Molecules in the Interstellar Medium

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CEFET-MG

Química Teórica: Reatividade e Estrutura Molecular

- Atmospheric chemistry
- Astrochemistry
- Adsorption & Catalysis

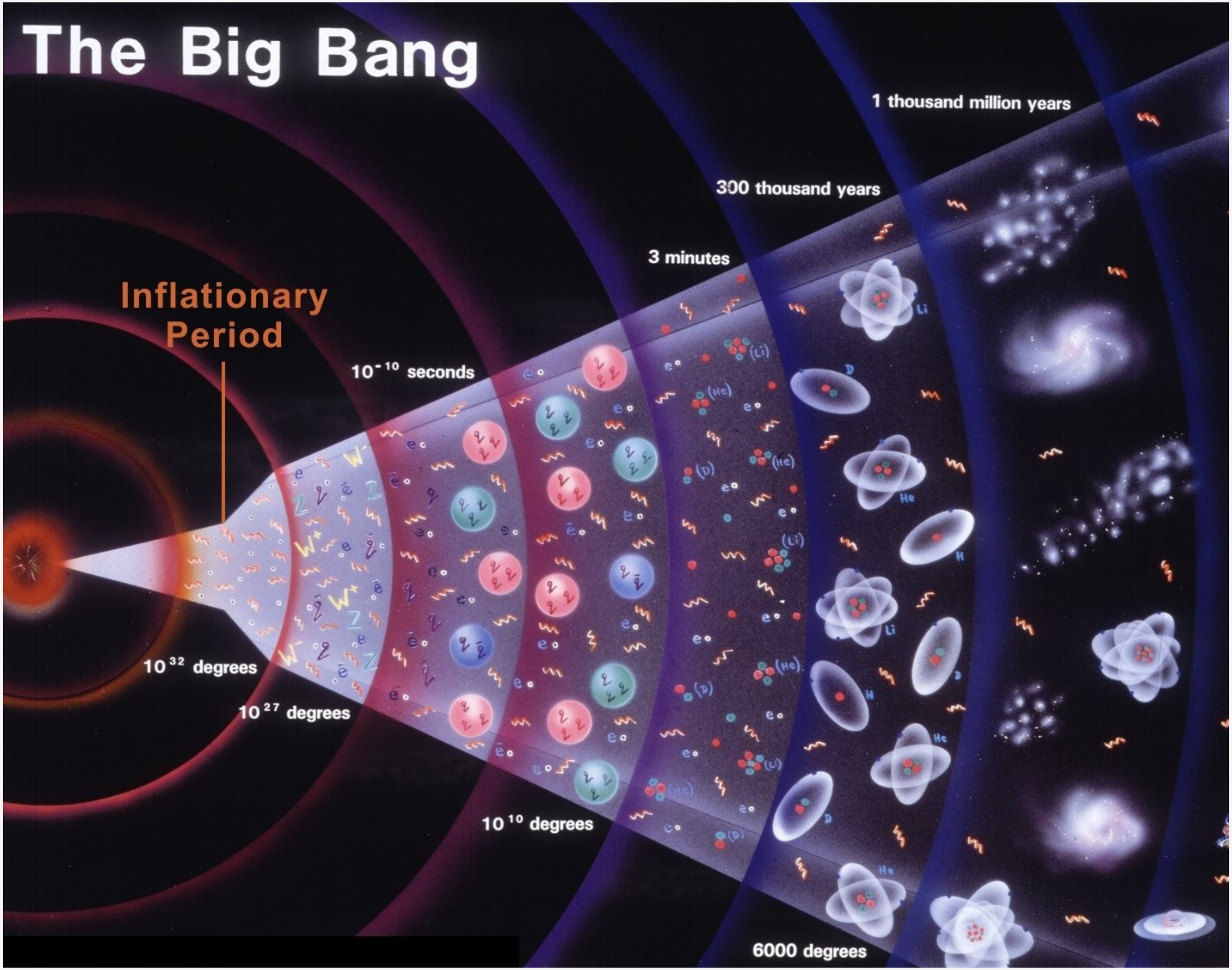
QuiTrem

Química Teórica: Reatividade e Estrutura Molecular

quitrem.cefetmg.br

- When does **electronic structure** begin?
- Where is condensed matter in the night sky?
- How do we study it?
- Selected results from our group

When did chemical bonds first formed?



When did chemical bonds first formed?

~100.000 yrs after the Big Bang:

1. Available: $\mathbf{H^+}$ e $\mathbf{He^{2+}}$
2. **He** gets electrons first
3. A lot of $\mathbf{H^+}$, some neutral **He**
4. Many collisions: He + H^+

