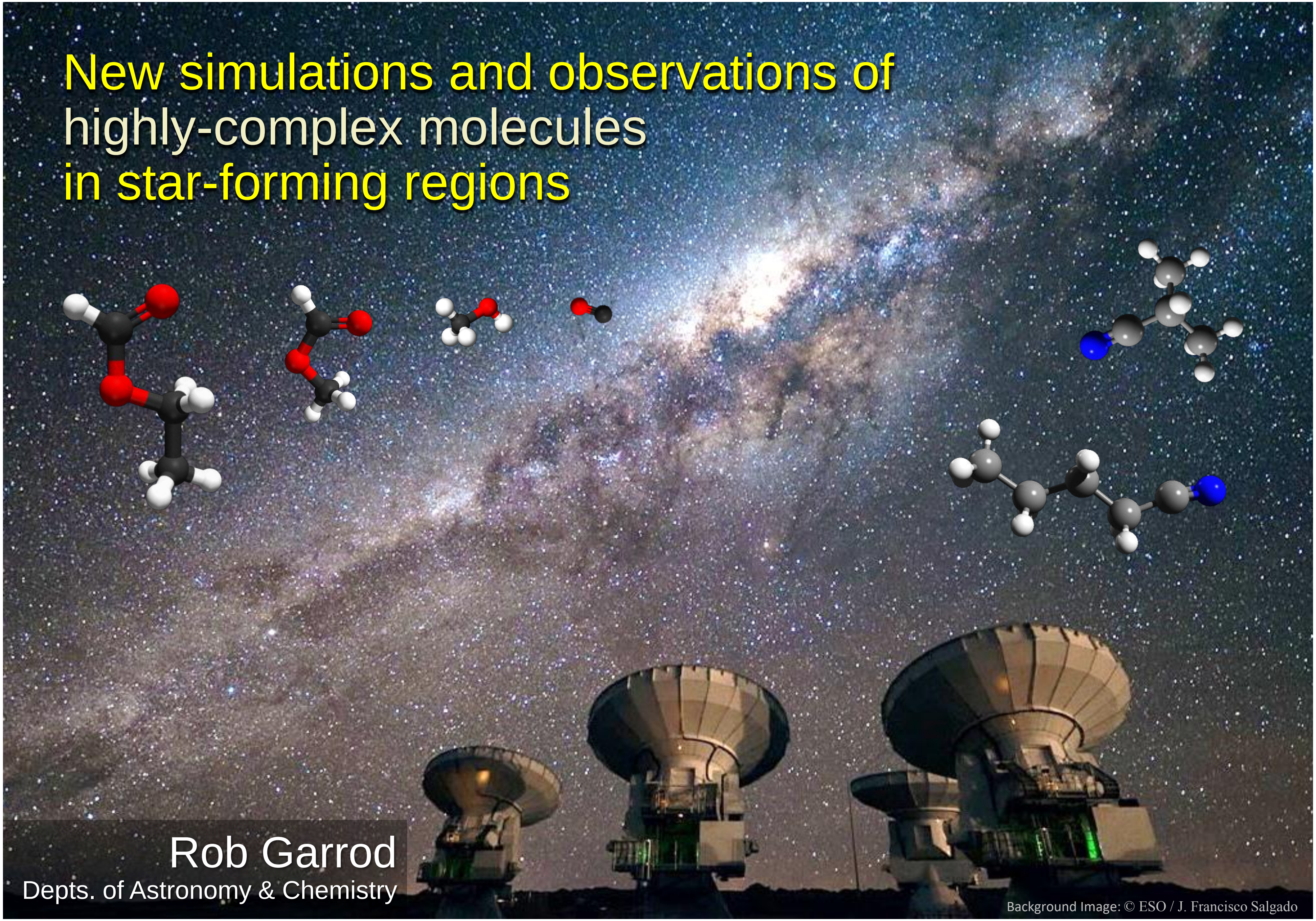


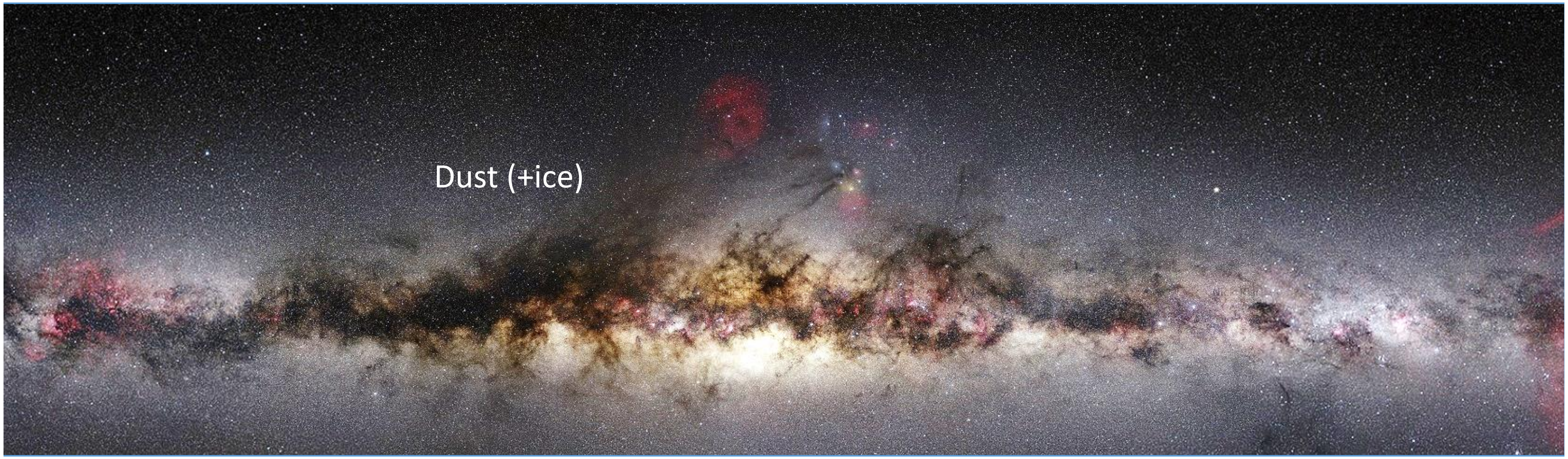
New simulations and observations of highly-complex molecules in star-forming regions

Rob Garrod
Depts. of Astronomy & Chemistry

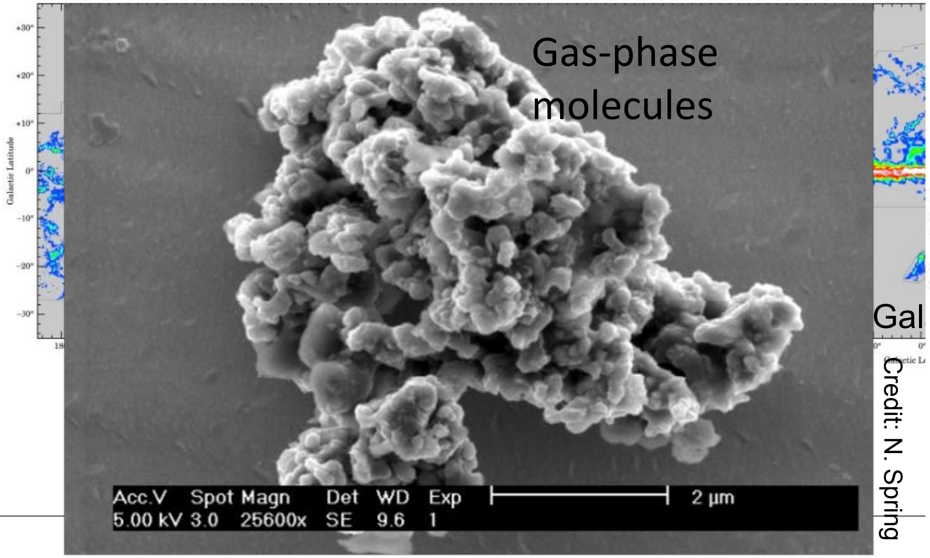
Background Image: © ESO / J. Francisco Salgado

UNIVERSITY of VIRGINIA

Molecules are observed throughout the Milky Way


Dust (+ice)

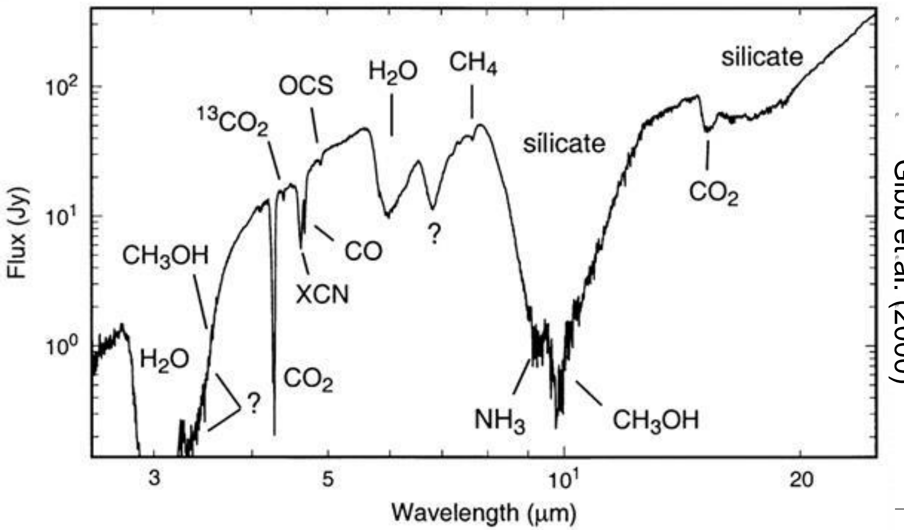
Interplanetary dust grain



Gas-phase molecules

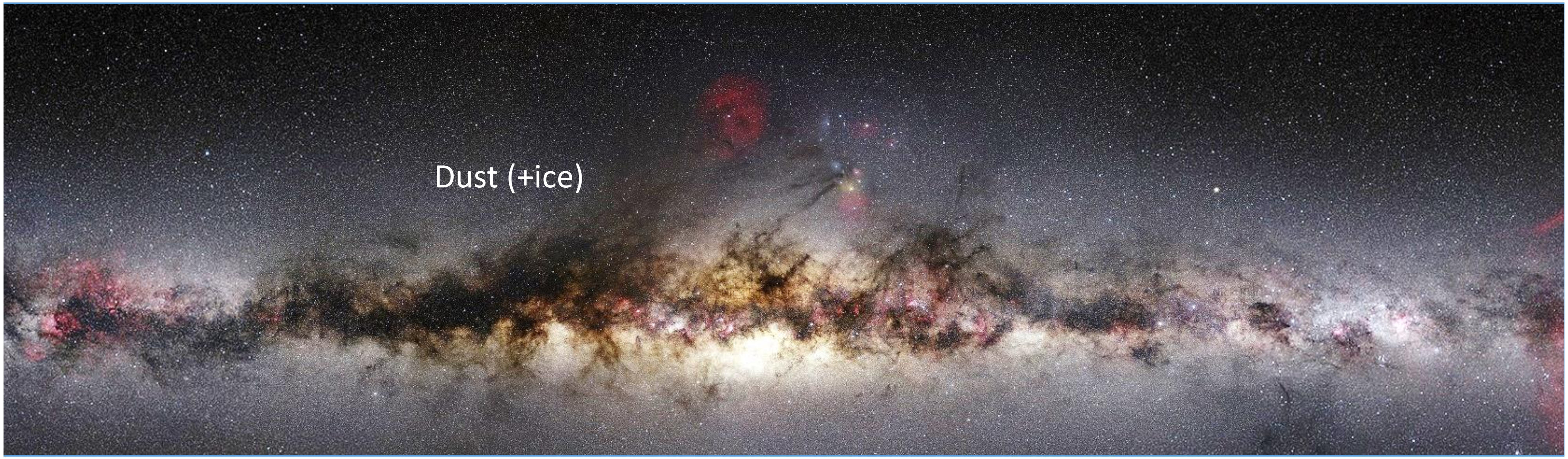
Gal

Credit: N. Spring

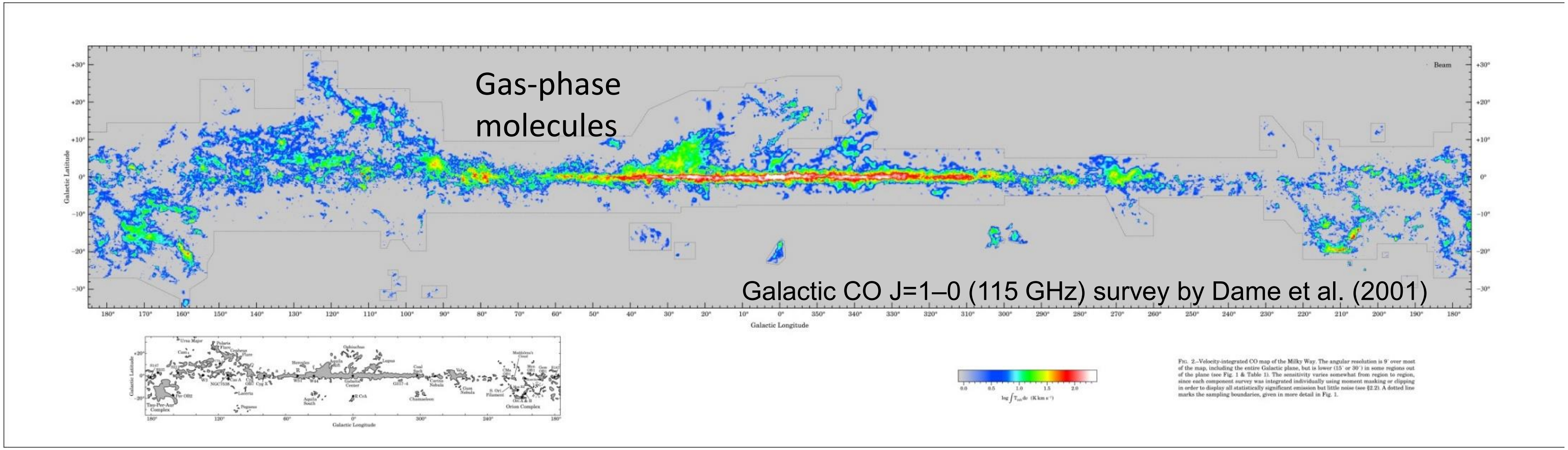


Gibb et.al. (2000)

Molecules are observed throughout the Milky Way



Dust (+ice)



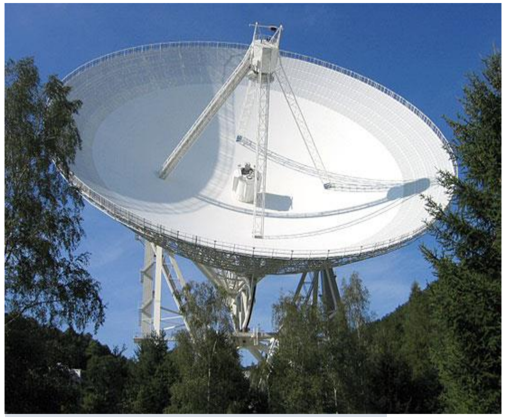
Gas-phase molecules

Galactic CO J=1–0 (115 GHz) survey by Dame et al. (2001)

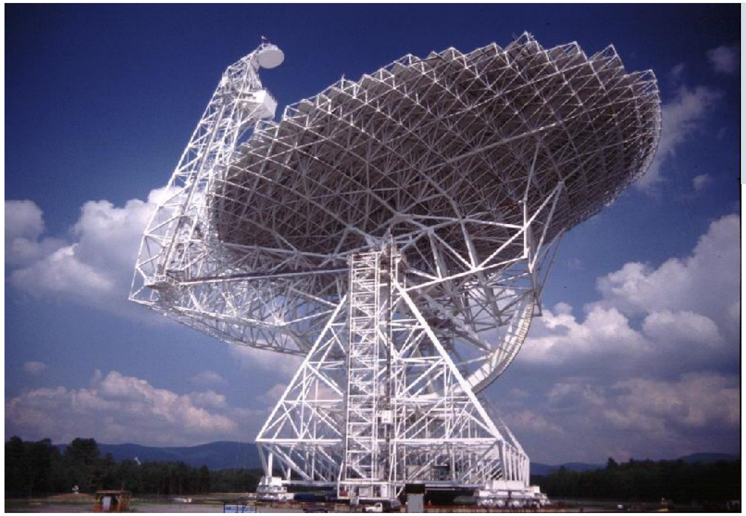
Fig. 2.–Velocity-integrated CO map of the Milky Way. The angular resolution is 9′ over most of the map, including the entire Galactic plane, but is lower (15′ or 30′) in some regions out of the plane (see Fig. 1 & Table 1). The sensitivity varies somewhat from region to region, since each component survey was integrated individually using moment masking or clipping in order to display all statistically significant emission but little noise (see §2.2). A dotted line marks the sampling boundaries, given in more detail in Fig. 1.

