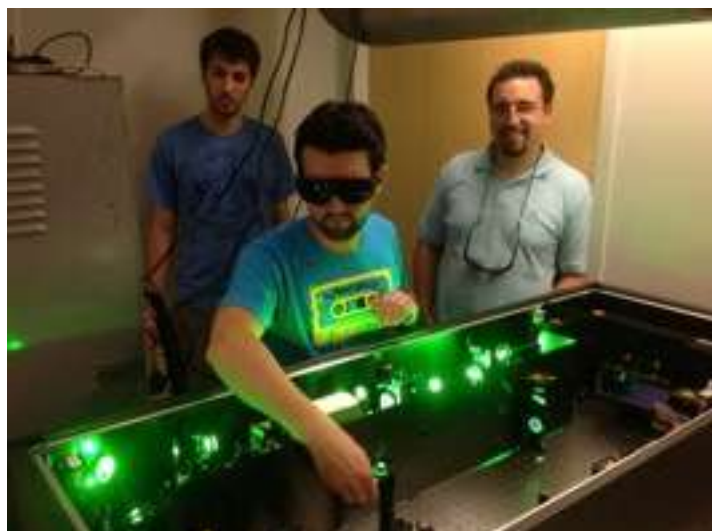


DELIVERABLES



- Spatial distributions
- Excitation conditions
- Column densities

LABORATORY ASTROPHYSICS



ASTROCHEMISTRY

Chemical Reactions, Kinetics, Thermodynamics

Species and Reactions of Interest

Extraordinarily
Broad Range of
Research

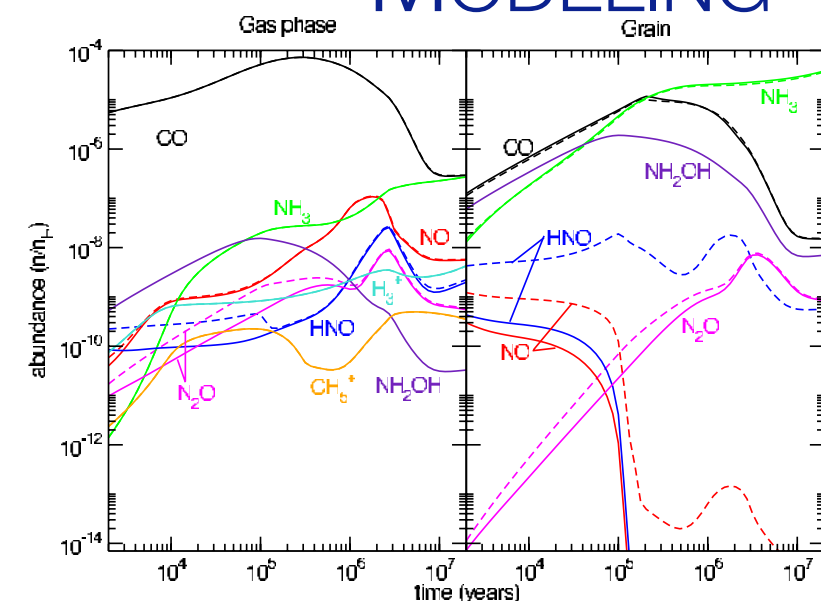
Temperatures, Abundances,
and Densities

Rotational, Vibrational,
and Electronic Spectra

Environments and Species
of Interest

Chemical Inventories
Temperatures, Abundances,