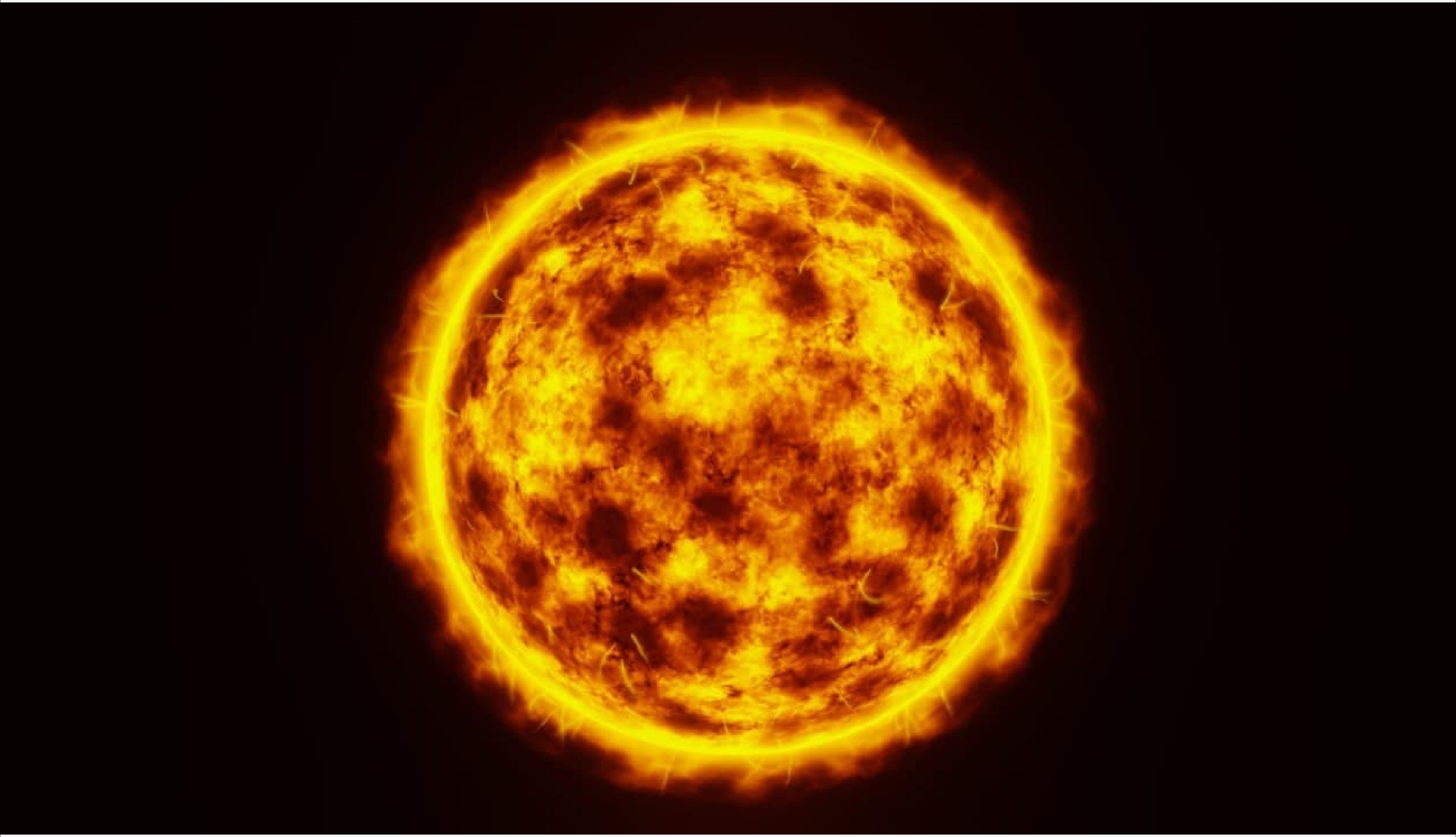
A primeira ligação química

Credit: Mondolithic Studios

1925: HeH^+ produced in lab
1978: Hypothesis: HeH^+ should still be present in space
2019: Detected

Nature **568**, 357 (2019)

Stars: mothers of heavier elements

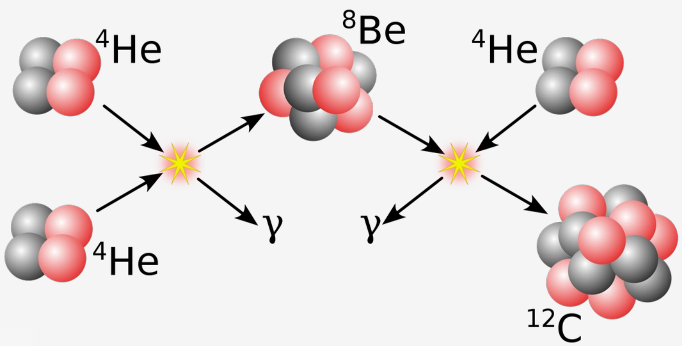


1^{st} stellar cycles:

few million yrs after big bang

1M$_\odot$:

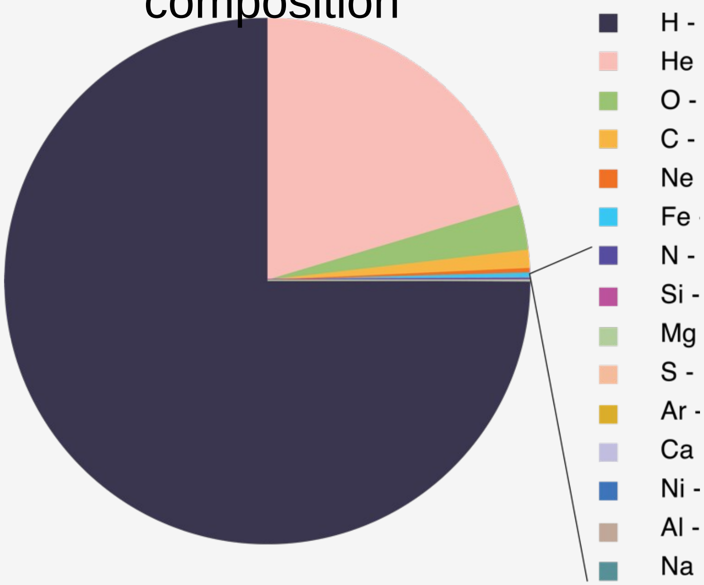
Triple alpha process

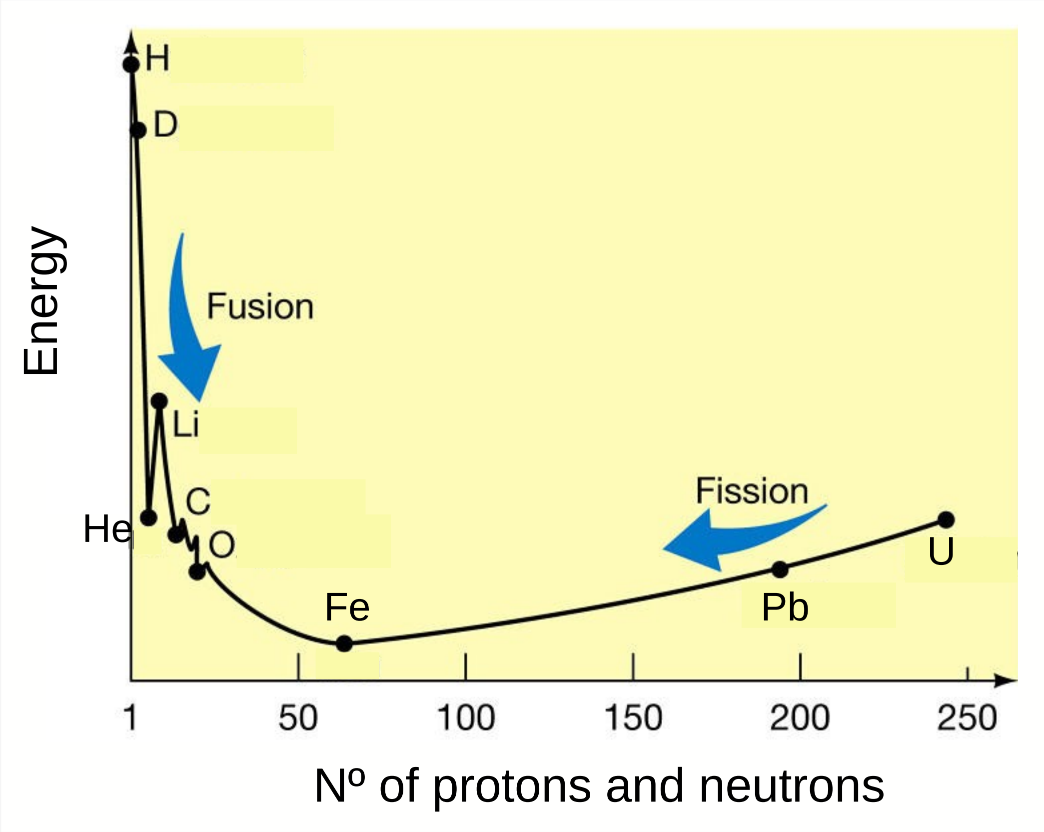


For stars with > 8M$_\odot$

- C burning up to Mg
- Ne burning up to Mg
- O burning up to S
- Si burning up to Fe, Ni

Current composition

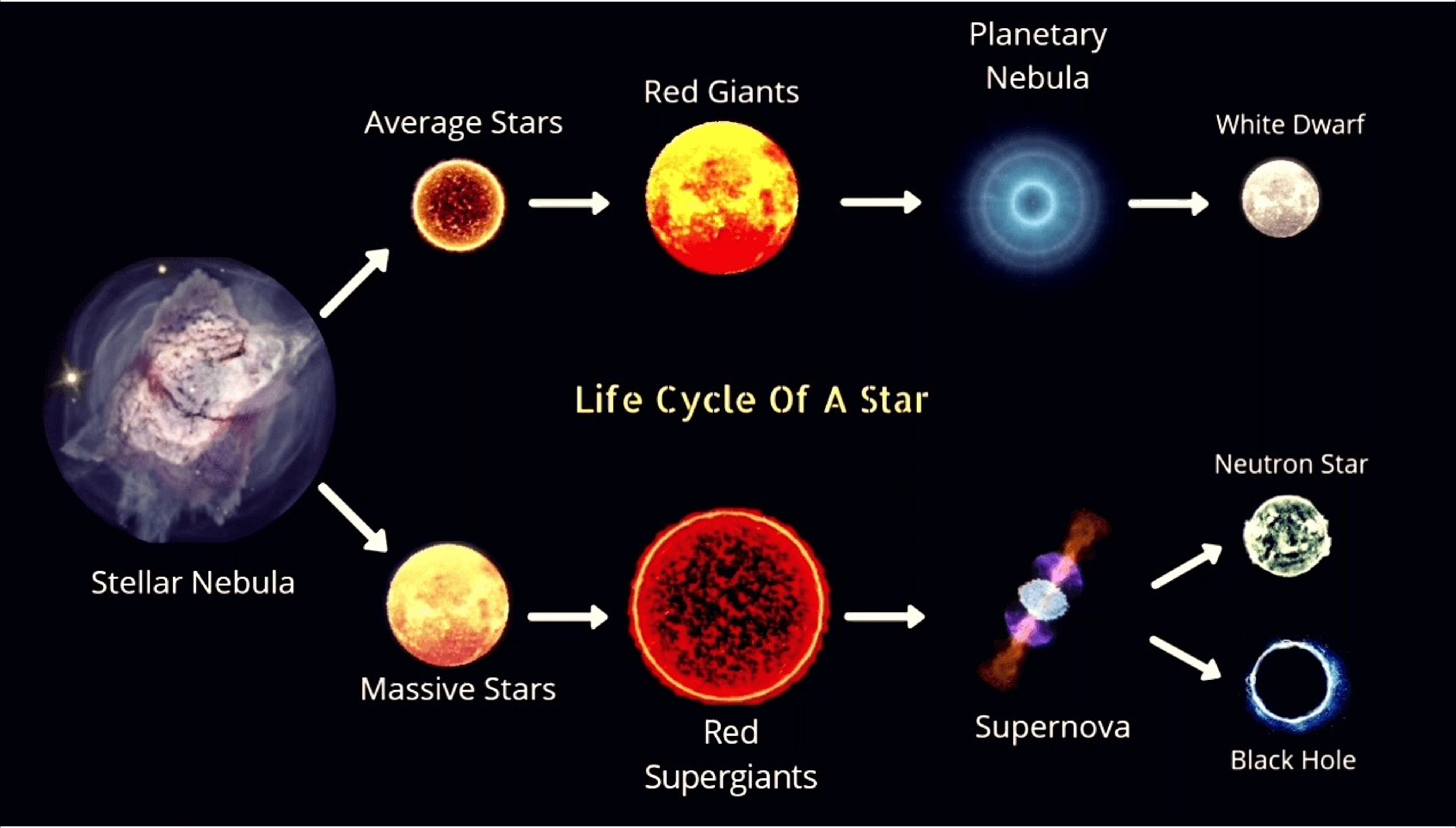




How the universe creates elements heavier than Fe?

Ex.: Ag, I, Au, Pb

Getting to heavier elements



Summary of chemical origins

BEGINING OF CHEMISTRY TIMELINE

1. **Big Bang**

2. **Recombination: 18-378 x10³ years**
   - 1st neutral atoms (H, He)
   - HeH^+