Detection of gas-phase interstellar molecules

– Rotational spectroscopy with radio-telescopes



Effelsberg telescope
Forest of Eiffel,
Germany
100m diameter



Green Bank telescope (GBT)
W. Virginia
100m diameter

IRAM telescope
Sierra Nevada,
Spain
30m diameter

Sub-Millimeter Array (SMA) interferometer
Mauna Kea,
Hawaii
8 x 6m antennas

ALMA – your new favorite radio-telescope

- Wavelengths: 0.32 – 8.6 mm (35 – 940 GHz)
- 5000 meters altitude.
- High spatial resolution (~0.01 arcsecond).
- The most sensitive mm/sub-mm instrument.
- Operating since 2011 (Cycle 0).

Atacama Large Millimeter/sub-mm Array
Llano de Chajnantor,
Atacama Desert, Chile
[12 x 7m] + [54 x 12m] antennas

Detected interstellar/circumstellar molecules

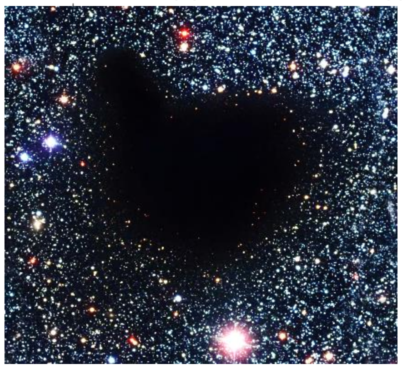
(~200 so far)

Number of atoms

2		3		4	5	6	7	8	9	10	11	12+
$AlCl$	PN	$AlNC$	NH_2	CH_3	C_5	c-H_2C_3O	c-C_2H_4O	CH_3C_3N	CH_3C_4H	CH_3COCH_3	HC_9N	c-C_6H_6
AlF	PO	$AlOH$	N_2H^+	l-C_3H	$NH_4{}^+$	$HNCHCN$	CH_3C_2H	$HCOCH_2OH$	CH_3OCH_3	$(CH_2OH)_2$	C_2H_5OCHO	n-C_3H_7CN
AlO	SiC	C_3	N_2O	l-C_3H^+	CH_4	C_2H_4	CH_3NH_2	$HCOOCH_3$	C_2H_5CN	C_2H_5CHO	CH_3COOCH_3	i-C_3H_7CN
C_2	SiN	C_2H	$NaCN$	c-C_3H	CH_3O	CH_3CN	CH_2CHCN	CH_3COOH	CH_3CONH_2	CH_3C_5N	CH_3C_6H	$C_2H_5OCH_3$ (?)
CF^+	SiO	C_2O	$NaOH$	C_3N	c-C_3H_2	CH_3NC	C_2H_3OH	C_6H_2	C_2H_5OH	CH_3CHCH_2O		
CH	SiS	C_2S	OCS	PH_3	l-C_3H_2	CH_3OH	C_6H	CH_2CHCHO	C_8H	CH_3OCH_2OH		c-C_6H_5CN
CN	TiO	C_2P	O_3	C_3O	H_2CCN	CH_3SH	CH_3NCO	CH_2CCHCN	HC_7O			C_{60}
CO	ArH^+	CO_2	SO_2	C_3S	H_2C_2O	l-H_2C_4	HC_5N	CH_3CHNH	HC_7N			$C_{60}{}^+$
CO^+	CH^+	$FeCN$	c-SiC_2	H_3O^+	H_2CNH	HC_3NH^+	CH_3CHO	C_7H	CH_3CHCH_2			C_{70}
CP	CN^+	$H_3{}^+$	$SiCN$	C_2H_2	H_2COH^+	NH_2CHO	HC_5O	NH_2CH_2CN	C_8H^-			
CS	CN^-	H_2C	$SiNC$	H_2CN	C_4H	C_5H	C_6H^-	l-HC_6H	CH_3NHCHO (?)			
FeO	HCl^+	H_2Cl^+	Si_2C	H_2CN^+	C_4H^-	C_5N		CH_3SiH_3	C_2H_5SH (?)			
H_2	NS	H_2O	TiO_2	H_2CO	HC_3N	HC_2CHO						
HCl	NS^+	CH_2	HS_2	H_2CS	$HCCNC$	SiC_3CN						
HF	SH	HO_2	HCO^+	$HCCN$	$HC(O)CN$	CH_2CNH (?)						

Complex, saturated organic molecules

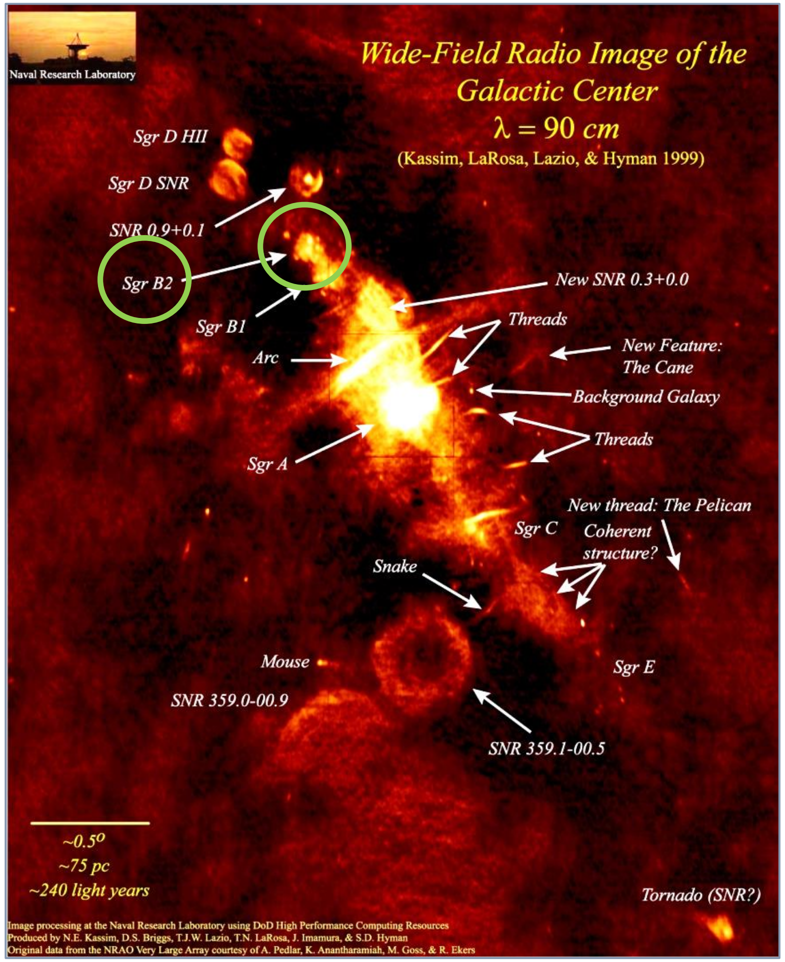
Diffuse clouds (e.g. *Zeta Ophiuchi*)



Dense, dark clouds (e.g. *B68*)

Molecular clouds / star formation

Complex organic molecules (COMs) in "***hot cores***"

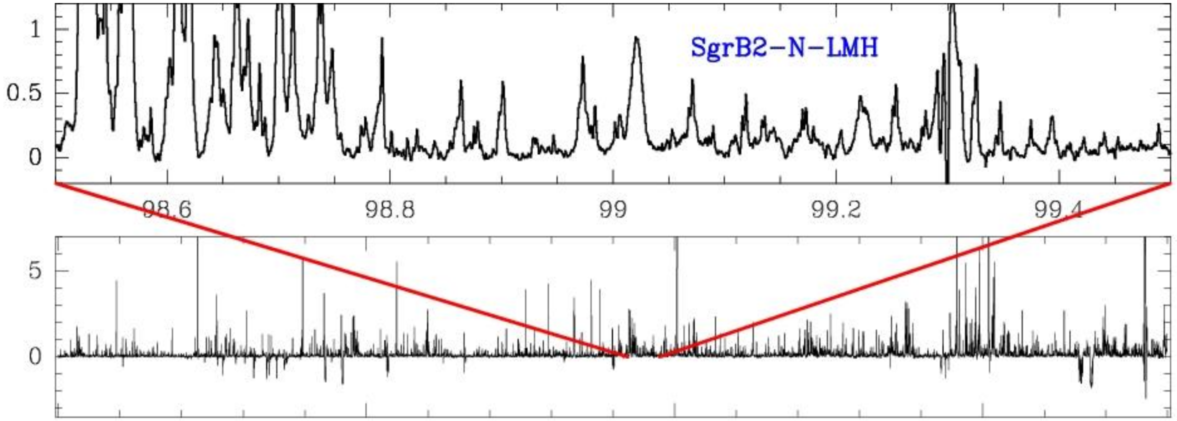


"Hot-core molecules"

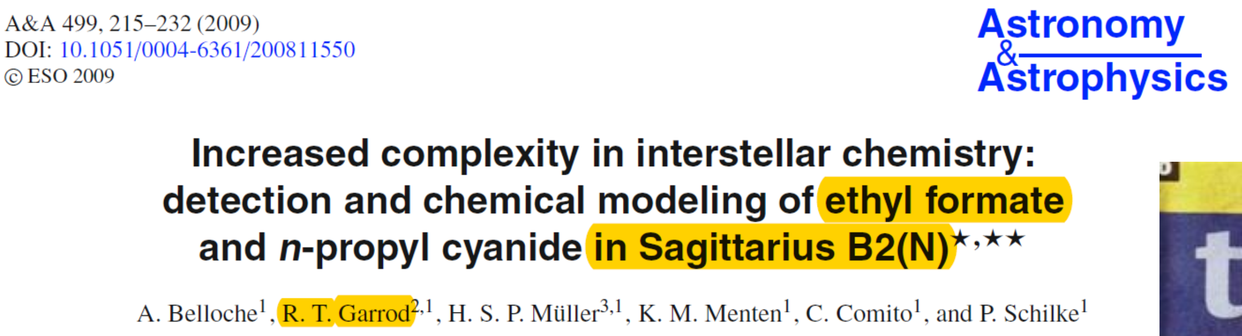
CH_3OH	CH_3CHO	CH_3OCH_3	$HCOOH$	$HCOCH_2OH$	CH_3CN
C_2H_5OH	NH_2CHO		CH_3COOH	$(CH_2OH)_2$	CH_3NC
		$HCOOCH_3$			C_2H_3CN
		$HCOOC_2H_5$			C_2H_5CN
					C_3H_7CN

Sagittarius B2(N) – the richest hot core

(Observed using IRAM 30m telescope)



Belloche et al. 2008

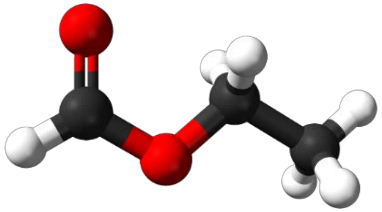


A&A 499, 215–232 (2009)
DOI: 10.1051/0004-6361/200811550

Astronomy & Astrophysics

Increased complexity in interstellar chemistry: detection and chemical modeling of ethyl formate and *n*-propyl cyanide in Sagittarius B2(N)★,★★

A. Belloche[1], R. T. Garrod[2,1], H. S. P. Müller[3,1], K. M. Menten[1], C. Comito[1], and P. Schilke[1]



Ethyl Formate

$HCOOC_2H_5$

An ester implicated in the flavor/smell of

RUM

and (perhaps)

RASPBERRIES

theguardian

bn
n for
ket

include
omes

dence that rising
house prices, and
will see the sharp-
gle year since 1945
the government's
c competence.
they trusted most
ugh the recession,
they preferred the
an eight-
the opposition

nfident that the
to ameliorate
will pay off later
measures to help
economy, is vital
admitting that
to £170bn in
he will find cash
and support
the construction

plan will include:
to take a stake in
work has stalled.
may also be used to
such as roads.
houses have been
because of falling
would be through
equity schemes and
ended for the pro-
housing.
trend of 30 years
of council houses.
holiday on prop-
until the year's end.
mortgage
evidence
ment is
ople with repossess-
last autumn.
ncement follows

4»

Taste test Why life is raspberry flavour

4»