and Densities

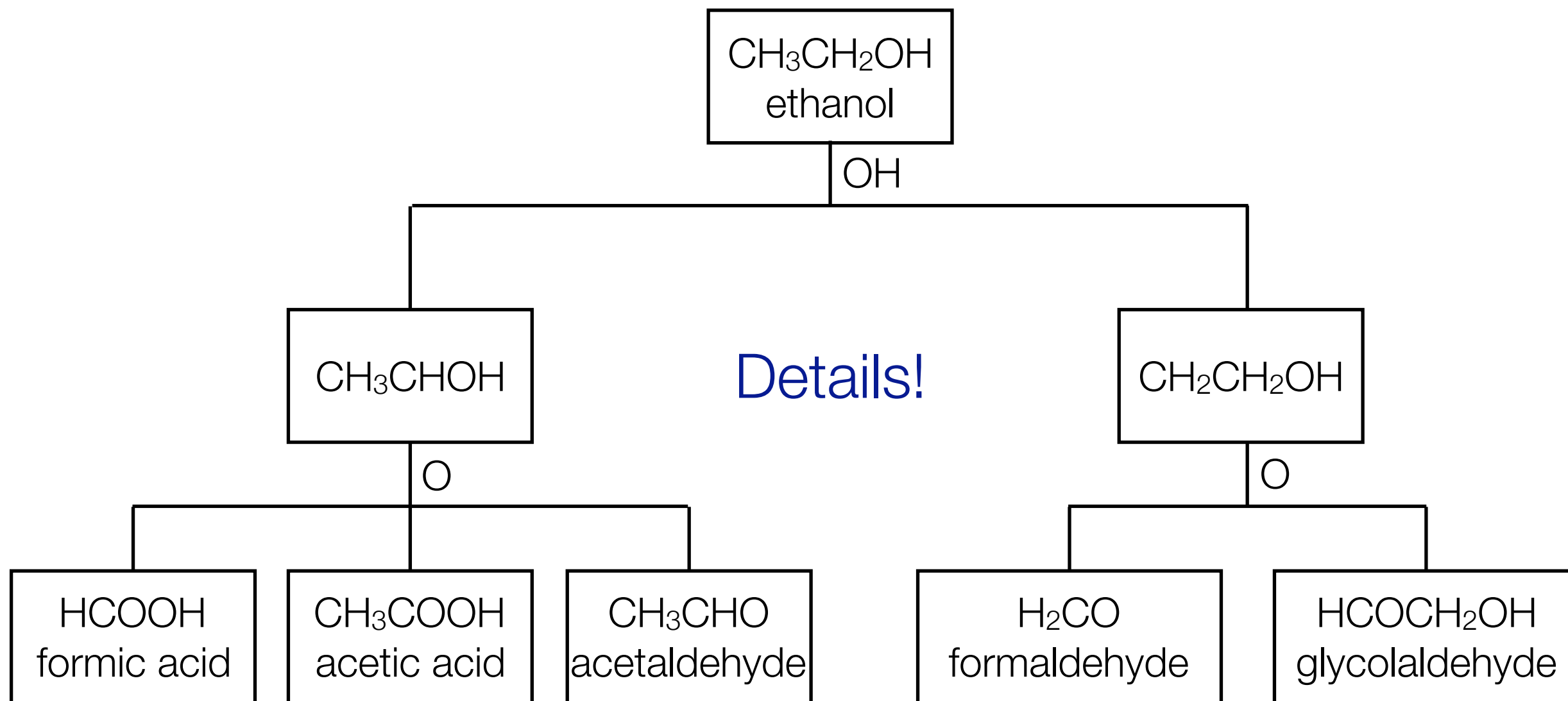
ASTROCHEMICAL MODELING



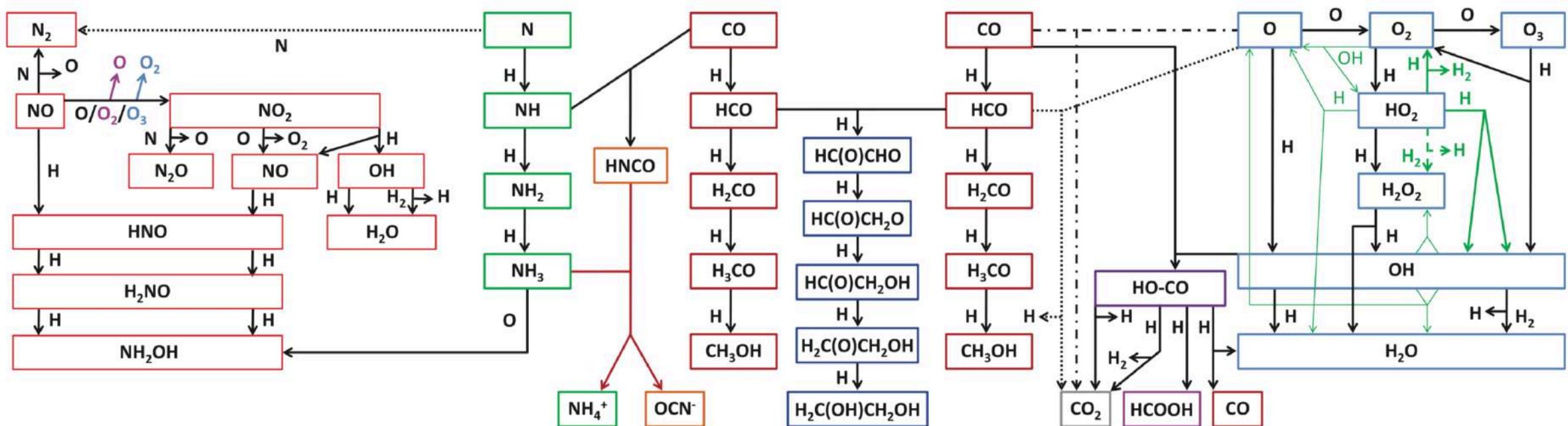
OBSERVATIONAL ASTRONOMY



CHEMICAL MODELING

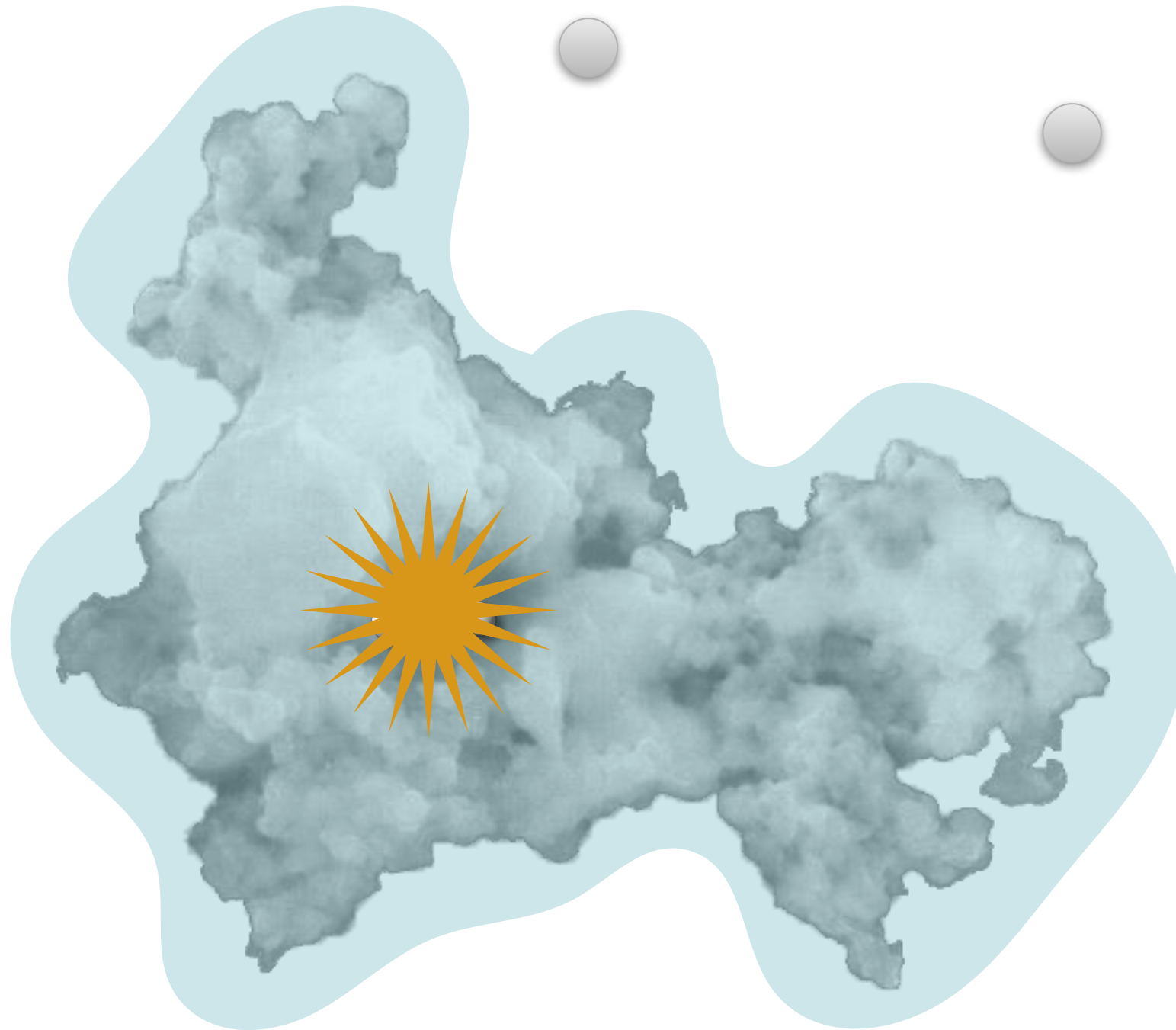


CHEMICAL MODELING



Typical networks have 800+ species and ~10,000 reactions

CHEMICAL MODELING



CHEMICAL MODELING - RATE EQUATIONS

$$\frac{dx}{dt} = \underbrace{\sum_y \sum_z k_{yz} n(y) n(z)}_{\text{Formation of } \mathbf{x}} - \underbrace{n(x) \sum_y k_{xy} n(y)}_{\text{Destruction of } \mathbf{x}}$$