3. **Dark Ages 0.38-150x10⁶ yrs**

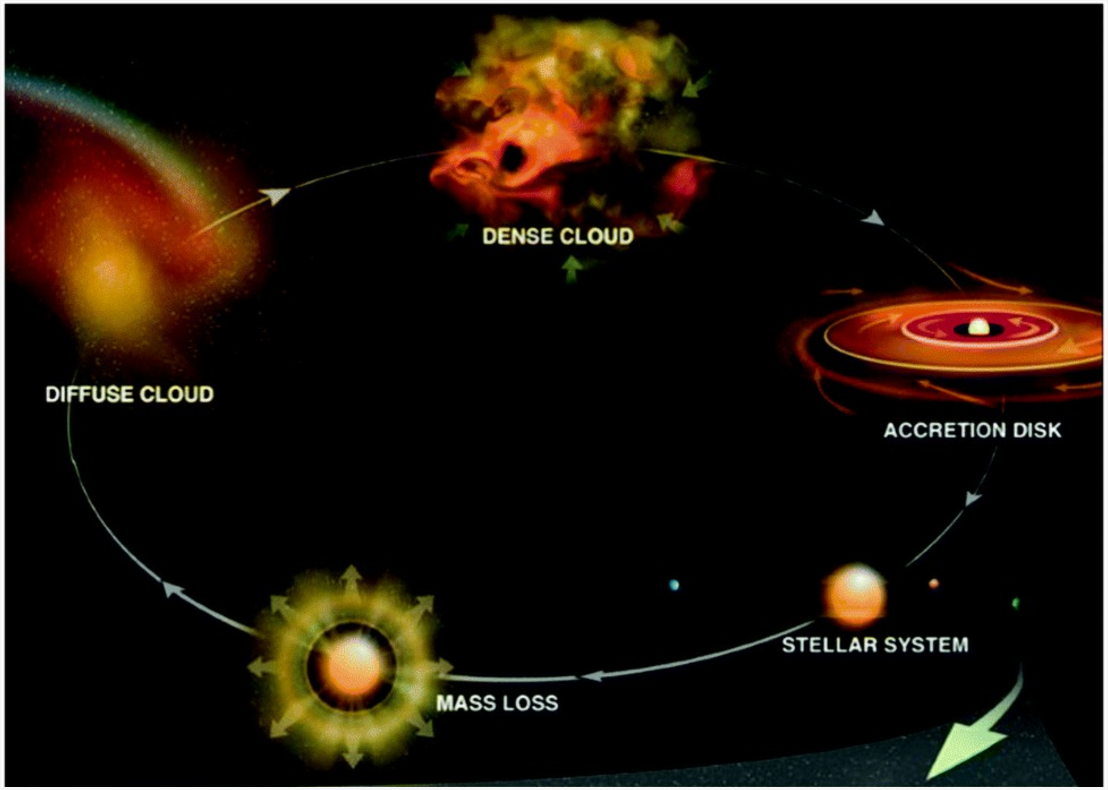
   Universe is transparent, but no stars yet.

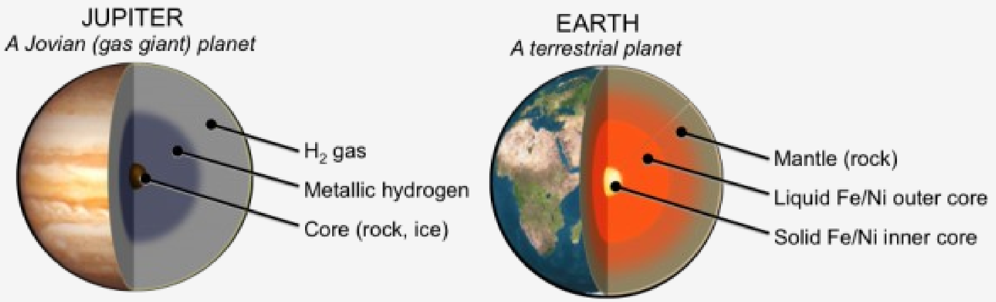
4. **Star and galaxy formation and evolution → 400x10⁶ yrs**

5. **Star cycle begins**

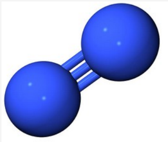
   Universe gets ever more rich on heavier elements

Rocky planets?

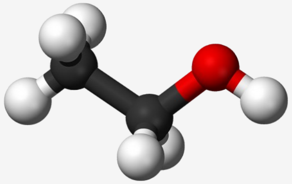

DENSE CLOUD
DIFFUSE CLOUD
ACCRETION DISK
STELLAR SYSTEM
MASS LOSS


JUPITER
A Jovian (gas giant) planet
H_2 gas
Metallic hydrogen
Core (rock, ice)
EARTH
A terrestrial planet
Mantle (rock)
Liquid Fe/Ni outer core
Solid Fe/Ni inner core

Where are the molecules in the night sky?