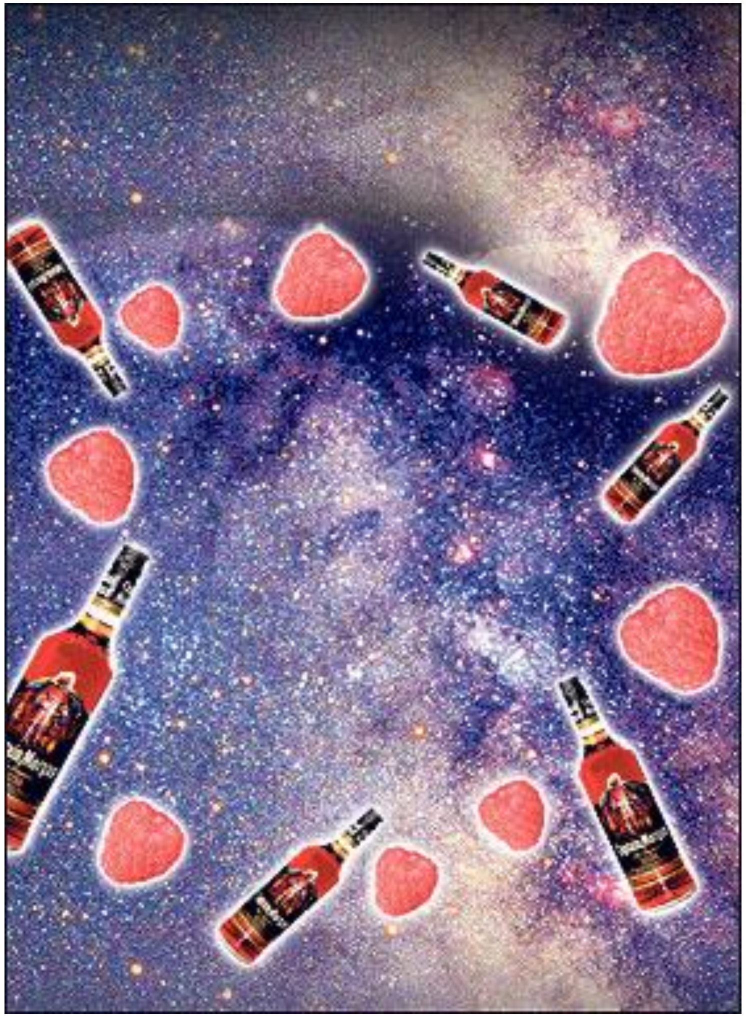
Astronomers searching the Milky Way for amino acids - the building blocks of life - found instead a chemical that flavours raspberries Photograph: Roger Tooth

THE Sun

Milky Way tastes of raspberry and rum

By GARY O'SHEA

Published: 22 Apr 2009



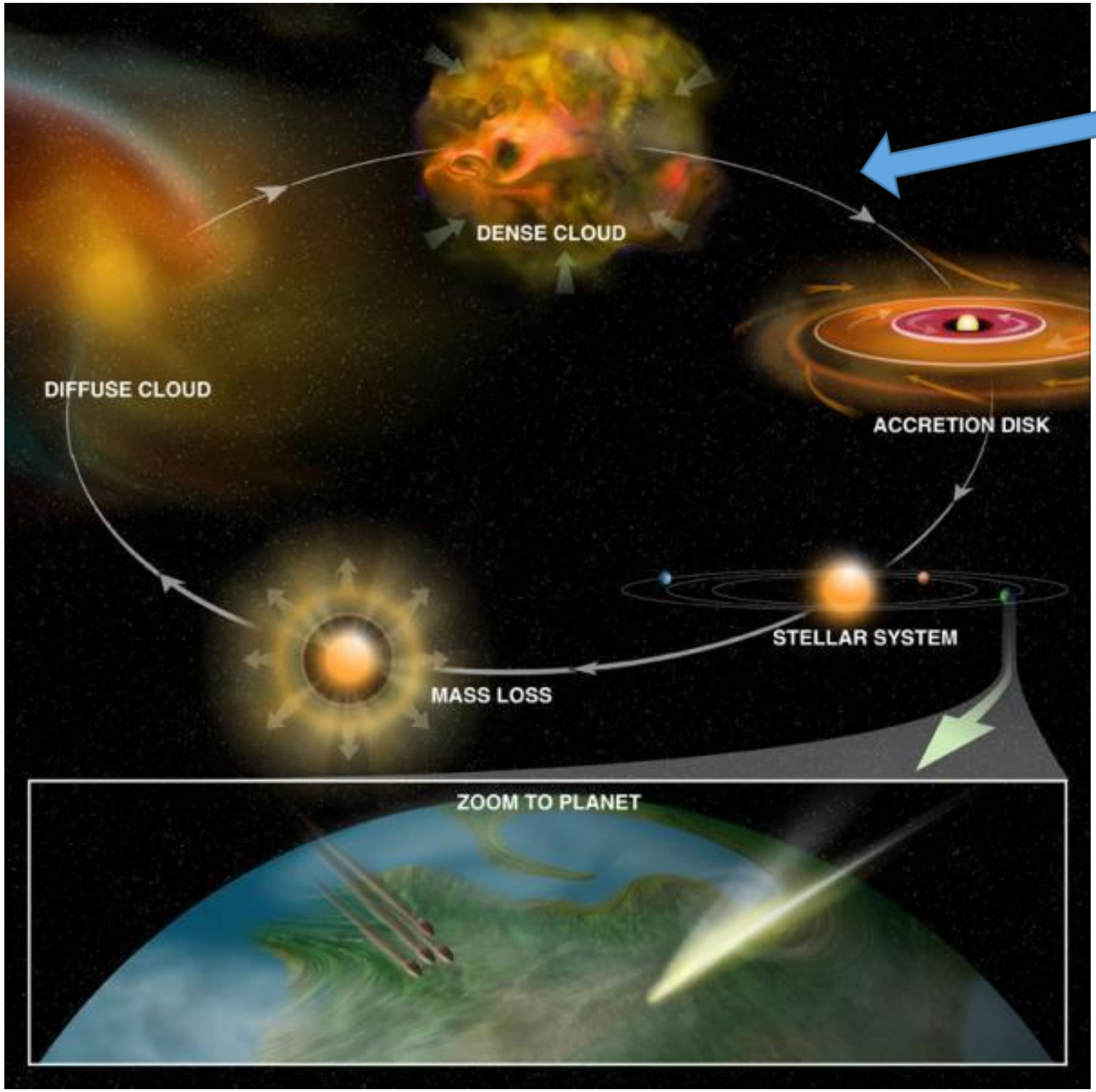
Astrochemistry goes to Hollywood

“Molly’s Game” (2017)

[redacted]

[redacted]

Life cycle of stars and planets



Credit: Bill Saxton

Complex organics begin to form around this point ("*Hot Core*" stage)

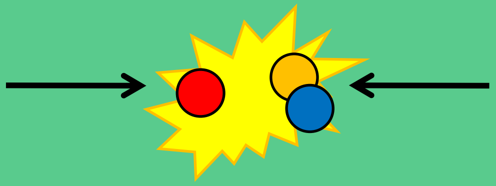
Are planetary systems seeded for life at **inception**?

Big questions

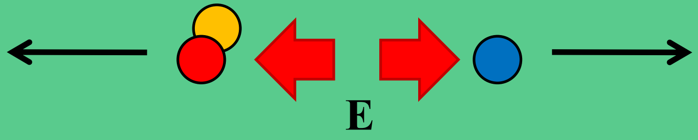
- How do interstellar complex organics form?
- How complex can they get?
- Can we use them to understand other properties of star-forming objects?

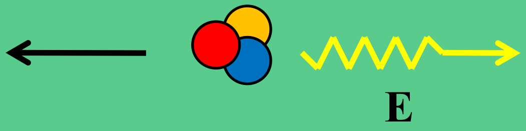
Gas Phase vs. Grain Surface Chemistry

- Free-roaming reactants collide/react.

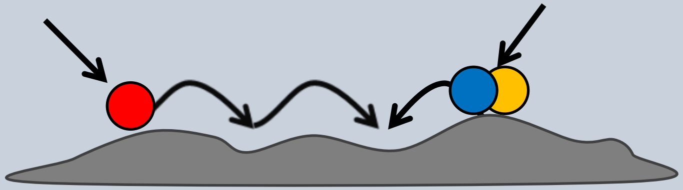


- Only break-up of complex, or photon emission, can stabilize products.

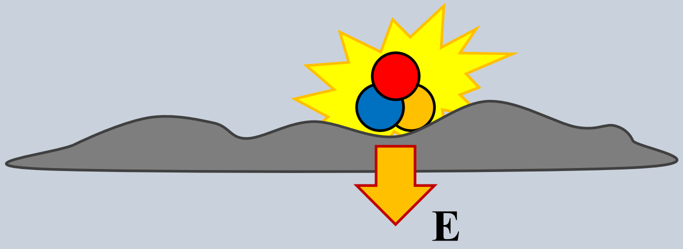




- Reactants accrete onto grain.
- Stick via van der Waals forces.
- Thermally migrate between binding sites (potential wells).



- Surface absorbs chemical energy, stabilizing product.



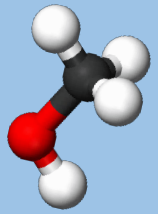
→ Can build molecules atom by atom, group by group.

What’s the interstellar recipe for complex organics?

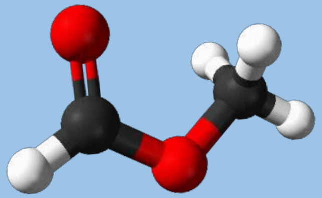
- Gas-phase mechanisms

  → *Not* very effective for highly-saturated organics.

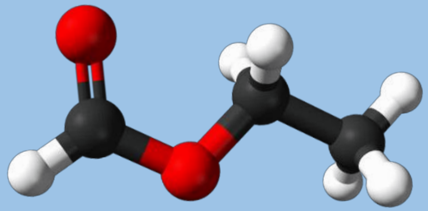
E.g.



Methanol



Methyl formate



Ethyl formate

- *Answer involves **grain-surface ice**…*

Diffusive chemistry on cold dust grains: H_2O

Atoms in the gas stick to cold (~10 K) grain surfaces

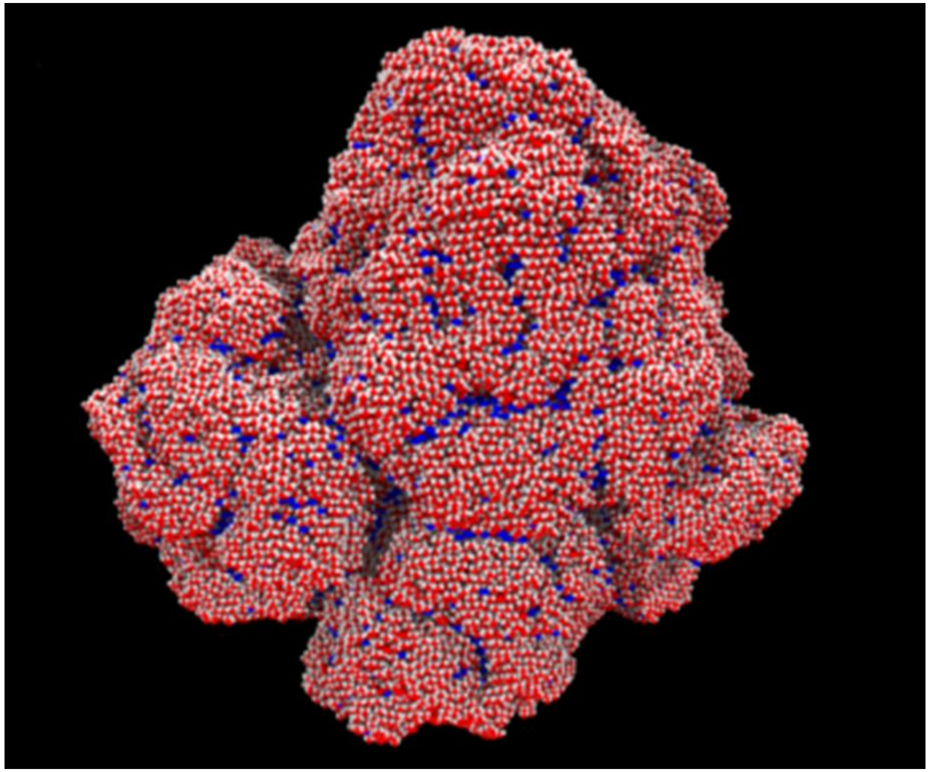
H (gas) → H (grain)
O (gas) → O (grain)

Atoms/molecules meet via diffusion

H: rapid
O: slow

$H + H \rightarrow H_2$
$H + O \rightarrow OH$
$H + OH \rightarrow H_2O$
$O + O \rightarrow O_2$
$OH + OH \rightarrow H_2O_2$

Simple molecules form on grains at low temperatures



- **Off-lattice Monte Carlo kinetics simulation (*Garrod 2013, ApJ, 778, 158*)**
- Accretion of H and O from the gas.
- Small, idealized grain (r = 16 Å).
- Model traces every:
  - *Thermal hop*
  - *Sticking event*
  - *Desorption event*
- ***Model explicitly traces the positions of surface particles.***

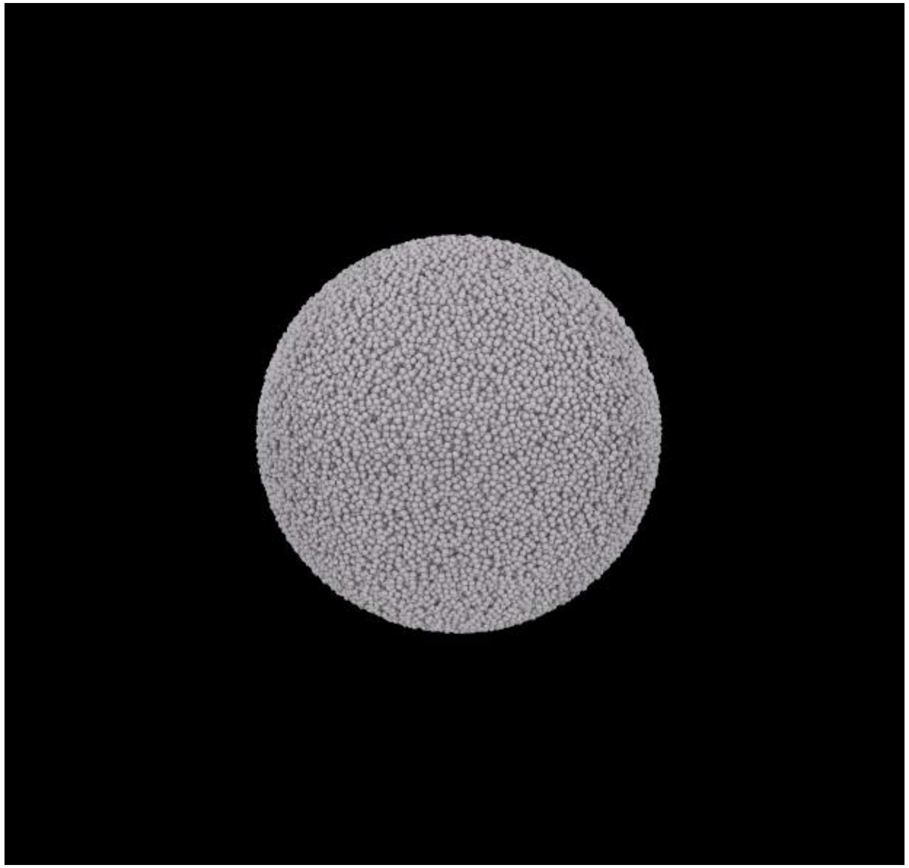
Updated model: *MIMICK*

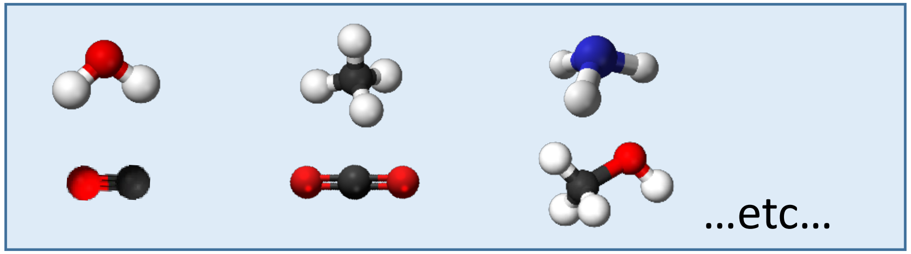
(Model for Interstellar Monte Carlo Ice Chemical Kinetics)