How molecule \mathbf{x} changes abundance with time \mathbf{t}

(~)Rate of the reaction between \mathbf{y} and \mathbf{z} to form \mathbf{x}

Abundance of species \mathbf{y} and \mathbf{z} that react to form \mathbf{x}

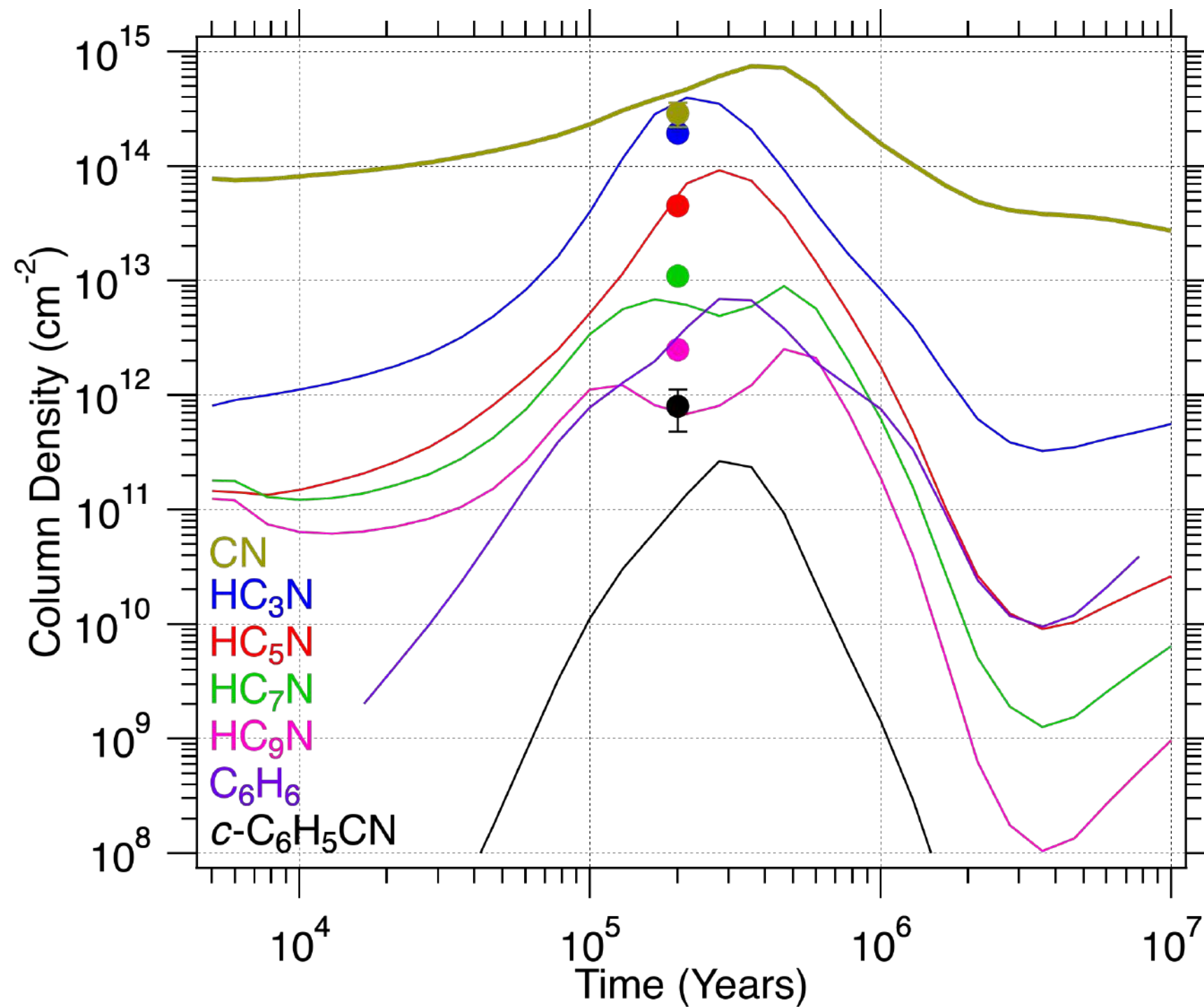
Abundance of \mathbf{x}

(~)Rate of the reaction with \mathbf{y} to destroy \mathbf{x}

Abundance of species \mathbf{y} that destroys \mathbf{x}

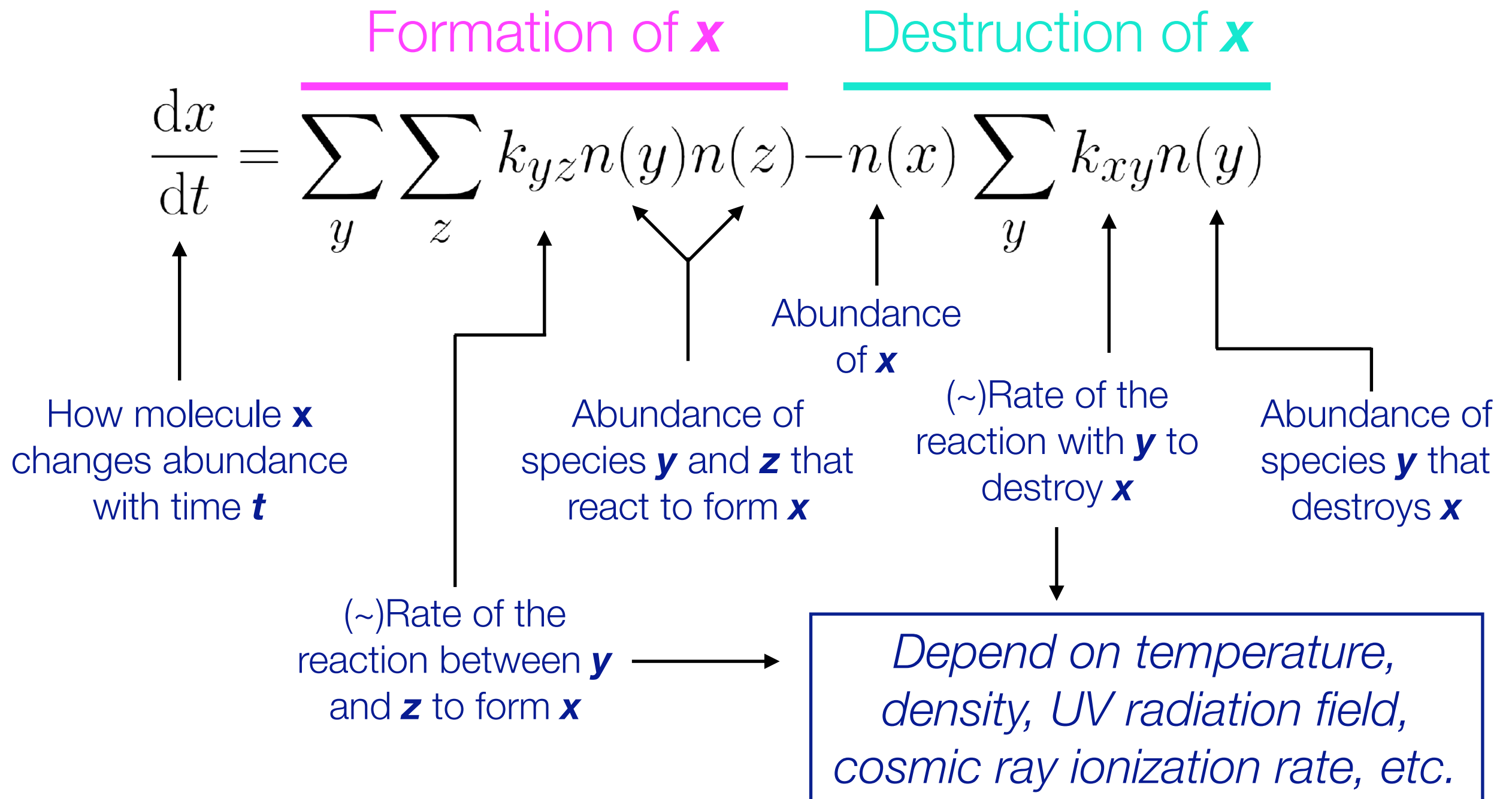
1 differential equation per molecule

CHEMICAL MODELING - RATE EQUATIONS

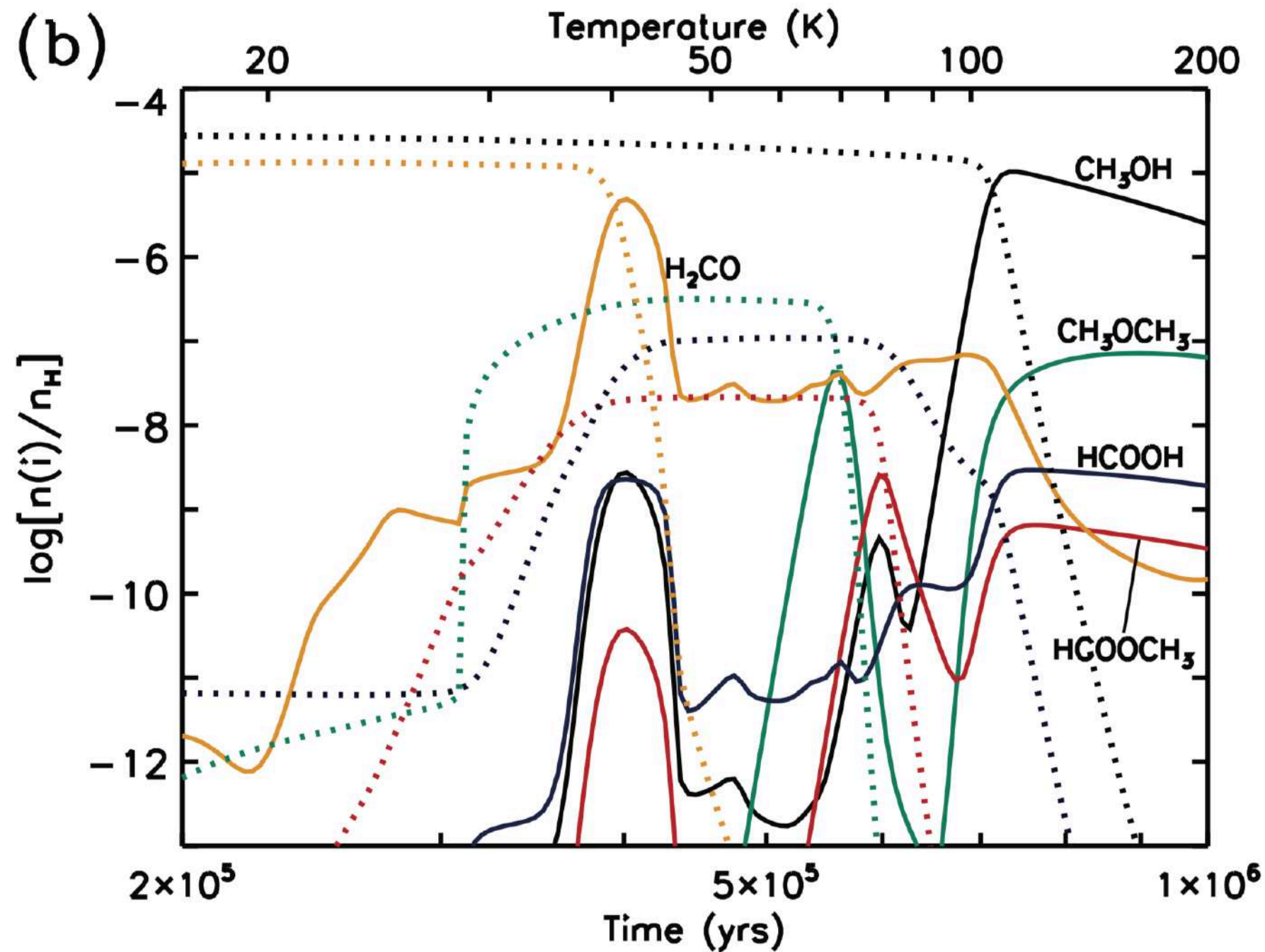


McGuire et al. 2018 *Science* 359, 202