N_2 dissociation 9.7eV



Ethanol combustion: 14eV

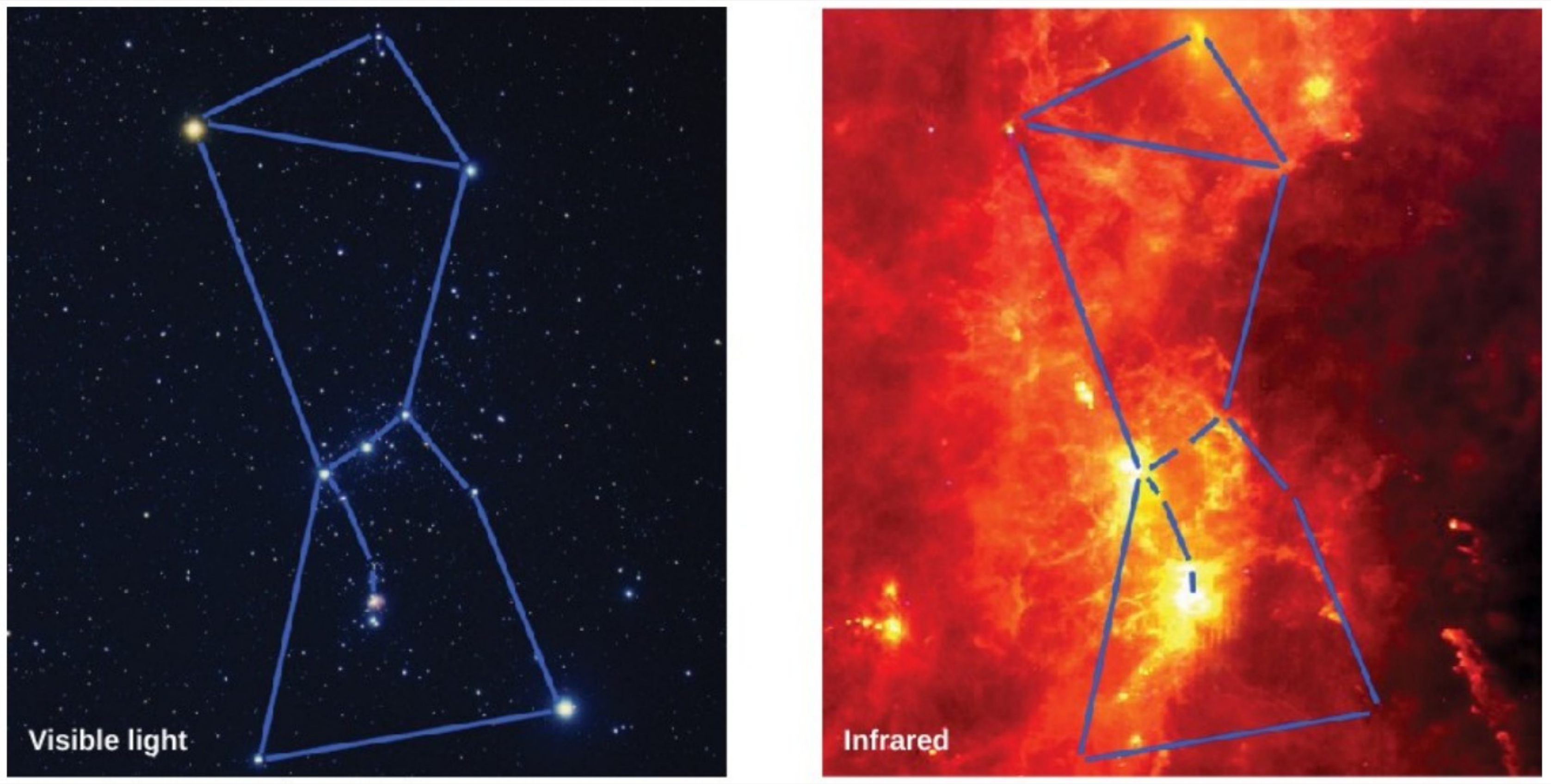
Ionization of **any element**: < 25eV

Stars: Mega eV!

Space is not empty!

A galaxy as the Milky Way has enough gas and dust to make **billions of stars** like the Sun!

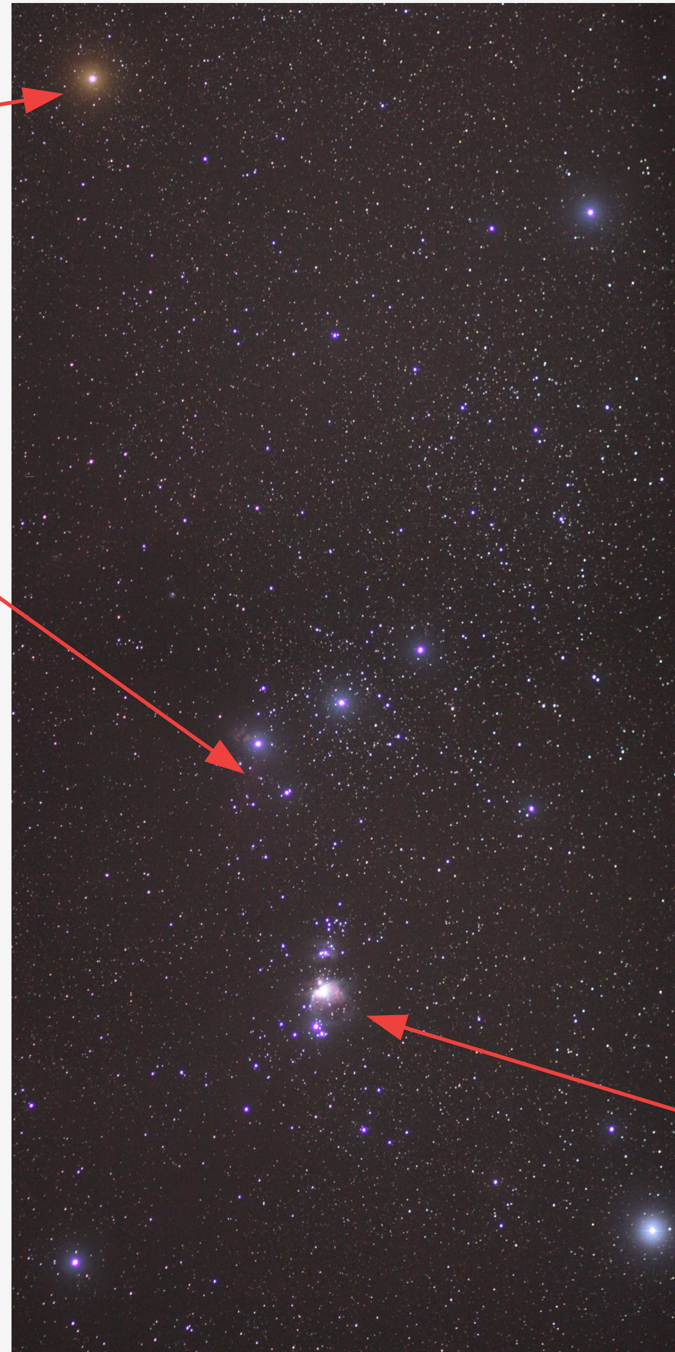
Orion Molecular Cloud Complex



Some stars cannot even be seen!

The interstellar medium

Betelgeuse



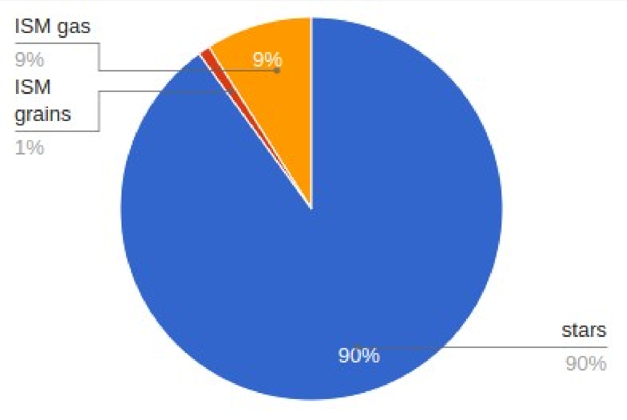
Orion molecular cloud:
200000 times the mass of the Sun

Horsehead Nebula

Orion Nebula:
closest region of **massive star formation** to Earth.