Garrod (in prep.)
Clements, Berk, Cooke & Garrod (2018)
Willis & Garrod (2017)

- Larger grain: *r* = 100 Å (amorphous)
- Larger network:
  - ***Accrete:*** **H, C, O, N, CO**
  - ***Form:*** **e.g. H_2O, CO_2, CH_4, NH_3, CH_3OH**
- Methanol (CH3OH)
  - a building block for larger things…

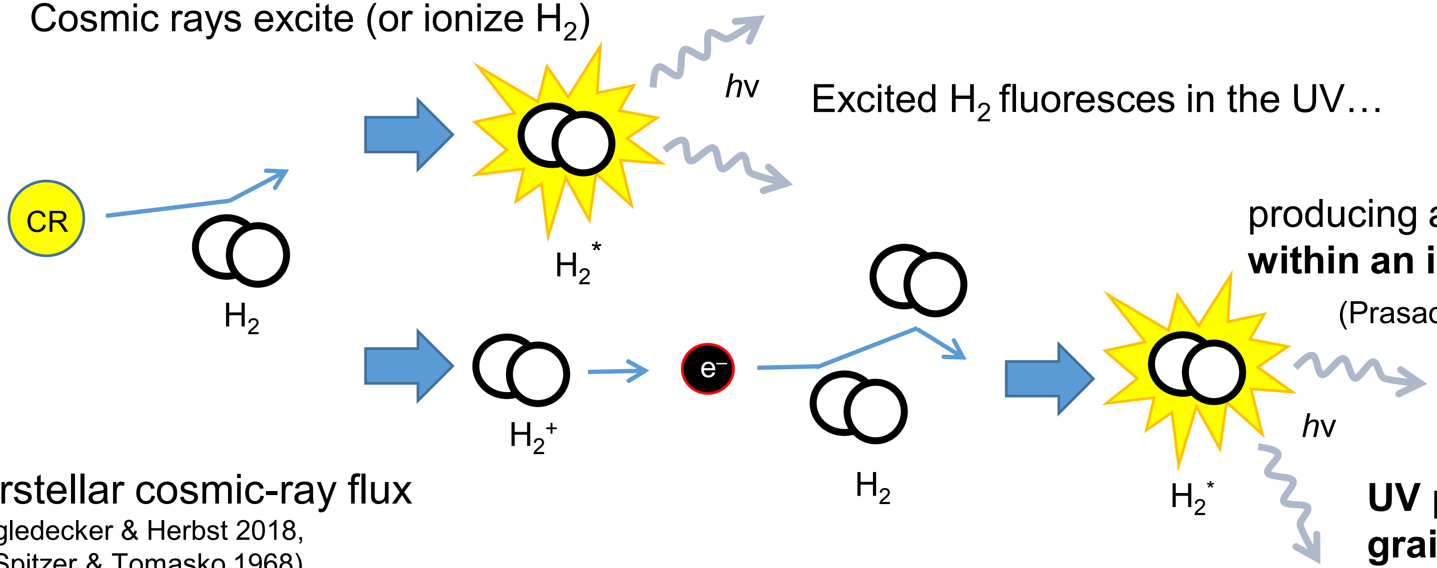
$$CO \xrightarrow{H} HCO \xrightarrow{H} H_2CO \xrightarrow{H} CH_3O \xrightarrow{H} \mathbf{CH_3OH}$$





…etc…

How are simple ices converted into gas-phase COMs?



Cosmic rays excite (or ionize H_2)

Excited H_2 fluoresces in the UV…

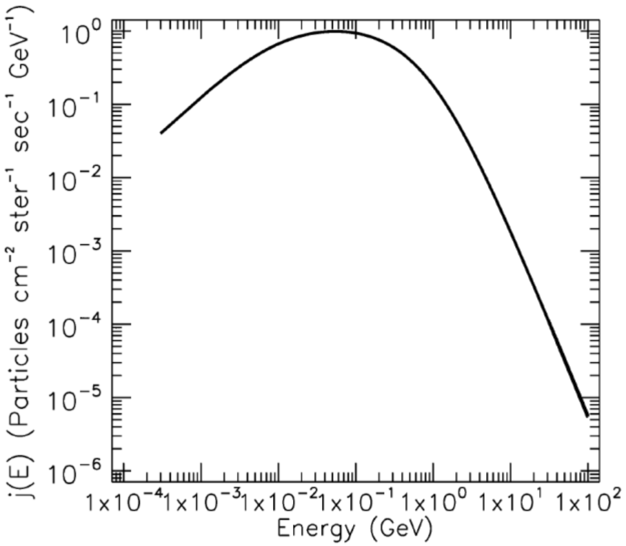
producing a **dissociating UV field within an interstellar cloud**…

(Prasad & Tarafdar 1983)

UV photons can dissociate grain-surface molecules…

Interstellar cosmic-ray flux

(Shingledecker & Herbst 2018, after Spitzer & Tomasko 1968)



Water:

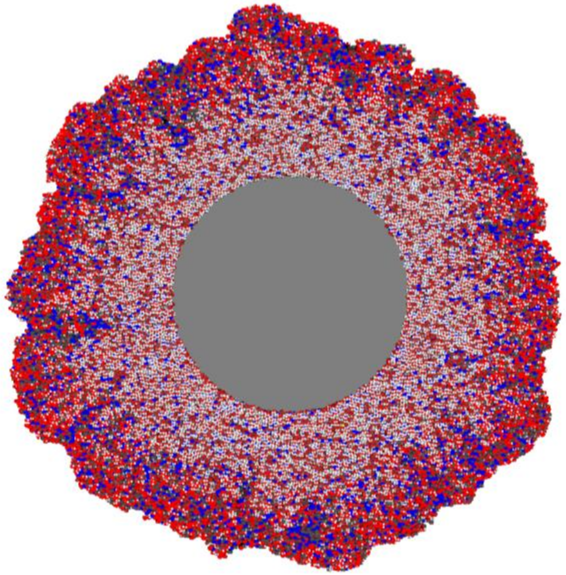
$H_2O + h\nu \rightarrow \mathbf{OH} + H$

Methanol:

$CH_3OH + h\nu \rightarrow \mathbf{CH_3} + OH$

$\rightarrow \mathbf{CH_3O} + H$

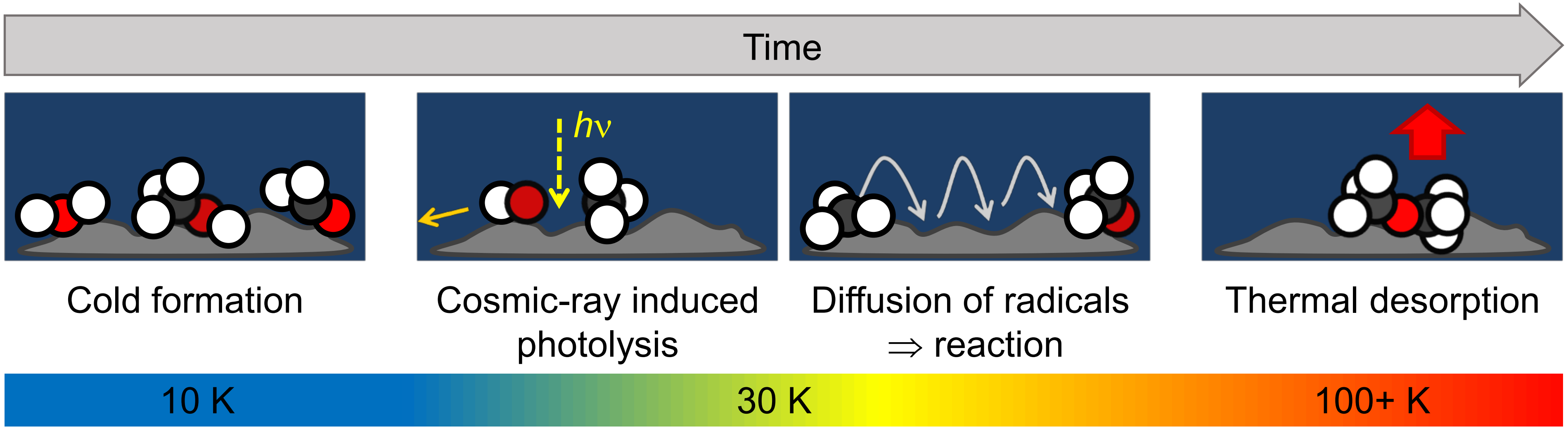
$\rightarrow \mathbf{CH_2OH} + H$



Current COM formation paradigm for hot cores:

Dissociation / diffusion / sublimation

- Ice forms on grains surfaces at low temps (~10K):
    - – atomic diffusion/addition of atoms/molecules from gas phase.
- Production of CR-induced photo-fragments (*radicals*).
- Warm temperatures ⇒ Radicals meet via diffusion: react to produce COMs
- Desorption into gas phase at high temps (>100 K)
- Destruction in gas phase caused by reactions with ions: *CR ionization rate matters*.



Time

Cold formation

Cosmic-ray induced photolysis

Diffusion of radicals ⇒ reaction

Thermal desorption

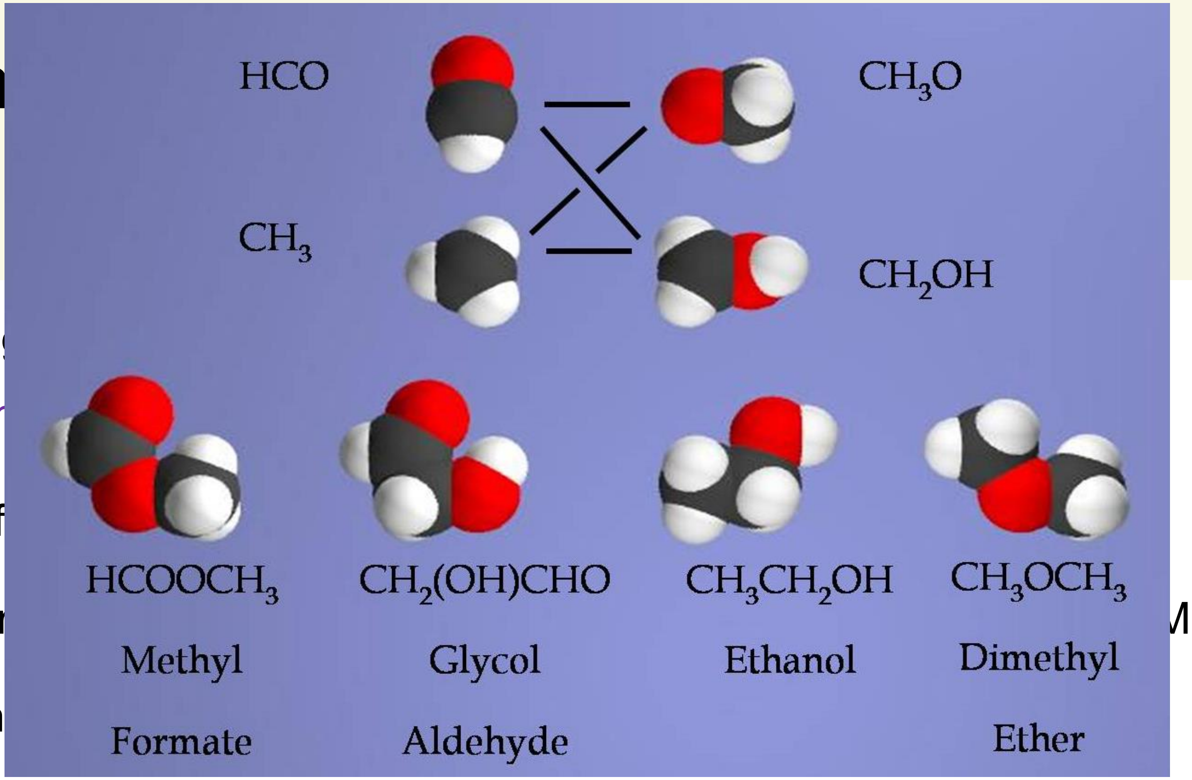
10 K

30 K

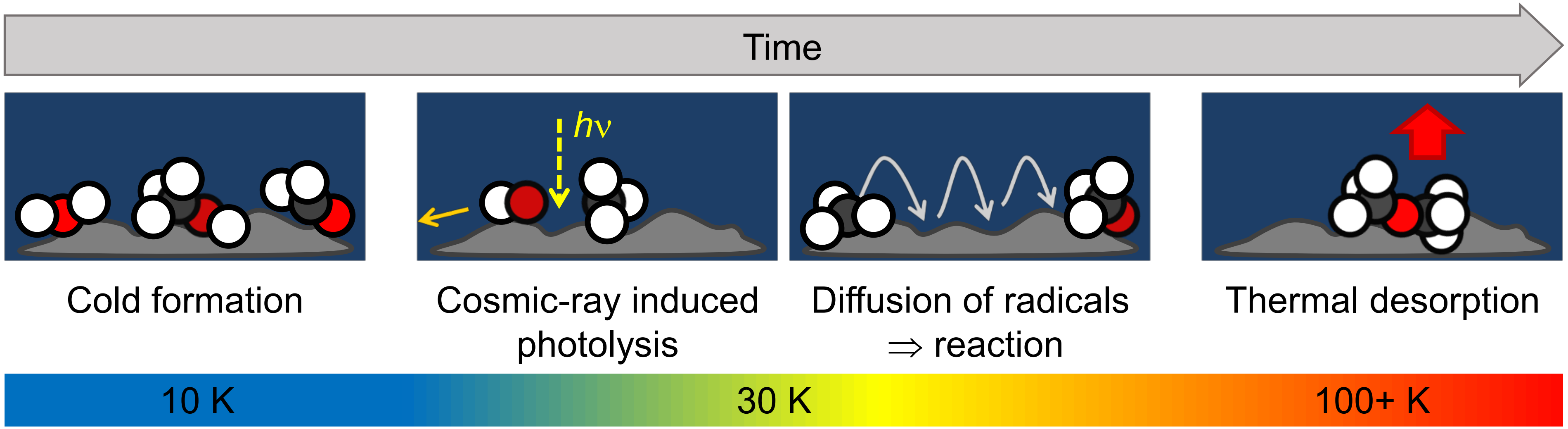
100+ K

Garrod & Herbst (2006), Garrod et al. (2008), etc.

Curren cores:



- Ice forms on
  - – ator
- Production of
- Warm temper Ms
- Desorption in
- Destruction in gas phase caused by reactions with ions: *CR ionization rate matters*.