CHEMICAL MODELING - RATE EQUATIONS

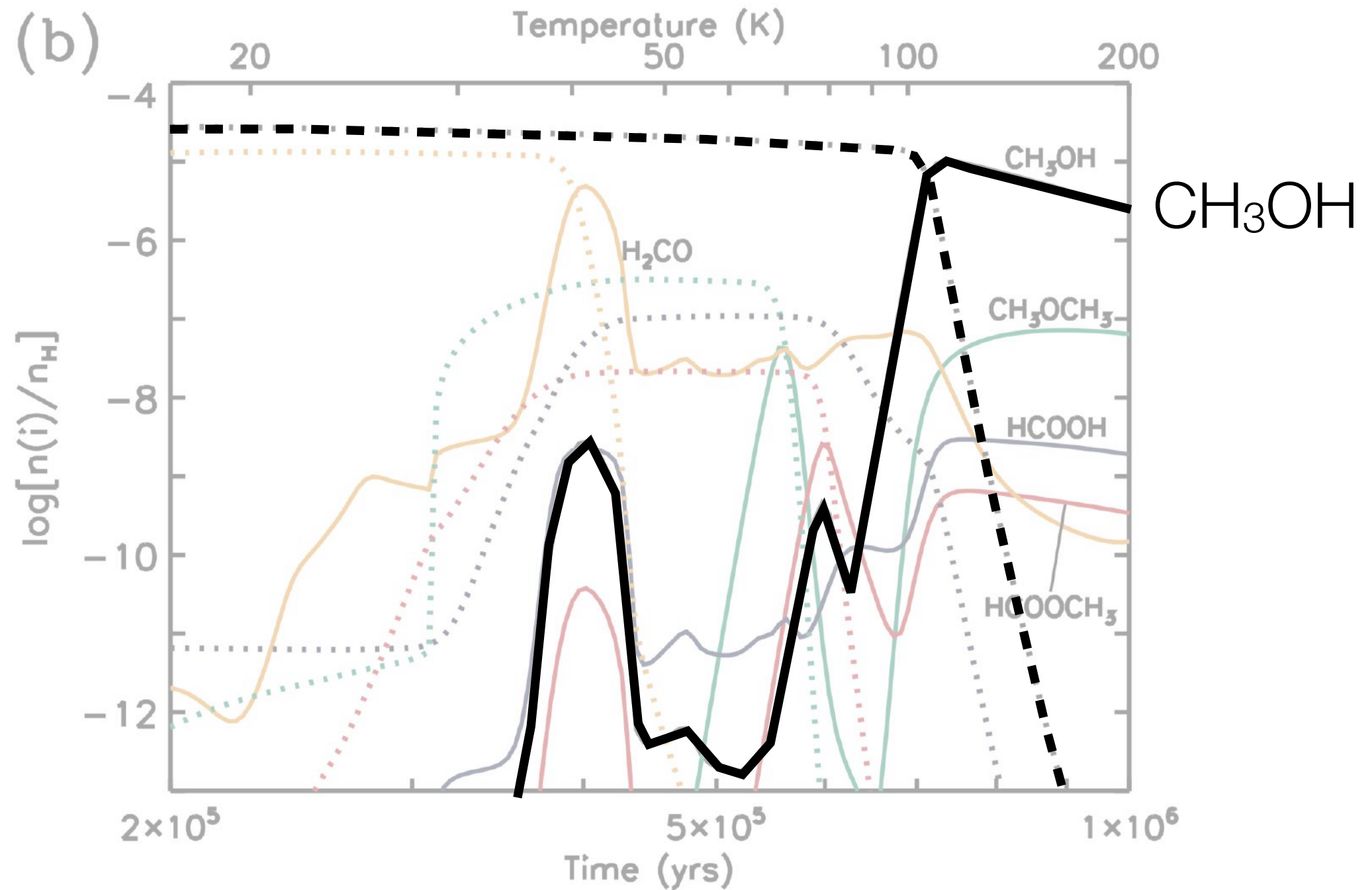


CHEMICAL MODELING - RATE EQUATIONS



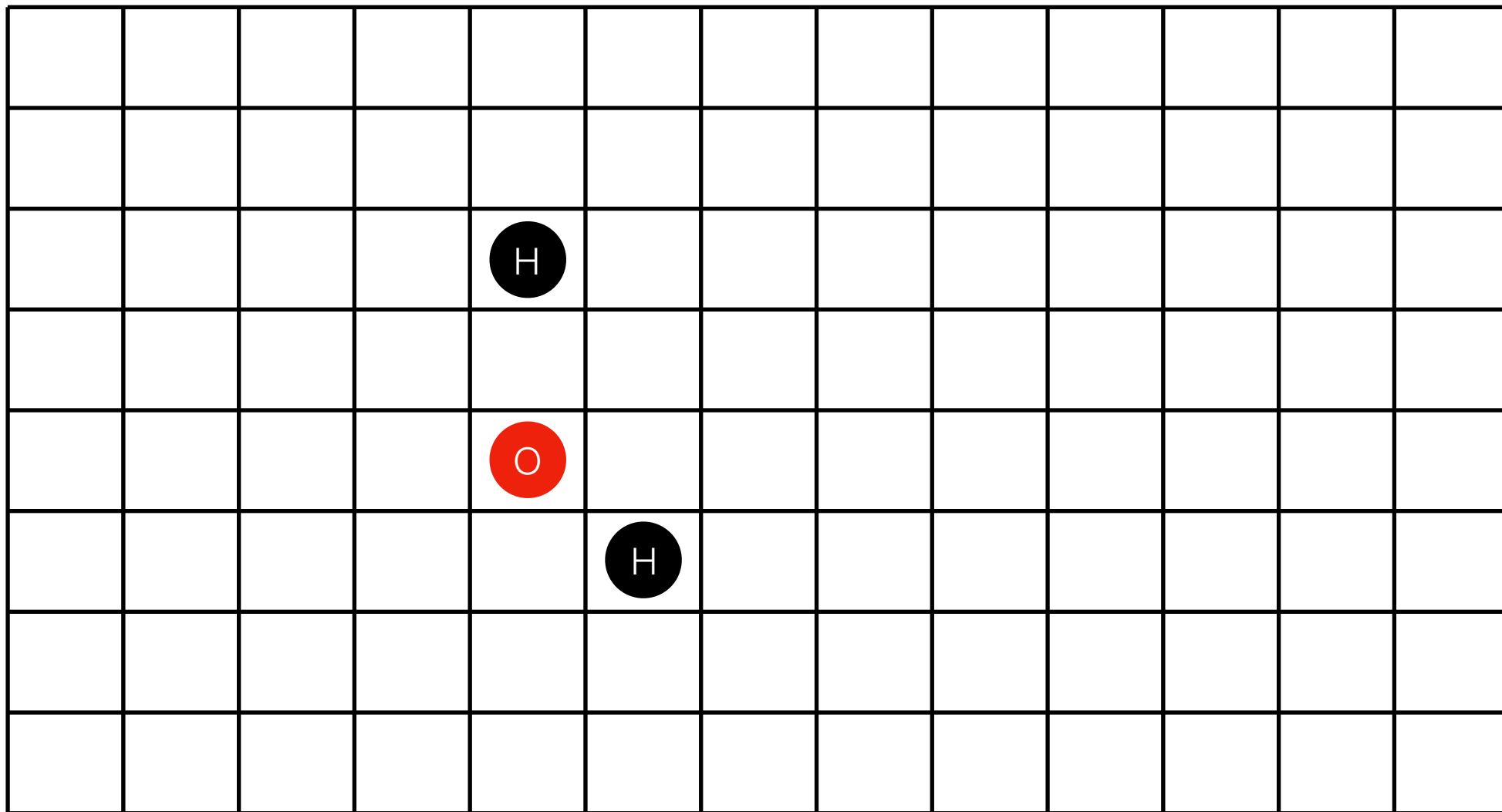
Garrod et al. 2008 *ApJ* 628, 283

CHEMICAL MODELING - RATE EQUATIONS

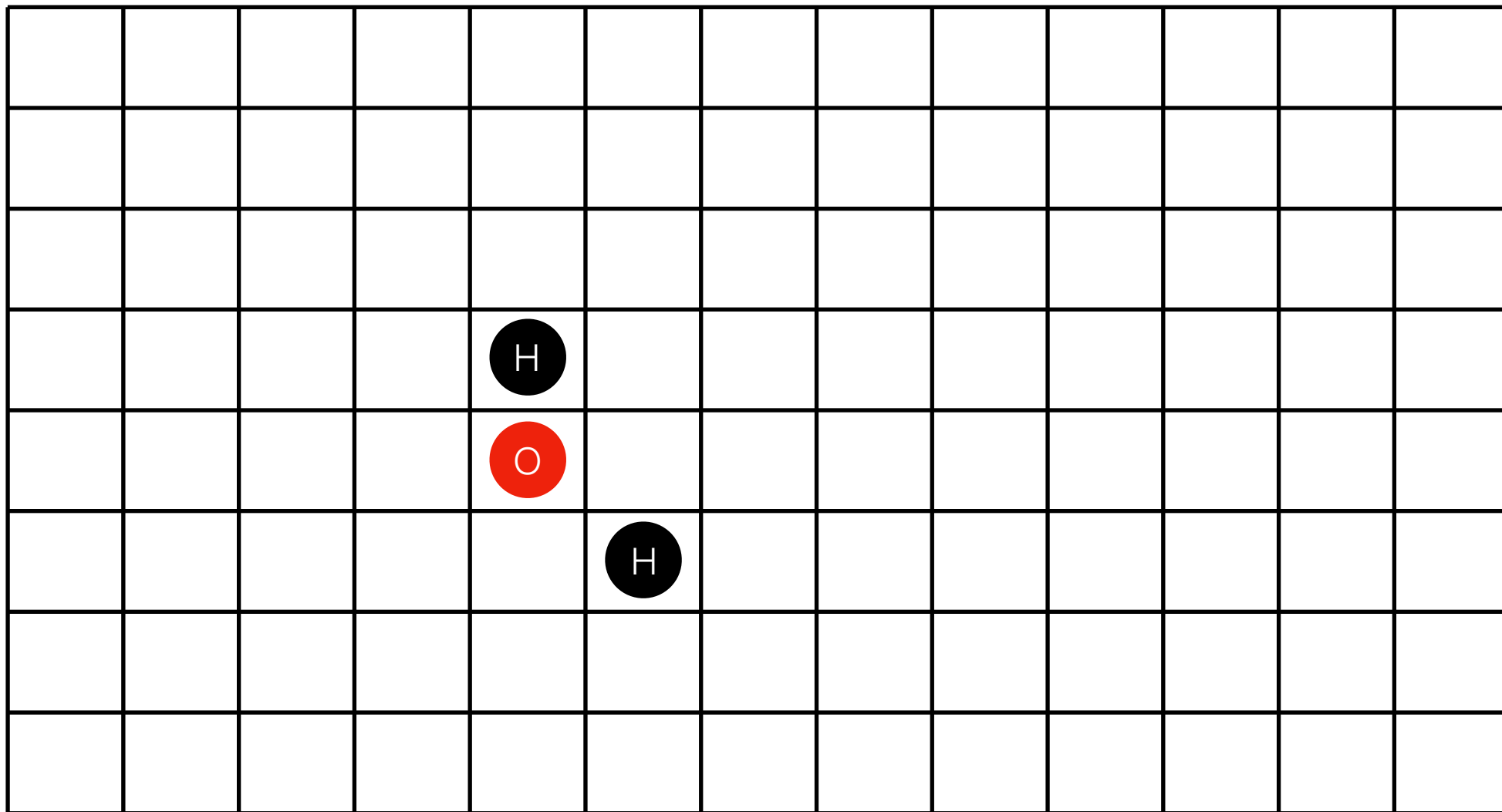


Garrod et al. 2008 *ApJ* 628, 283

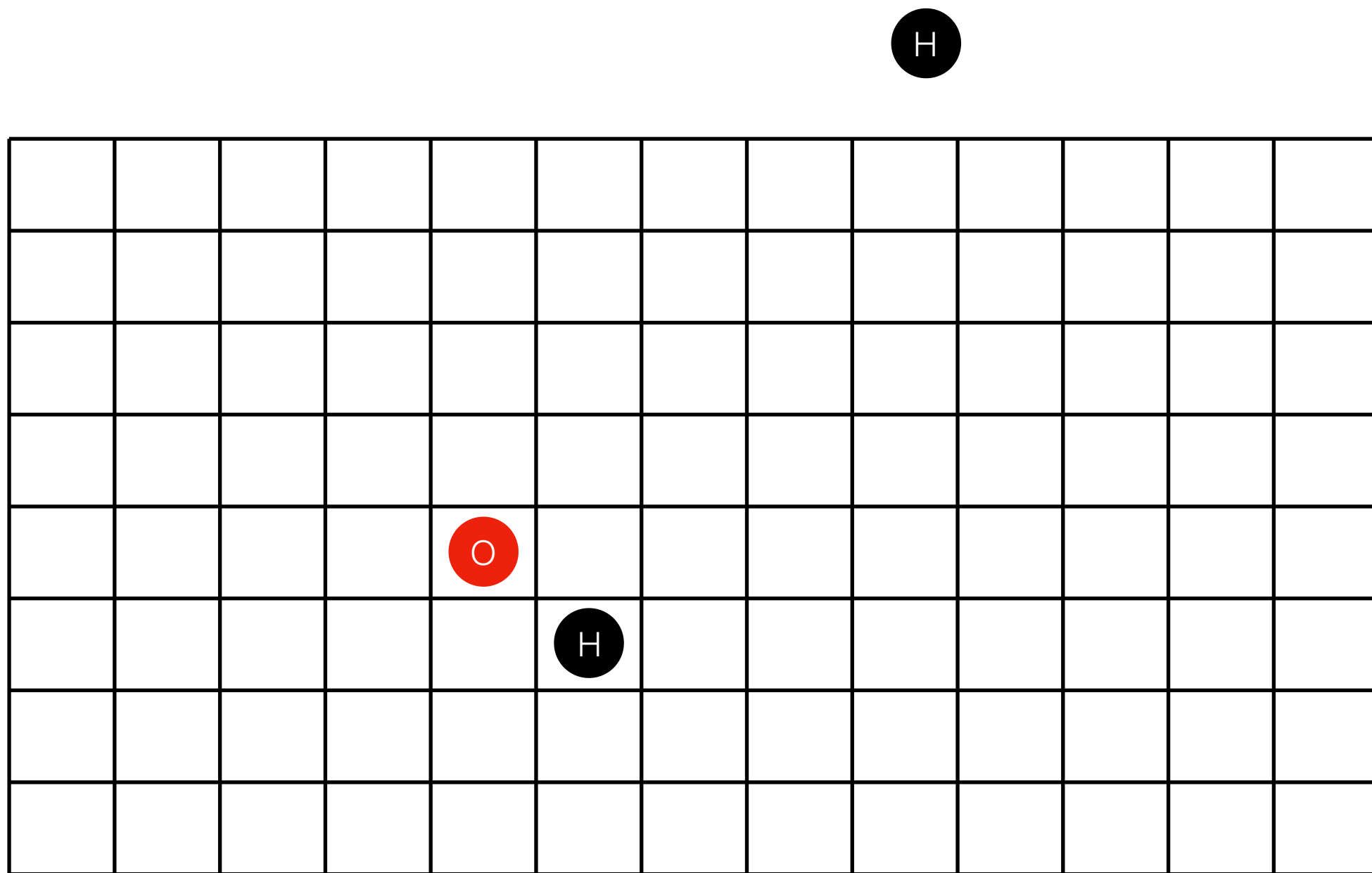
CHEMICAL MODELING - MONTE CARLO



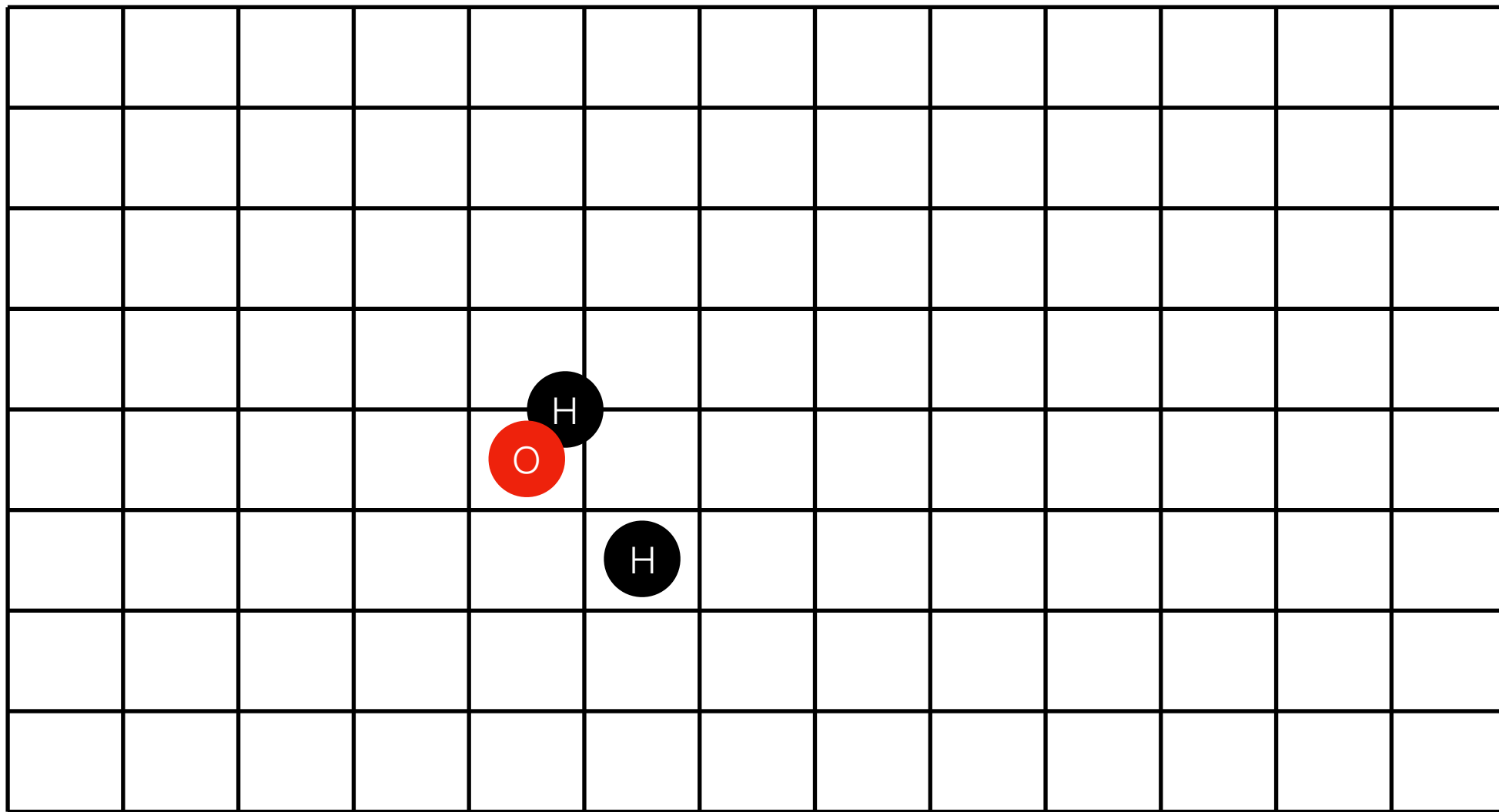
CHEMICAL MODELING - MONTE CARLO



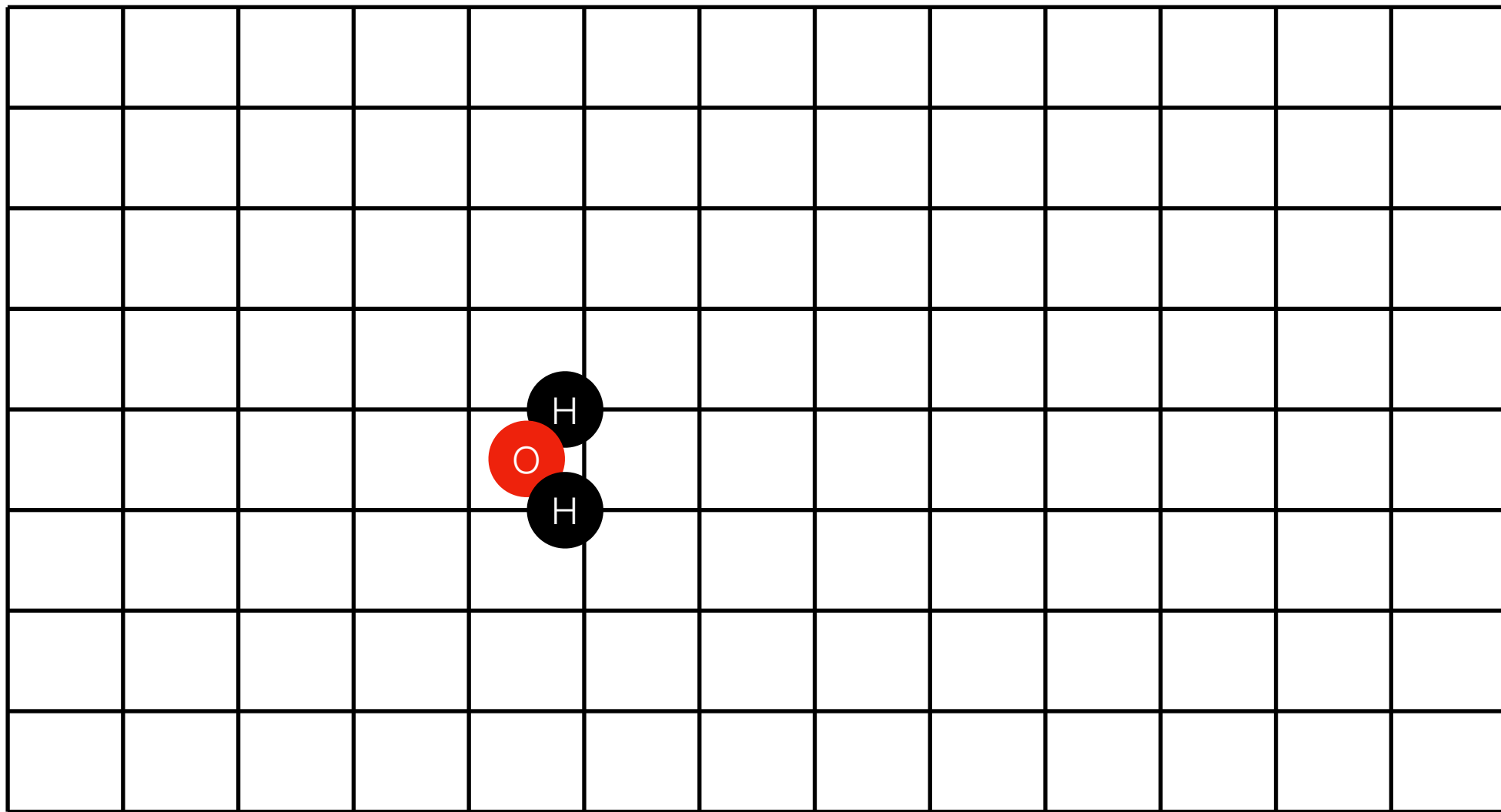
CHEMICAL MODELING - MONTE CARLO



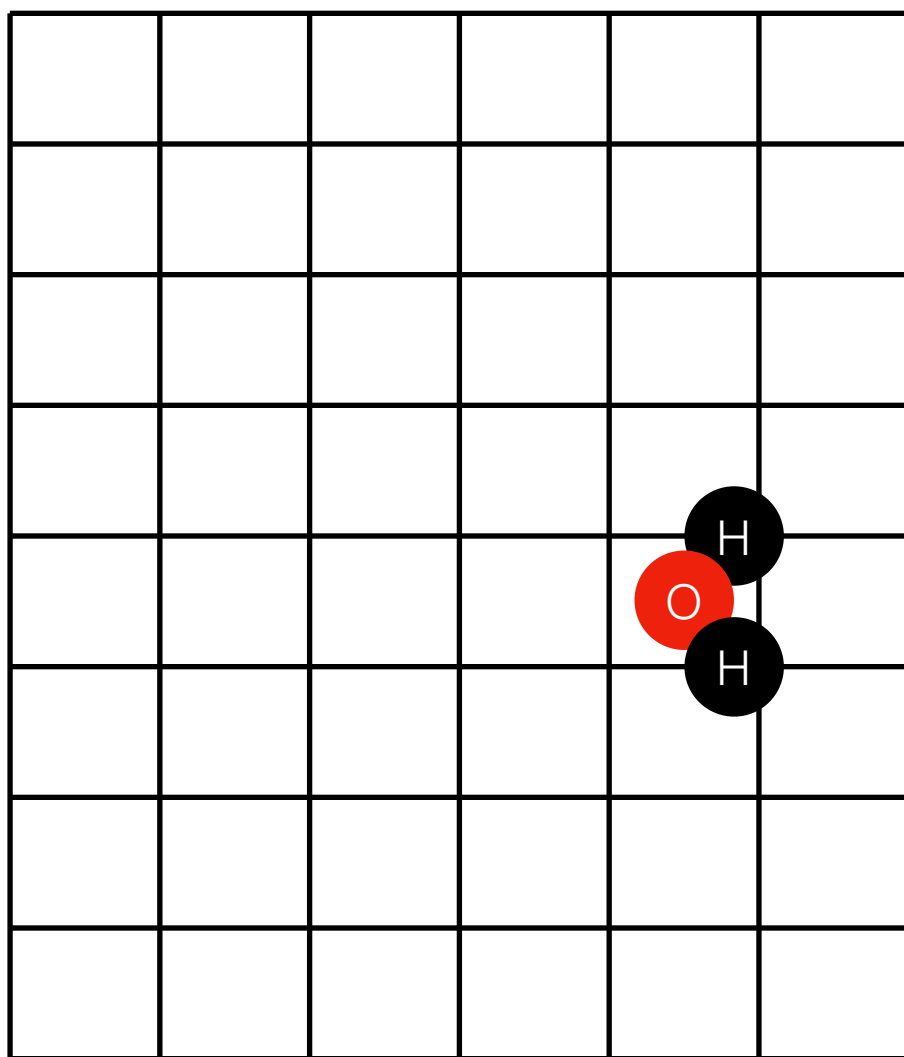