Facts about the ISM

Milky way's mass:



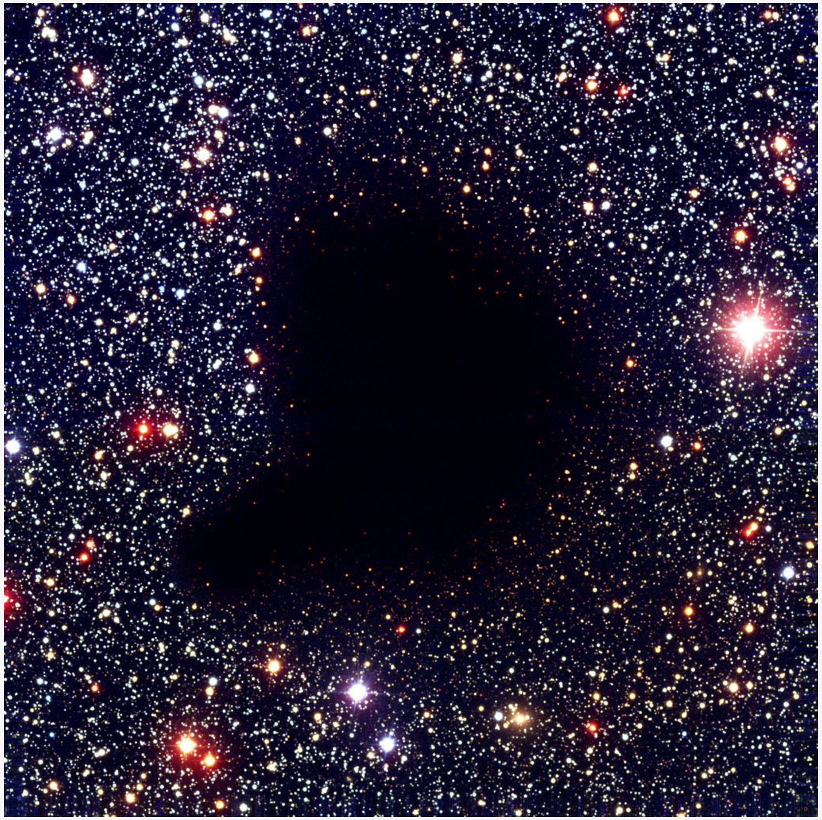
average number densities:
~ 1 H atom/cm^3
~ 10^{-11} grains/cm^3

Comparing:

Earth, 0°C, 1 atm: 2.7×10^{19} molecules/cm^3

ISM pressure is ~4.0×10^{-22} atm beyond any ultrahigh vacuum achieved on earth so far

B68 Molecular cloud



400 light-years: so close that not a single star can be seen behind

The regions of the interstellar medium

$\sim 10^{16}$ m

Matter is not uniformly distributed

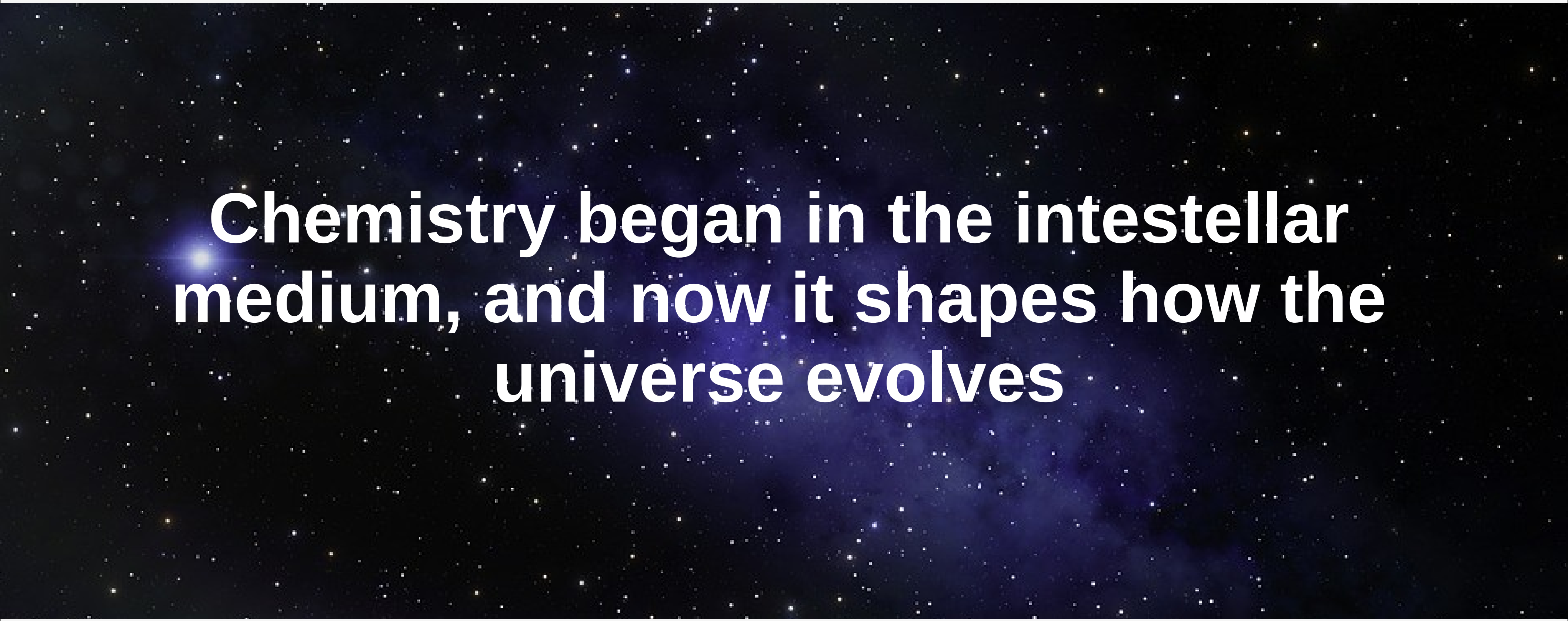
Diffuse medium
N~ 10 cm^3
T~ 50 K

Dense molecular cloud
N~ 10^3 cm^3
T~ 10 K

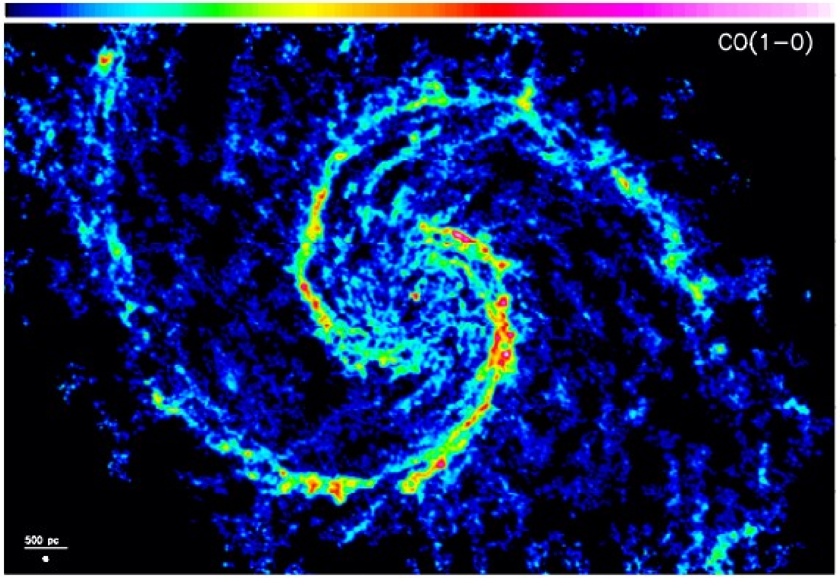
Earth (sea level)
N~ 10^{19} cm^3
T~ 300 K