Cold formation

Cosmic-ray induced photolysis

Diffusion of radicals ⇒ reaction

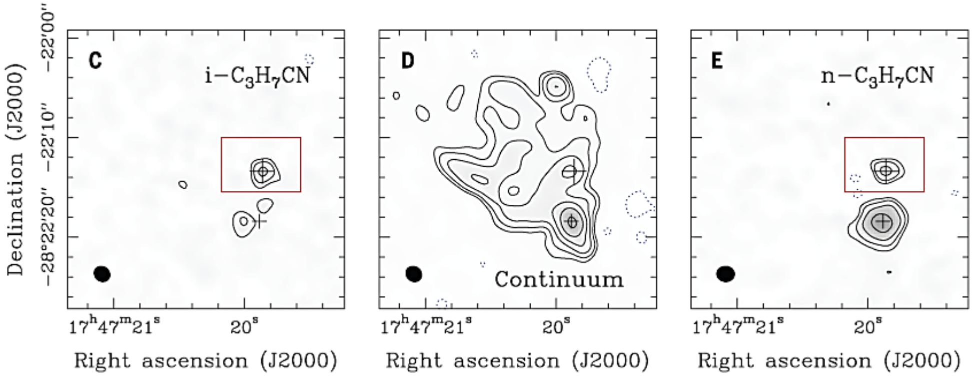
Thermal desorption

Garrod & Herbst (2006), Garrod et al. (2008), etc.

Exploring Molecular Complexity with ALMA (EMoCA)

Sagittarius B2(N): High-mass star-forming core(s)

Full 3-mm (band 3; 84 – 114 GHz) unbiased line survey of Sgr B2(N) (cycle 0/1 data)



Belloche (PI), Garrod, Mueller & Menten (2014): *i*-C_3H_7CN

Belloche, Mueller, Garrod & Menten (2016): Deuterated organics

Mueller et al. (2016): Alkanethiols & alkanols

Margules et al. (2016): ^{13}C-substituted C_2H_5CN

Mueller et al. (2016): vib. excited *n*-C_3H_7CN

Garrod et al. (2017): Butyl cyanide models

Belloche, Meshcheryakov, Garrod, et al. (2017): CH_3NCO, CH_3NHCHO

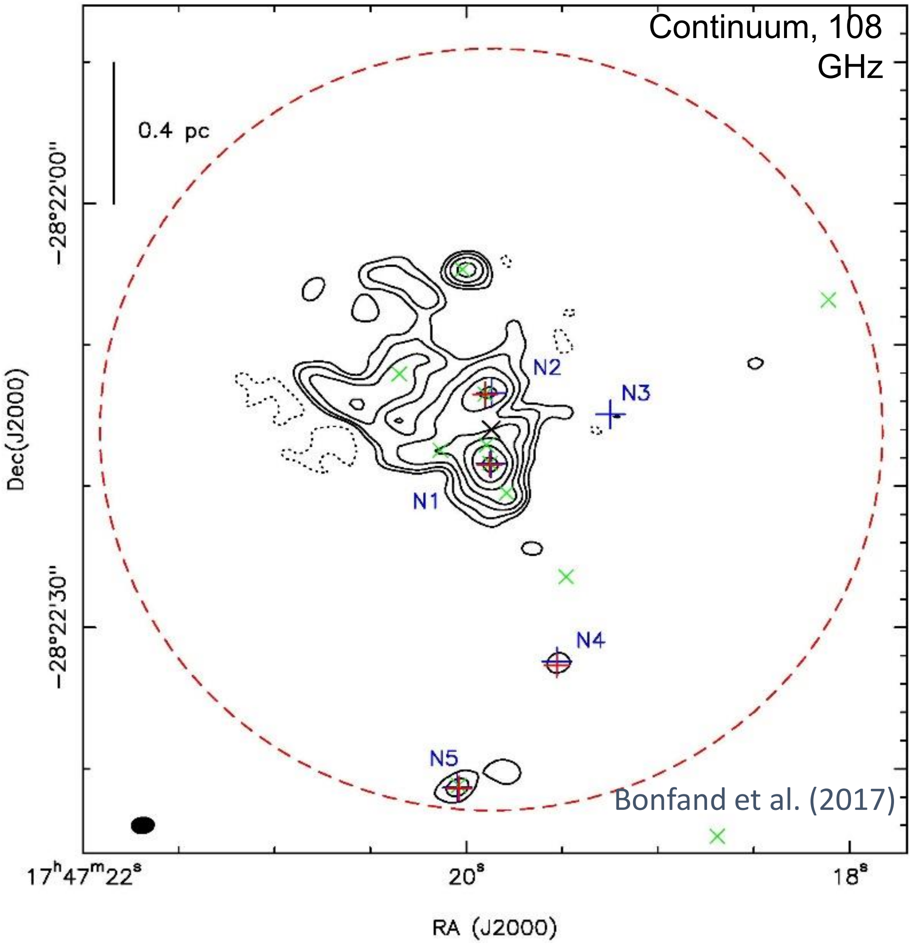
Bonfand, Belloche, Menten, Garrod & Mueller (2017): 3 new hot cores

Thiel, Belloche, Menten, Garrod & Mueller (2017): COMs in diffuse clouds

Bizzocchi et al. (2017): HC_3N

Richard et al. (2018): Aminopropionitrile (search)

EMoCA results for Sgr B2(N)

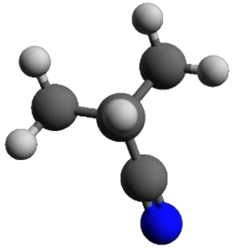


Bonfand et al. (2017)

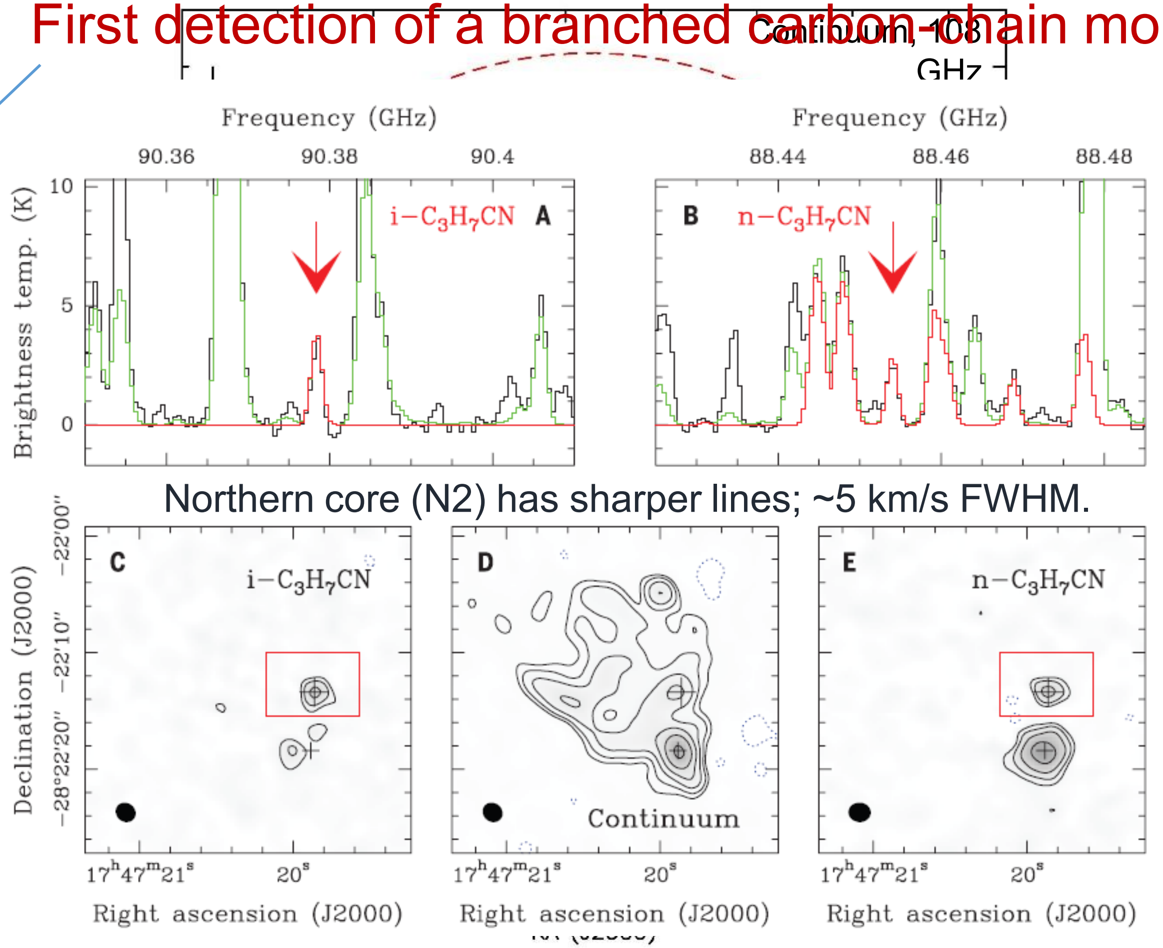
EMoCA results for Sgr B2(N)

First detection of a branched carbon-chain molecule

iso-propyl cyanide

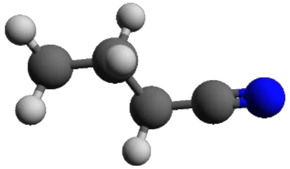


50 lines



Northern core (N2) has sharper lines; ~5 km/s FWHM.

normal-propyl cyanide



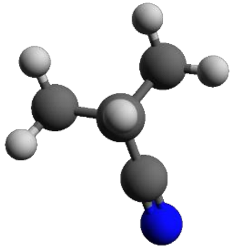
120 lines

Belloche, Garrod, Müller, & Menten, 2014, *Science*, 345, 1584

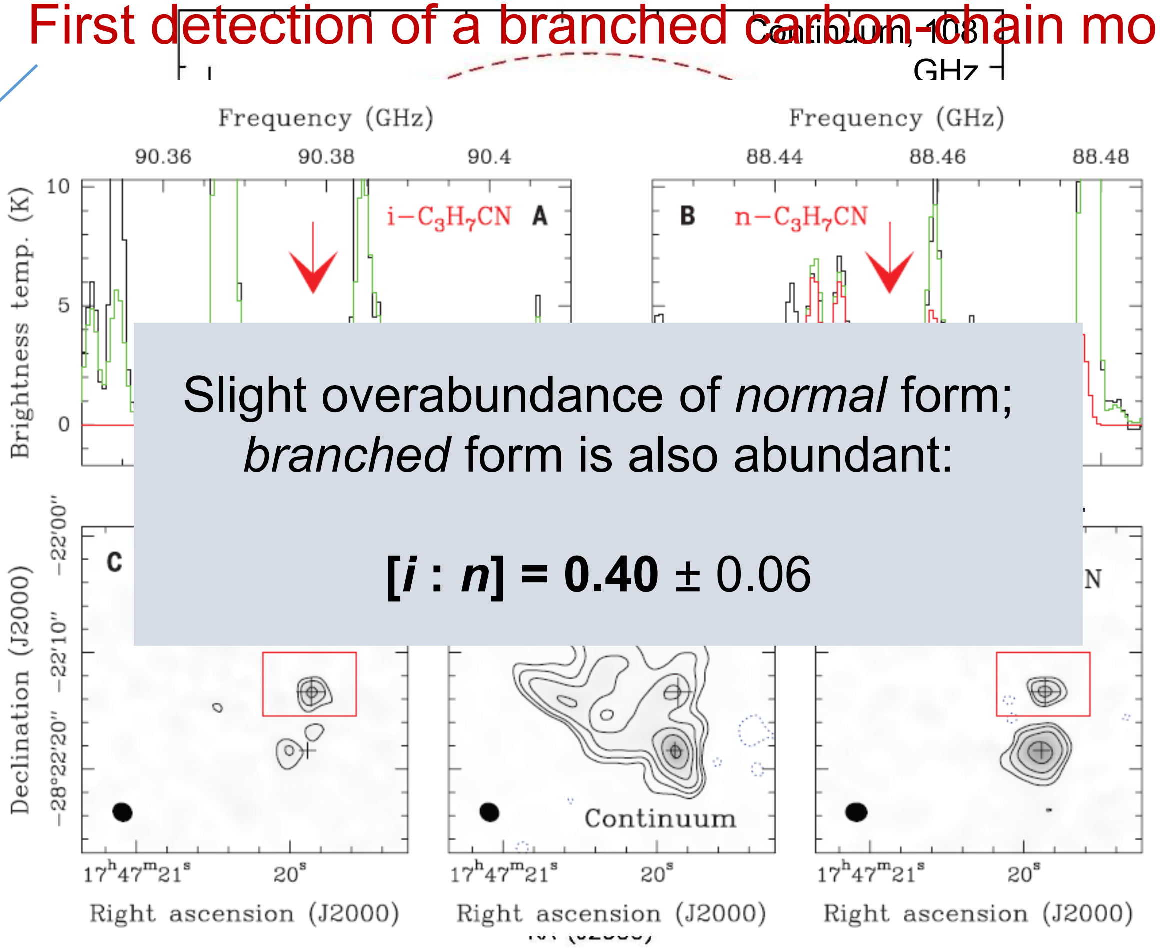
EMoCA results for Sgr B2(N)

First detection of a branched carbon-chain molecule

iso-propyl cyanide



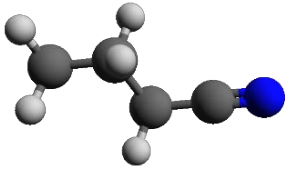
50 lines



Slight overabundance of *normal* form;
branched form is also abundant:

[*i* : *n*] = 0.40 ± 0.06

normal-propyl
cyanide



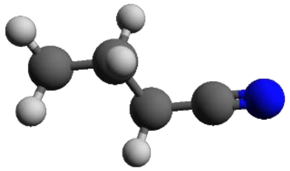
120 lines

Belloche, Garrod, Müller,
& Menten, 2014,
Science, 345, 1584

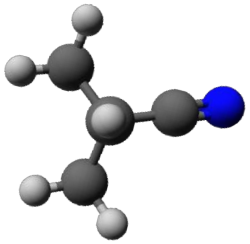
Branched carbon chains

- *New class* of interstellar molecule
  - ⇒ No previous interstellar detections
- Not present in chemical models
- Branching is found in e.g. amino acids on Earth/in meteorites.

normal-propyl
cyanide



iso-propyl
cyanide

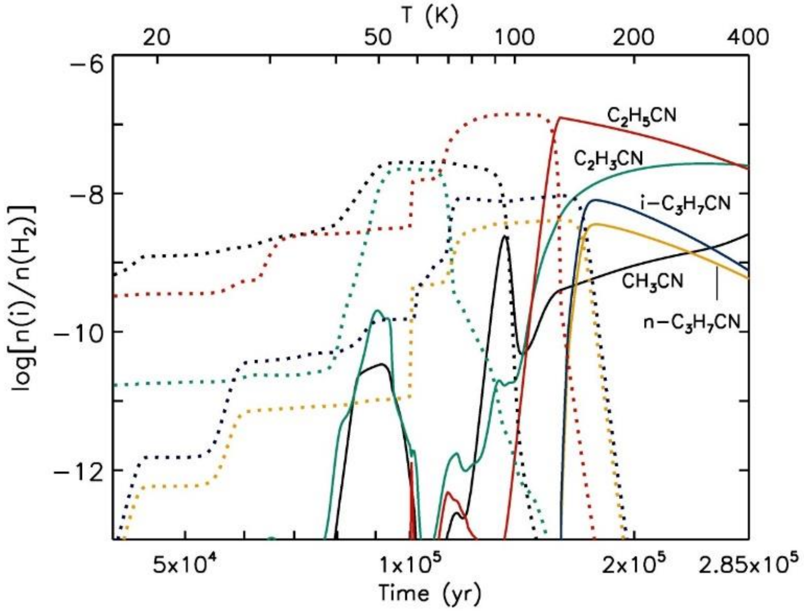


Need gas-phase and grain-surface reaction network

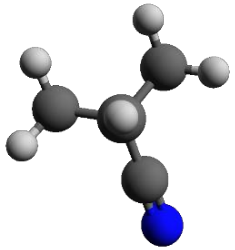
Belloche, Garrod, Müller, & Menten,
2014, *Science*, 345, 1584