CHEMICAL MODELING - MONTE CARLO



CHEMICAL MODELING - MONTE CARLO



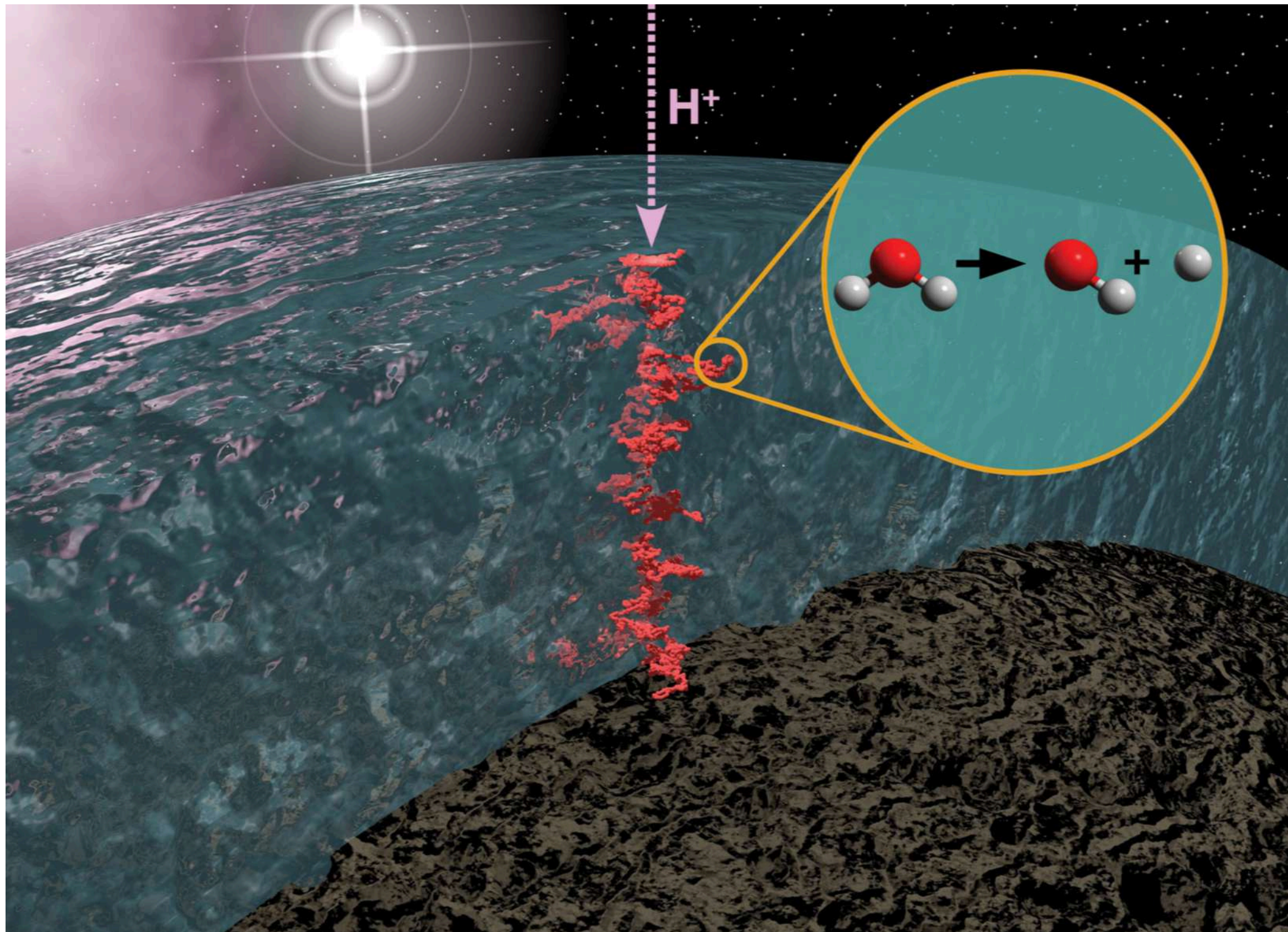
CHEMICAL MODELING - MONTE CARLO



Provides ability to trace the complete and discrete history of any individual item

Can model complex physical issues like crystallinity and porosity of ices or the extremely complex effects of a cosmic ray impact

CHEMICAL MODELING - MONTE CARLO



CHEMICAL MODELING

Rate Equations

Computationally inexpensive

‘Easy’ to implement new chemistry, physics, rapidly adapt model

Can model an arbitrarily long timescale by simply altering time step; time steps need not be linear