Hot-Core
(star forming region)
N~ 10^7 cm^3
T~ 100-300 K

Grains lose water, collisions dominate


Chemistry began in the intestellar medium, and now it shapes how the universe evolves

100 years ago:
"It is difficult to admit the existence of molecules in interestellar space, because once a molecule becomes dissociated, there seems no chance of the atoms joining up again ."
Sir Arthur Eddington, 1926
(1st to speculate nuclear reactions in stars)



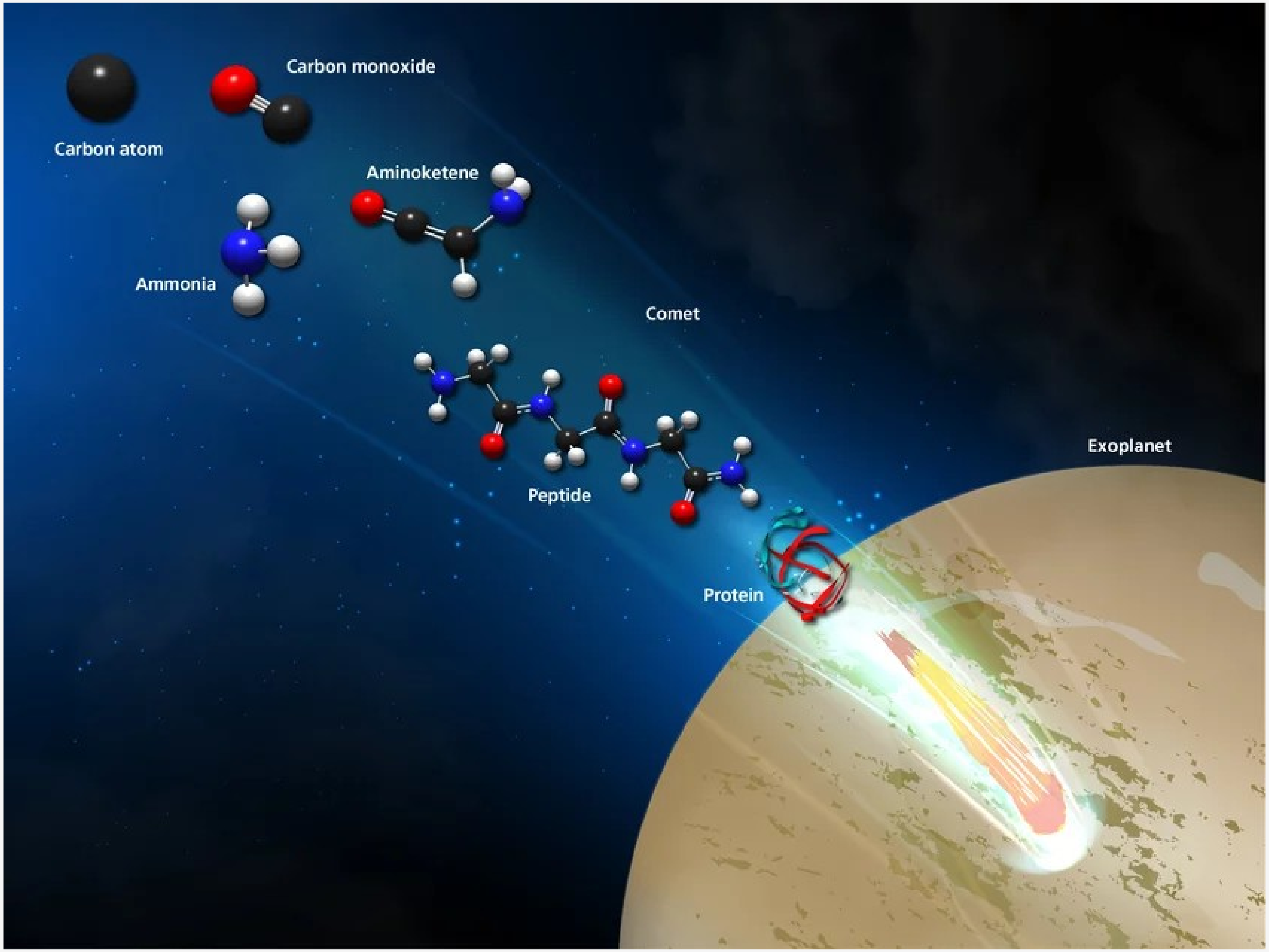
M51 galaxy as seen by the CO J = 1 − 0 line
ApJ, 779, 42 (2013)

Past 20 years
(specially after IR and submillimeter window were opened)

Molecules are now :
- thermometers/barometers in space
- relevant in the evolution of galaxies
- probe the dynamics of interesting objects