Iso-/normal- propyl cyanide model results

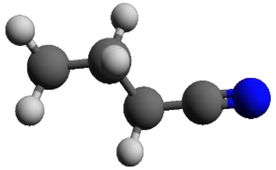
(Belloche, Garrod, Müller, & Menten, 2014)



i-C_3H_7CN



n-C_3H_7CN



Observations

N = 7.2 ± 1.4 x 10^{16} cm^{-2} — N = 1.8 ± 0.4 x 10^{17} cm^{-2}

T_{rot} = 153 ± 12 K — T_{rot} = 153 ± 12 K

[*i* : *n*] = 0.40 ± 0.06

Chemical models

[*i*-PrCN]/[H_2] = 8.0 x 10^{-9} — [*n*-PrCN]/[H_2] = 3.6 x 10^{-9}

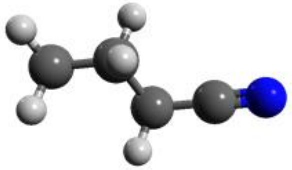
T_{peak} = 160 K — T_{peak} = 160 K

[*i* : *n*] = 2.2

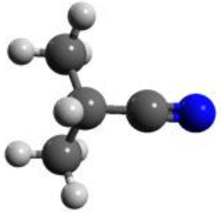
New/recent additions to the network

(Garrod, Belloche, Müller & Menten, 2017)

Propyl cyanides
(already present)



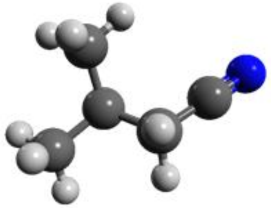
n-C_3H_7CN



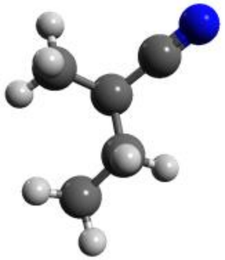
i-C_3H_7CN

Butyl cyanides

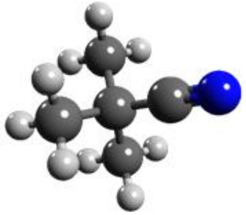
n-C_4H_9CN



i-C_4H_9CN

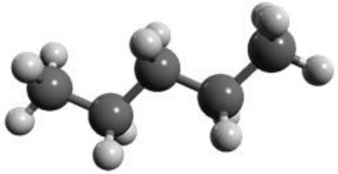


s-C_4H_9CN

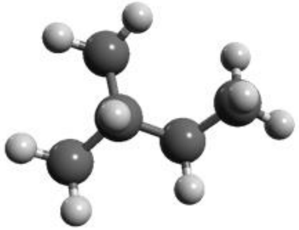


t-C_4H_9CN

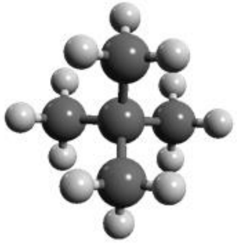
Pentanes



n-C_5H_{12}



i-C_5H_{12}



neo-C_5H_{12}

Image credit:
E. Willis

(Smaller alkanes and alkyl cyanides were already present in 2014 network)

Butyl cyanide production *on dust grains* via radical addition

$$\begin{array}{rcllr}
\dot{C}H_3 & + & \dot{C}H_2CH_2CH_2CN & \rightarrow & n\text{-}C_4H_9CN \\
\dot{C}H_2CH_3 & + & \dot{C}H_2CH_2CN & \rightarrow & n\text{-}C_4H_9CN \\
\dot{C}H_2CH_2CH_3 & + & \dot{C}H_2CN & \rightarrow & n\text{-}C_4H_9CN \\
\dot{C}H_2CH_2CH_2CH_3 & + & \dot{C}N & \rightarrow & n\text{-}C_4H_9CN \\
\dot{C}N & + & C_4H_8 & \rightarrow & CH_3CH_2\dot{C}HCH_2CN \\
H & + & CH_3CH_2\dot{C}HCH_2CN & \rightarrow & n\text{-}C_4H_9CN \\[1ex]
\dot{C}H_3 & + & CH_3\dot{C}HCH_2CN & \rightarrow & i\text{-}C_4H_9CN \\
CH_3\dot{C}HCH_3 & + & \dot{C}H_2CN & \rightarrow & i\text{-}C_4H_9CN \\
\dot{C}H_2CH(CH_3)CH_3 & + & \dot{C}N & \rightarrow & i\text{-}C_4H_9CN \\[1ex]
\dot{C}H_3 & + & CH_3CH_2\dot{C}HCN & \rightarrow & s\text{-}C_4H_9CN \\
\dot{C}H_3 & + & \dot{C}H_2CH(CH_3)CN & \rightarrow & s\text{-}C_4H_9CN \\
\dot{C}H_2CH_3 & + & CH_3\dot{C}HCN & \rightarrow & s\text{-}C_4H_9CN \\
CH_3\dot{C}HCH_2CH_3 & + & \dot{C}N & \rightarrow & s\text{-}C_4H_9CN \\[1ex]
\dot{C}H_3 & + & CH_3\dot{C}(CH_3)CN & \rightarrow & t\text{-}C_4H_9CN \\
CH_3\dot{C}(CH_3)CH_3 & + & \dot{C}N & \rightarrow & t\text{-}C_4H_9CN
\end{array}$$

CN radical has some special reactions…

Crucial additions to (grain-surface) reaction network:

Barriers from gas-phase experimental data by Gannon et al. (2008)

$\mathbf{\dot{C}N + C_3H_6} \rightarrow CH_3\dot{C}HCH_2CN$ ($E_A = 0$)

$CH_3\dot{C}HCH_2CN + H \rightarrow$ ***n*-C_3H_7CN** (*n*-propyl cyanide)

$CH_3\text{-}CH\text{=}CH_2$

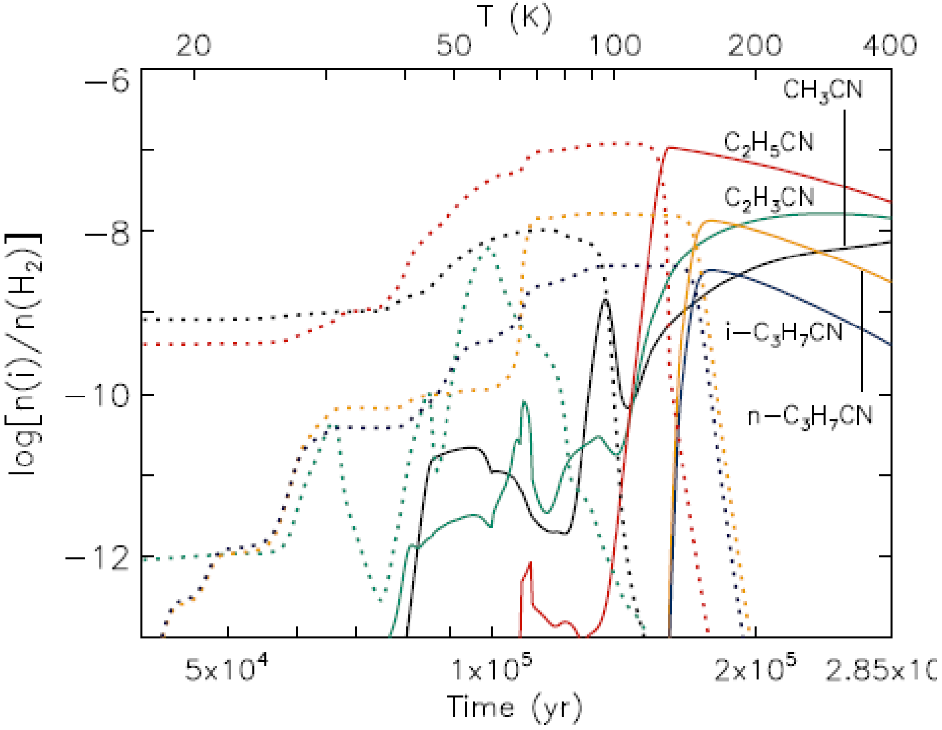
$\mathbf{\dot{C}N + C_4H_8} \rightarrow CH_3CH_2\dot{C}HCH_2CN$ ($E_A = 0$)

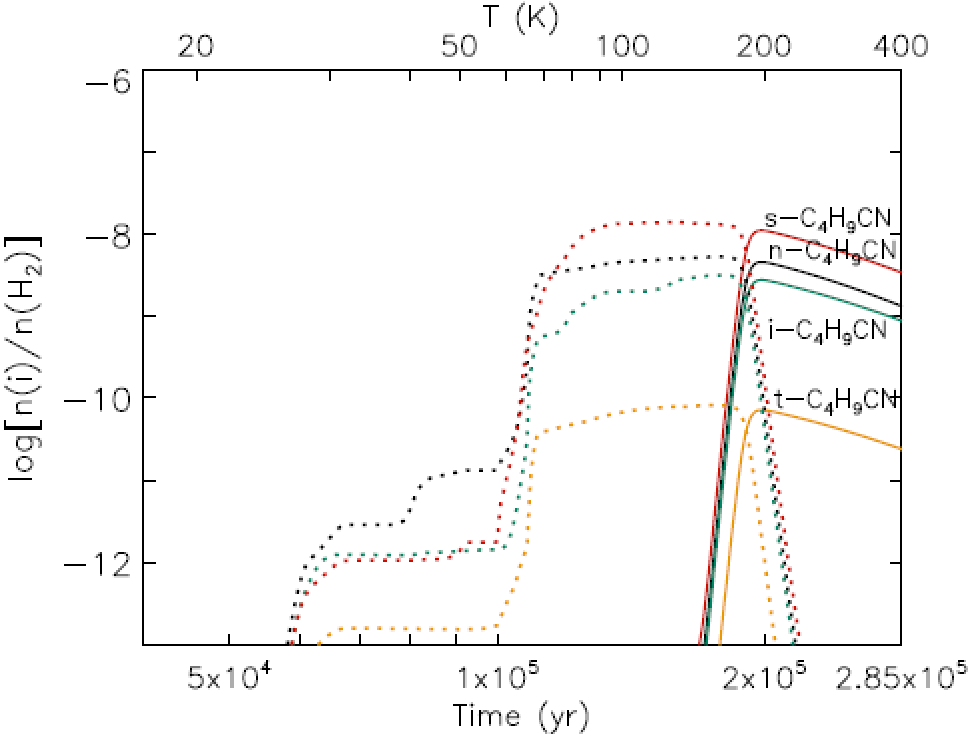
$CH_3CH_2\dot{C}HCH_2CN + H \rightarrow$ ***n*-C_4H_9CN** (*n*-butyl cyanide)

$CH_3\text{-}CH_2\text{-}CH\text{=}CH_2$

- Without these reactions, branching dominates the chemistry!

Nitrile predictions



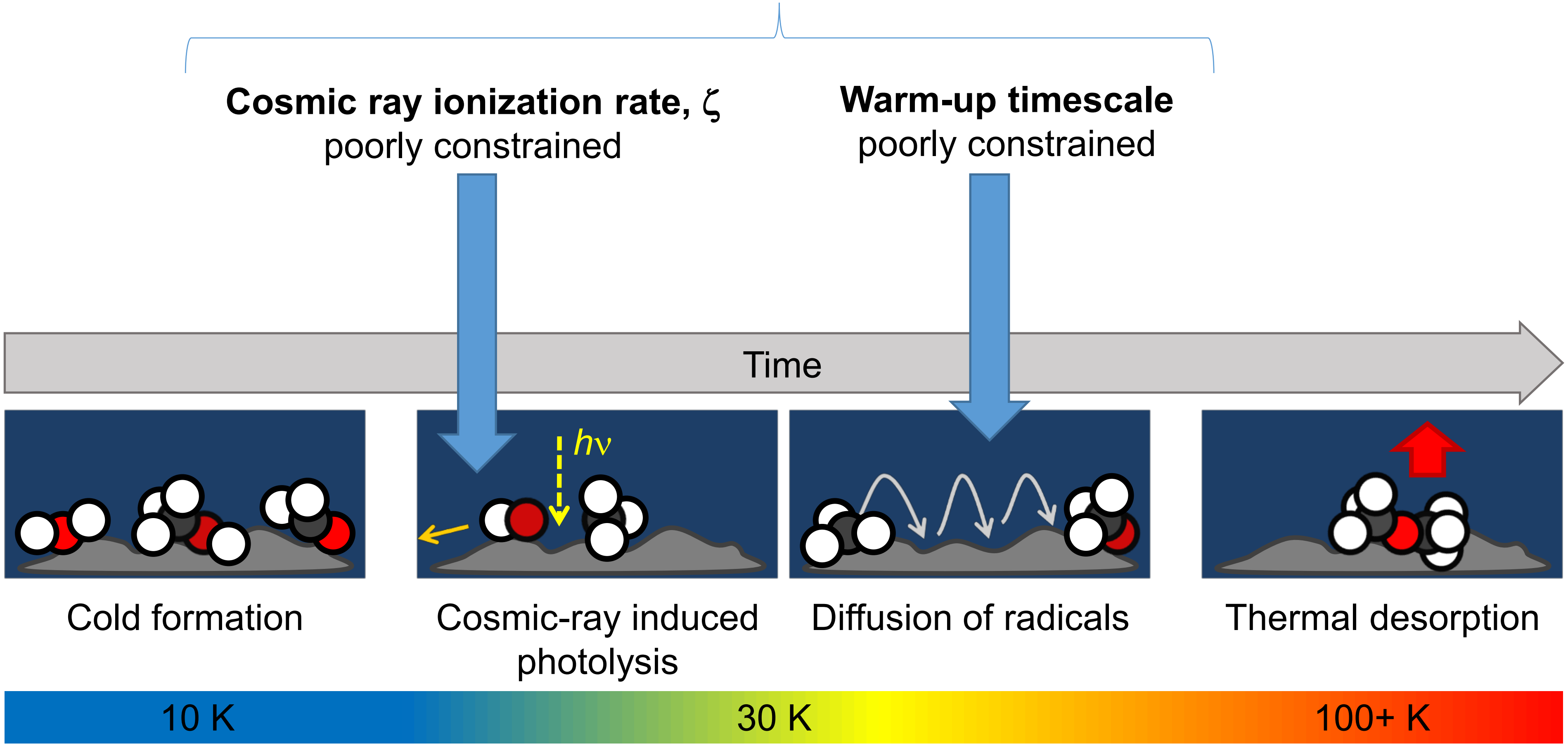


- *n*-propyl cyanide is correctly more abundant than the *iso* form (i.e. better than our previous model).
- Attack of CN on propylene seems to be the critical mechanism.