‘Hard’ to implement microscopic properties - ice structure, diffusion, environment-sensitive issues

Models the entire cloud - bulk gas and bulk surface

Monte Carlo

Computationally v. expensive

(Not so) ‘easy’ to implement new chemistry, physics, rapidly adapt model

Can model an arbitrarily long timescale by simply altering time step; time steps need not be linear

Get a ‘complete’ physical picture of the system. System is typically ~1 gas-grain interface

More physically ‘realistic’



CHEMICAL MODELING - A FINAL NOTE

Astrochemical models are almost always completely incapable of correctly reproducing reality

BUT

They are still incredibly useful and important for:

Identifying gaps in our understanding of pertinent reactions, species, and physical processes

Suggesting reasonable explanations for observations, and necessary follow-up observational or laboratory tests

LABORATORY ASTROPHYSICS



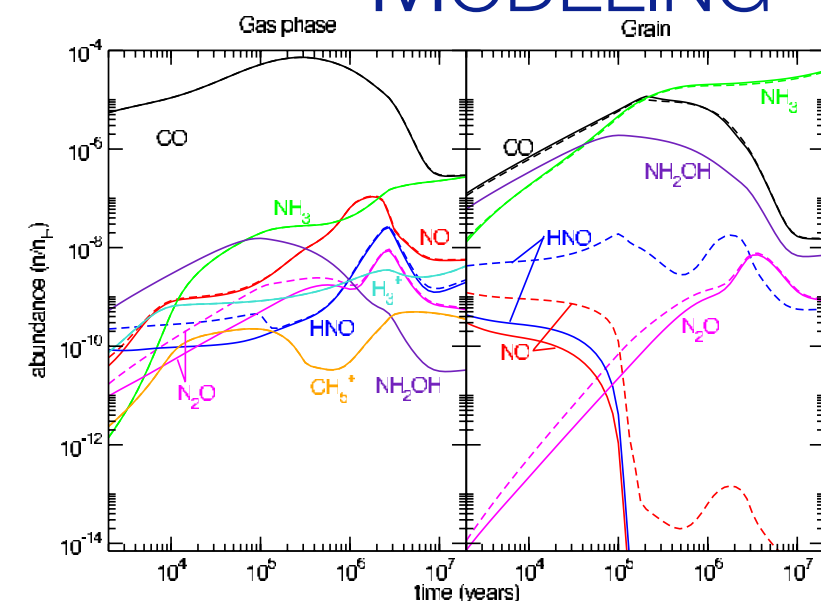
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ASTROCHEMICAL MODELING



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Rotational, Vibrational,
and Electronic Spectra

Environments and Species
of Interest

Chemical Inventories
Temperatures, Abundances,
and Densities

OBSERVATIONAL ASTRONOMY



PARTING THOUGHTS

Astrochemistry seeks to understand the evolution of molecular complexity through cosmic time and its influence on the dynamical evolution of our universe.

Molecular lines aren't noise - they're invaluable information on the current conditions and evolutionary history of the source you're studying! Don't ignore them!

Molecules can be valuable probes/tracers of physical conditions, but only when interpreted in context. If in doubt, ask an astrochemist!