- The branched *sec*-BuCN dominates the butyl cyanides.
- Comparable to *n*-PrCN abundance ⇒ detectable?
- *tert*-BuCN is formed, but very unlikely to be detectable.

Can COMs constrain physical parameters?

Both may vary by object



Cosmic ray ionization rate, ζ
poorly constrained

Warm-up timescale
poorly constrained

Time

Cold formation

Cosmic-ray induced photolysis

Diffusion of radicals

Thermal desorption

10 K

30 K

100+ K

Need to constrain these values somehow

Cosmic-ray ionization

- $H_2 + CR \rightarrow H_2^+$ (+CR)

  …is the main source of ionization in dark/dense interstellar clouds.

- Canonical rate is $\zeta = 1.3 \times 10^{-17}\ s^{-1}$ – but poorly constrained,

  and *only measured for diffuse gas*.

- CR ionization rate determines ambient UV field (fluorescence of H_2)

  ⇒ **Promotes formation of COMs on grains**

- CR ionization chemistry destroys gas-phase molecules

  ⇒ **Promotes destruction of COMs in gas-phase**

Perhaps we can tune ζ to reproduce observations…

Cosmic-ray ionization in hot cores

(Barger & Garrod, *in prep.*)

- Run **grid of models** with **varying CR ionization rate** and **warm-up timescales**.
- Why also timescale? – Timescale and CR flux may be degenerate…

Work by UVa grad student *Chris Barger*.

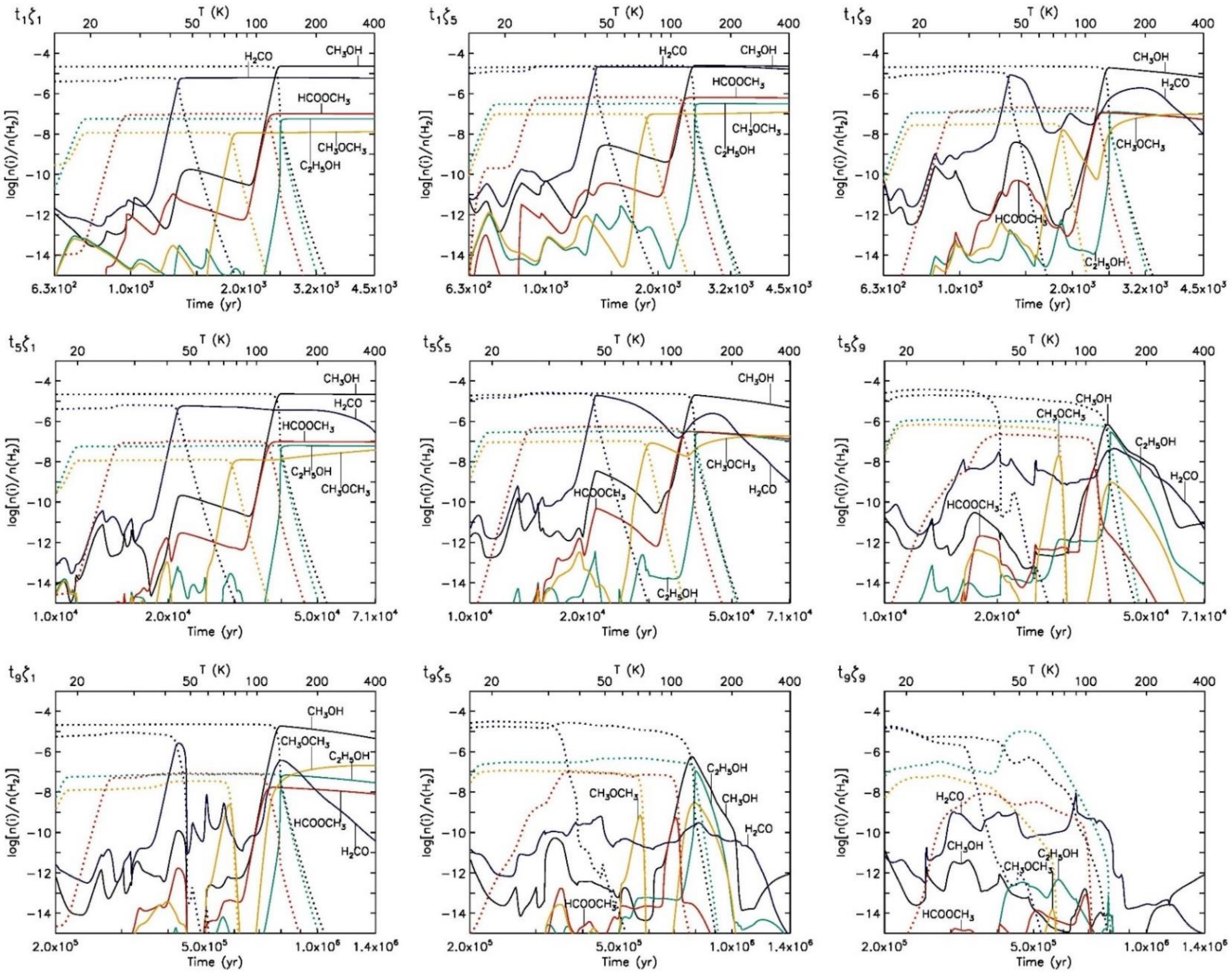
Warm-up Timescale		Cosmic-ray Ionization Rate	
Notation	Time to reach 200K (yr)	Notation	$\zeta(\mathrm{s}^{-1})$
t_1	3.13×10^{3}	ζ_1	2.60×10^{-18}
t_2	6.25×10^{3}	ζ_2	5.81×10^{-18}
t_3	1.25×10^{4}	$\zeta_3{}^*$	1.30×10^{-17}
t_4	2.50×10^{4}	ζ_4	2.60×10^{-17}
$t_5{}^*$	5.00×10^{4}	ζ_5	5.20×10^{-17}
t_6	1.00×10^{5}	ζ_6	1.04×10^{-16}
$t_7{}^*$	2.00×10^{5}	ζ_7	2.08×10^{-16}
t_8	4.50×10^{5}	ζ_8	4.16×10^{-16}
$t_9{}^*$	1.00×10^{6}	ζ_9	8.32×10^{-16}

*Original parameters from G13

Model outputs for COMs

Increasing cosmic ray flux, ζ

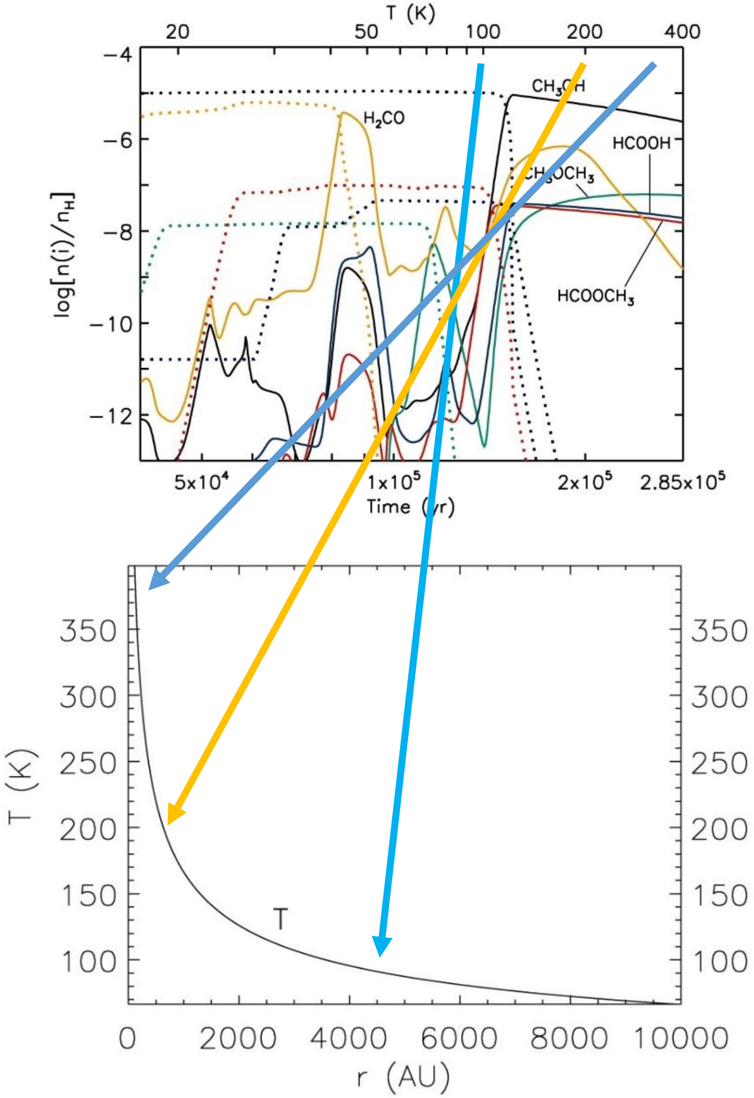
Increasing warm-up timescale



Actual:
9x9 grid

Chemical/physical model mapping to sources

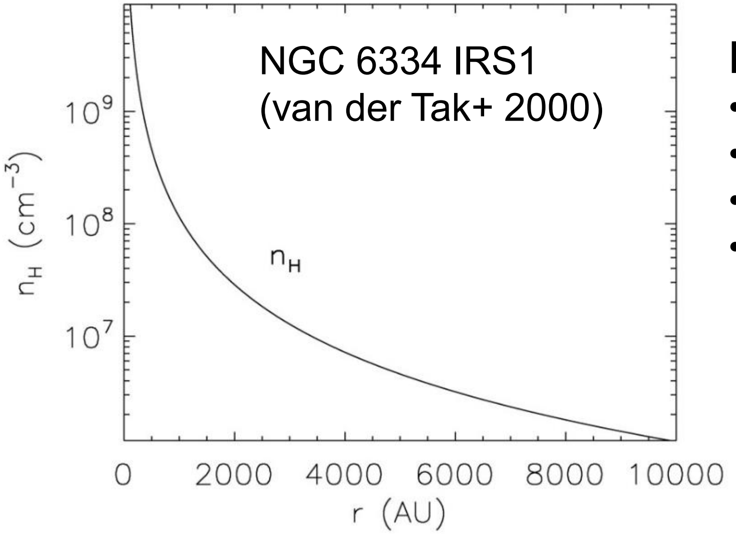
We map the chemical model results to observational physical profiles, based on temperature. (see Garrod 2013)



Calculate simple LTE molecular line radiative transfer for abundance-populated hot-core profiles.

Convolve with observational beam profile.

⇒ **Compare simulated line integrated intensities** w/ JCMT/IRAM observations (Bisschop+ 2007)


NGC 6334 IRS1
(van der Tak+ 2000)

Hot cores:

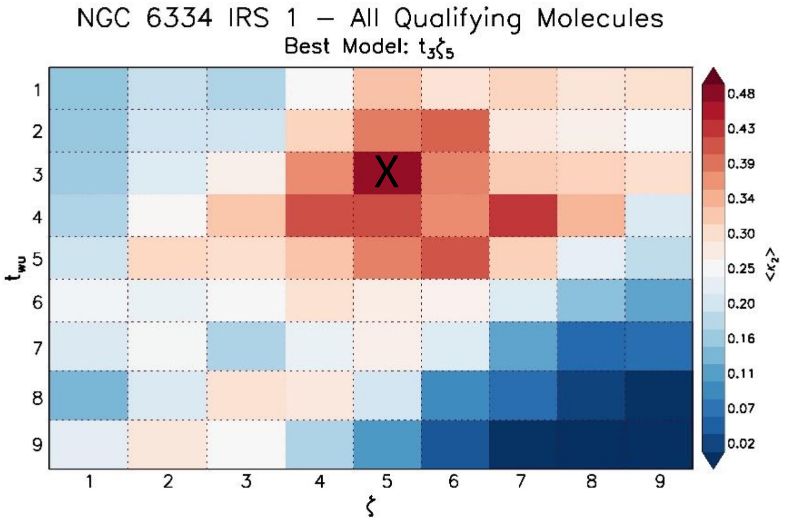
- NGC 6334 IRS1
- NCG 7538
- W3 (H_2O)
- W33A

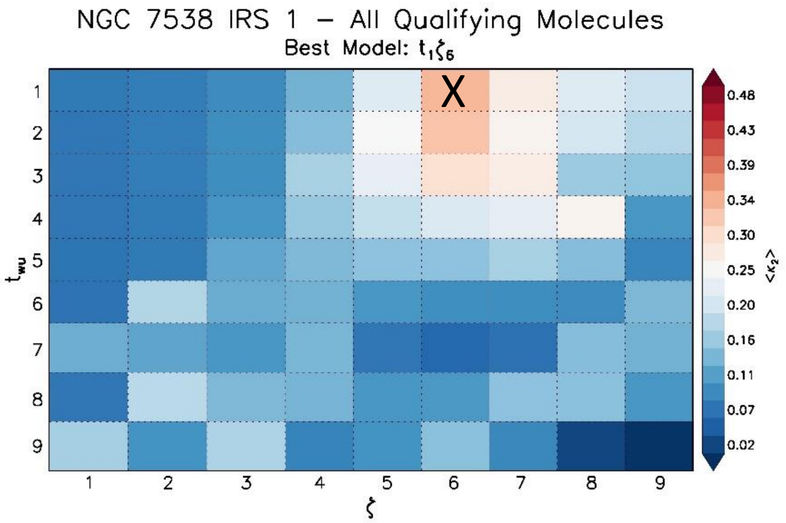
Cumulative line-emission matches for all four sources

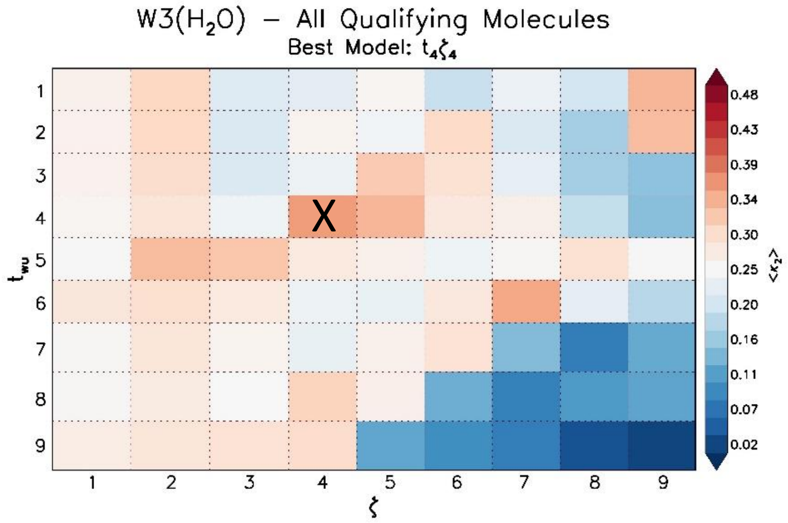
Matches based on line-emission int. intensities for 11 molecules studied by Bisschop+ (2007):

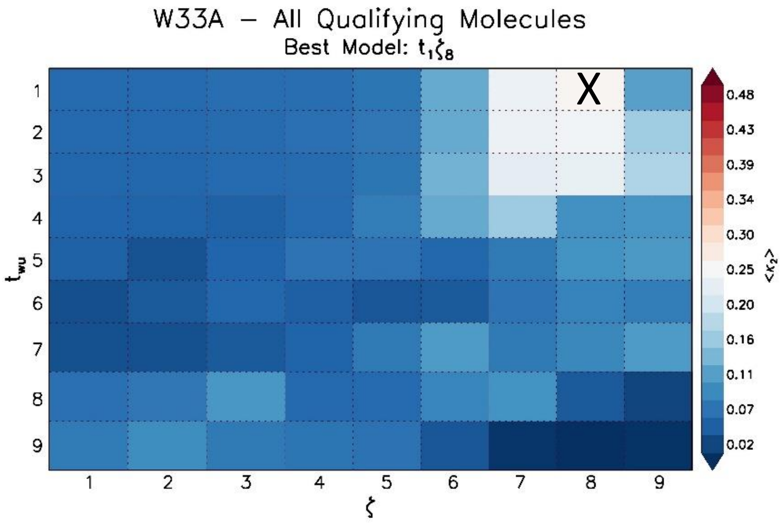
H_2CO
CH_3OH
C_2H_5OH
HNCO
CH_3CN
C_2H_5CN
$HCOOCH_3$
CH_3OCH_3
CH_2CO
CH_3CHO
C_3H_4
~~HCOOH~~
~~NH_2CHO~~

Red = good
Blue = poor


NGC 6334 IRS 1 – All Qualifying Molecules
Best Model: $t_3\zeta_5$


NGC 7538 IRS 1 – All Qualifying Molecules
Best Model: $t_1\zeta_6$


W3(H_2O) – All Qualifying Molecules
Best Model: $t_4\zeta_4$


W33A – All Qualifying Molecules
Best Model: $t_1\zeta_8$

Best-model matches for all four sources

Source	Best Model	κ	Fit to ζ (s^{-1})	# lines
NGC 6334 IRS 1	$t_3\zeta_5$	0.471	$3.68 - 7.35 \times 10^{-17}$	137
NGC 7538 IRS 1	$t_{1.5}\zeta_6$	0.337	$7.35 \times 10^{-17} - 1.47 \times 10^{-16}$	72
W3(H_2O)	$t_4\zeta_4$	0.357	$1.84 - 3.68 \times 10^{-17}$	82
W33A	$t_0\zeta_{7.5}$	0.261	$2.08 - 4.16 \times 10^{-16}$	52

“Match” parameter, κ = mean(κ_i)

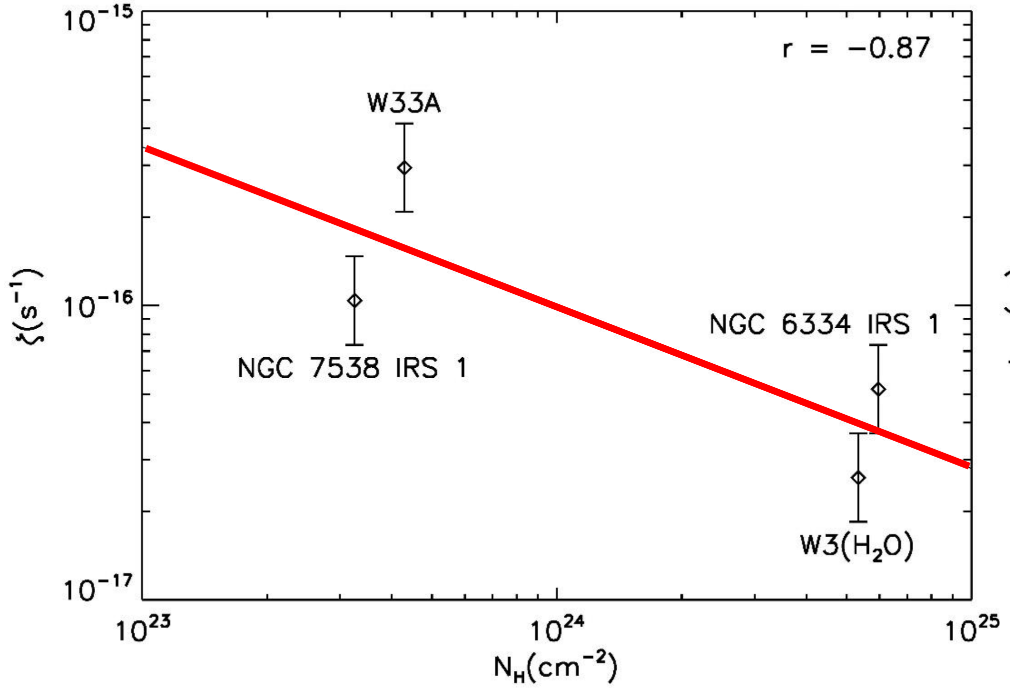
$$\kappa_i = erfc(|log_2([\int T_B(\nu)d\nu]_i) - log_2([\int T_B(\nu)d\nu]_{obs,i})|)$$

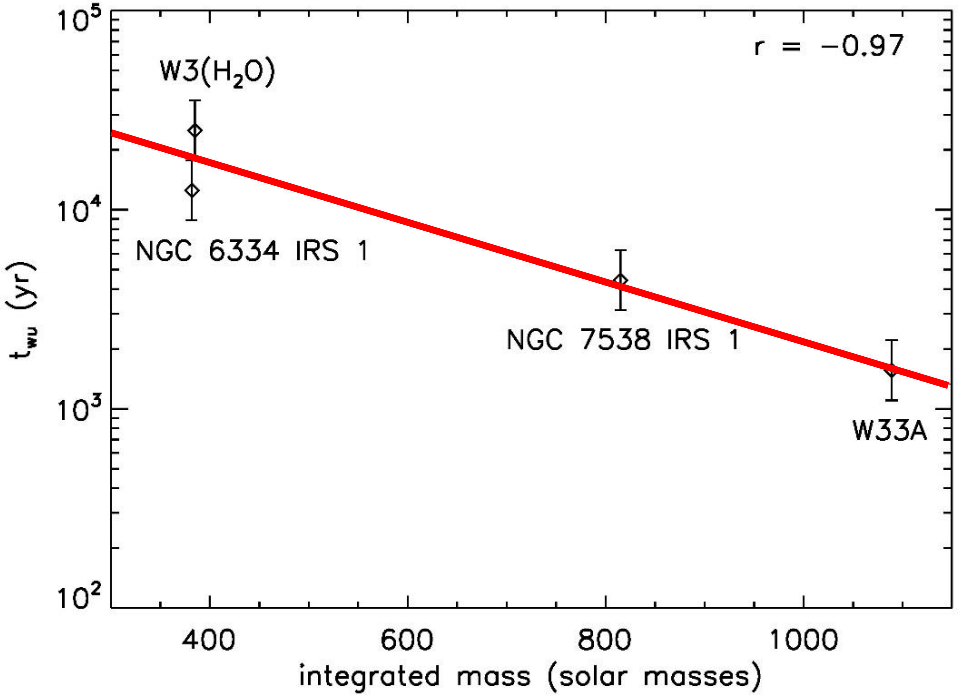
- **Optimal CR <u>ionization rates are higher than typically adopted</u> values ($1.3\text{x}10^{-17}$ s^{-1}).**

- **Optimal warm-up <u>timescales are shorter than the usual</u> “fast” warm-up timescale.**

ζ vs. N_H

Warm-up timescale vs. mass





Log-log correlation between:

- N_H (from van der Tak dust model)
- CR ionization rate

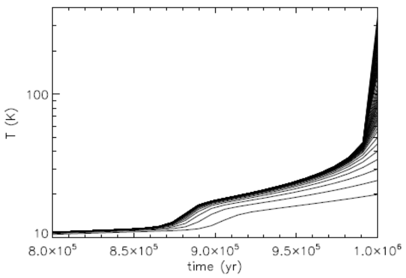
Log-linear correlation between:

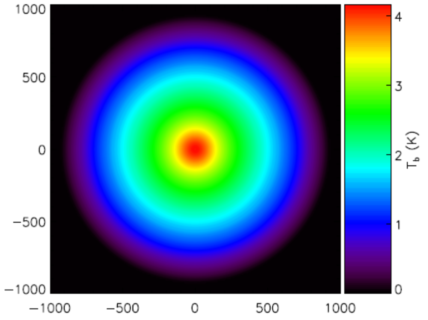
- Integrated core mass
  (from van der Tak dust model)
- Warm-up timescale

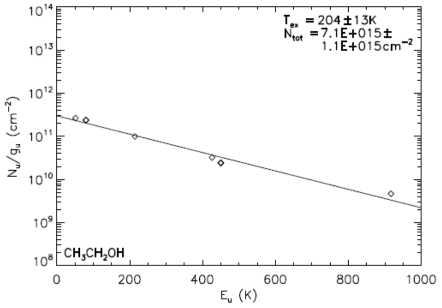
What comes next?

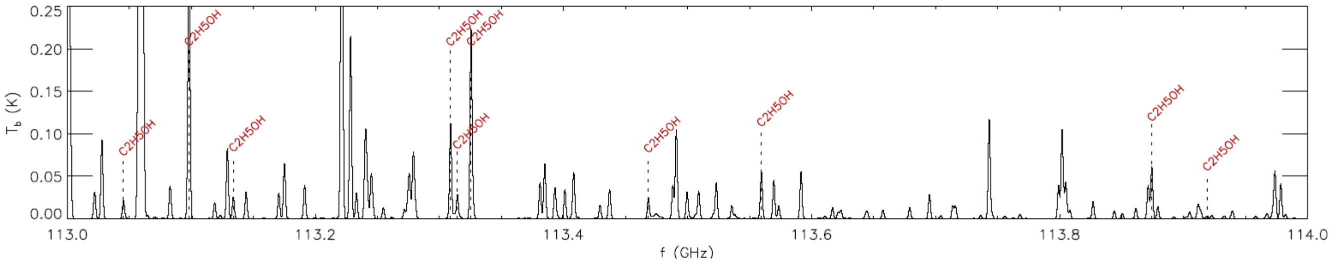
Combined simulations of hot-core hydrodynamics / chemistry / molecular emission

- Funded by NASA Astrophysics Theory Program.
- Will produce 2-D and 3-D hydro+radiation simulations, and combine them with MAGICKAL chemistry model and spectral simulation code.
- UVa co-I’s Herbst (Chem/Astro), Li (Astro) and Davis (Astro).
- Grad students Chris Barger (Chem) and Andy Lam (Astro) working on it…

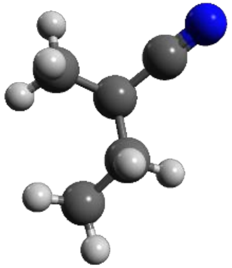








Conclusions



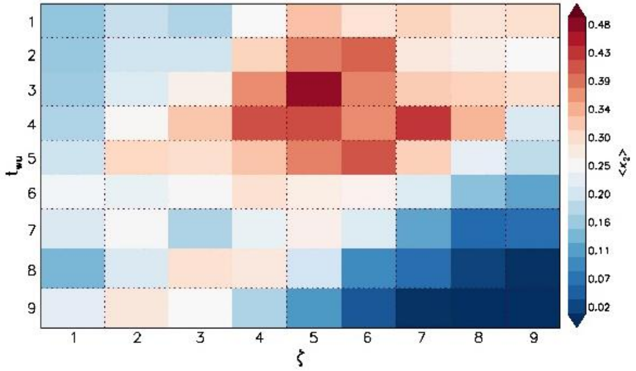
- **Branching in molecular structures opens a new frontier in astrochemistry.**

- Degree of molecular branching appears to increase with larger molecules.

- Dominance of *straight-chain* PrCN related to CN insertion into unsaturated hydrocarbons.

- **Molecules with different functional groups may show yet greater branching**

  $\Rightarrow$ lack of insertion routes (high activation barriers)



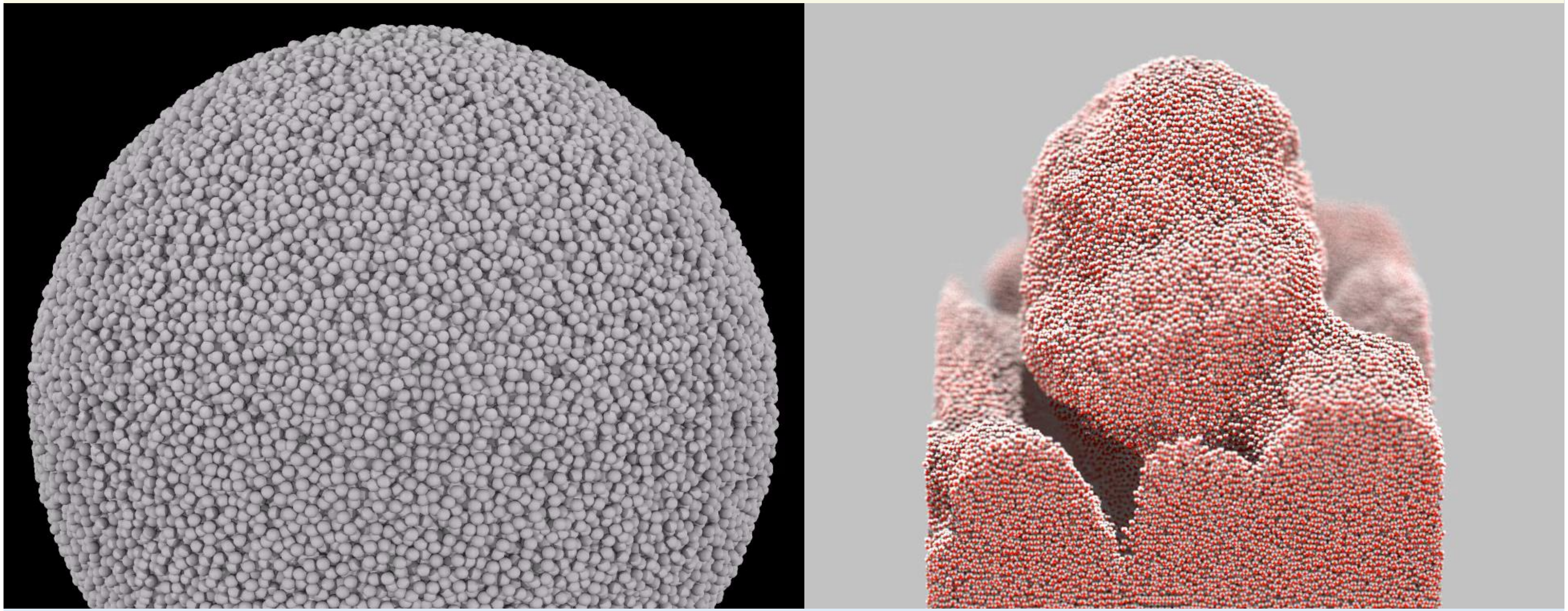
- **COMs may be a useful diagnostic of CR ionization rates.**

- *Rapid warm-up and high CR ionization rates*

  $\Rightarrow$ better match to observations.

- Strong correlations with mass and H column density.

Thanks for listening



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