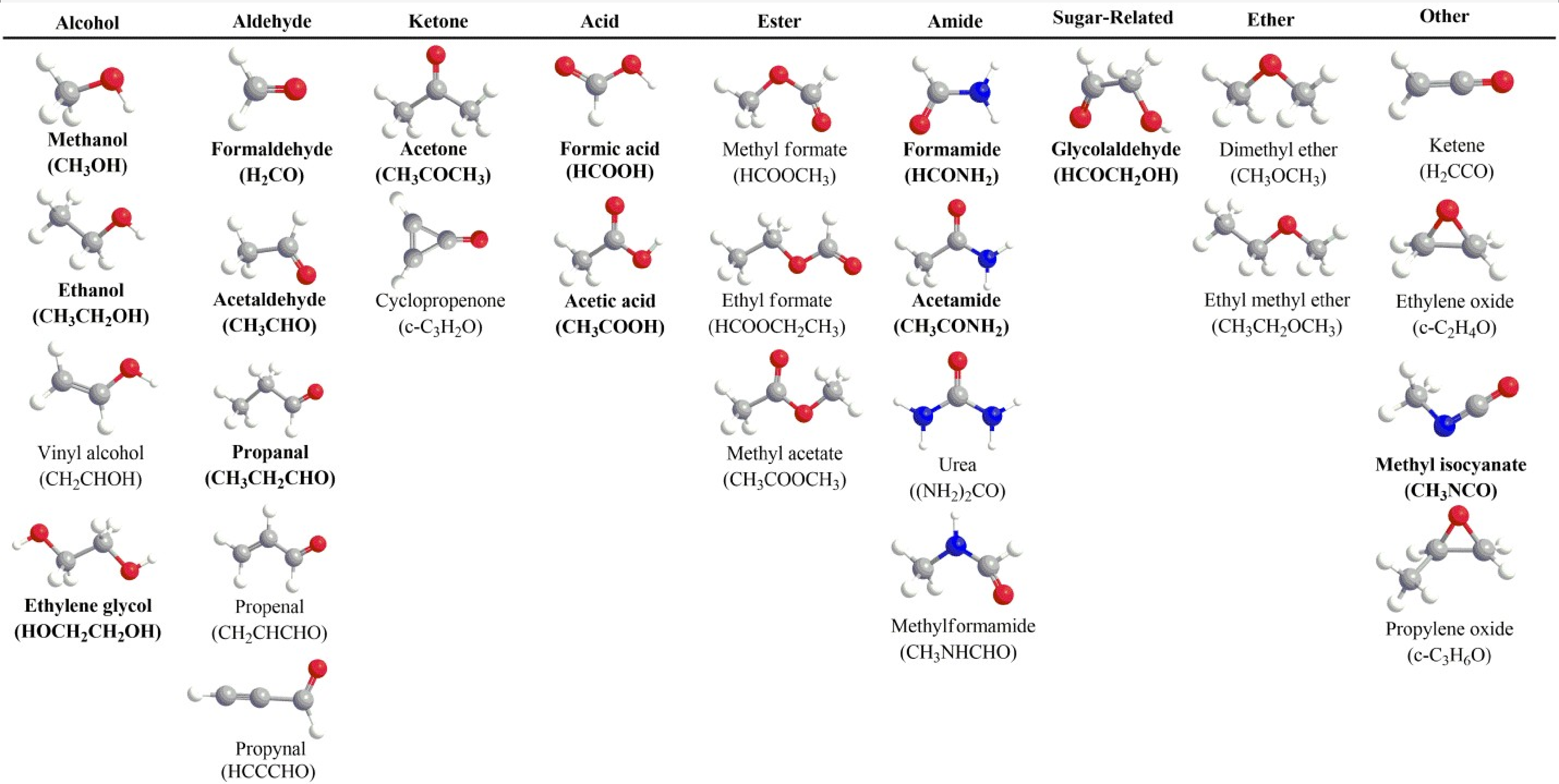
Regions of planet formation are rich in organic molecules!
Prebiotic roots?

Molecular Astrophysics
A.G.G.M. Tielesns
Cambridge University Press, **2021**



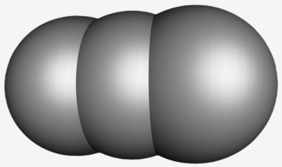
Ex.: Asteroide Ryugu:
Em 2023, uracila (base nitro. RNA) e vitaminina B3 foram detectadas!
Coletada direto do asteroide, e não na terra!!!

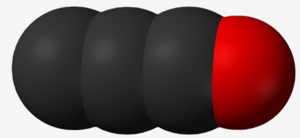
Detected Molecules

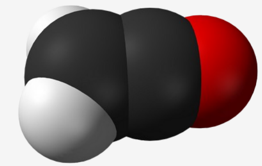


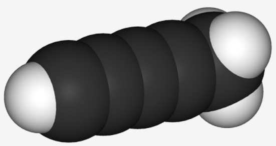
Cologne Database for Molecular Spectroscopy
CDMS – molecules in Space
https://cdms.astro.uni-koeln.de/classic/molecules

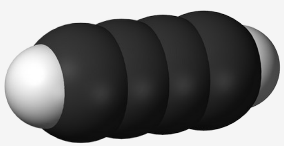
Detected Molecules

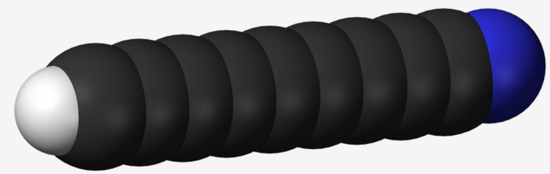


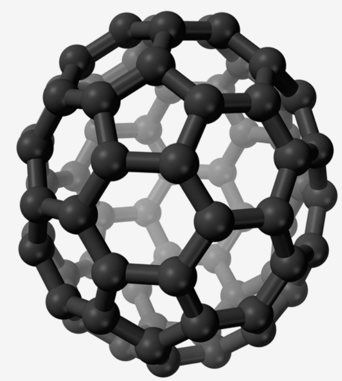












$H-C\equiv C-C\equiv N$

$H-C\equiv C-C\equiv C-C\equiv C\bullet$

$H-C\equiv C-C\equiv C-C\equiv C-C\equiv C\bullet$

Cologne Database for Molecular Spectroscopy
CDMS – molecules in Space
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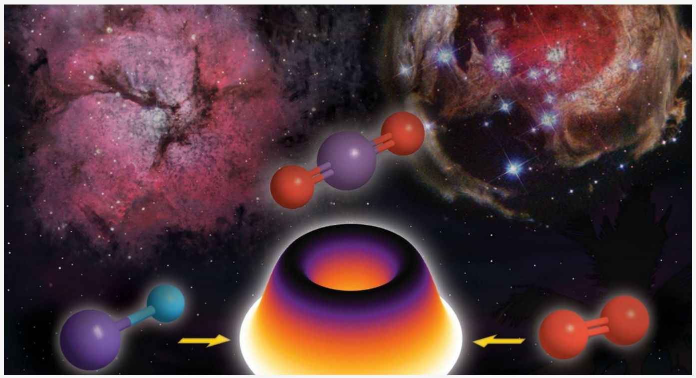
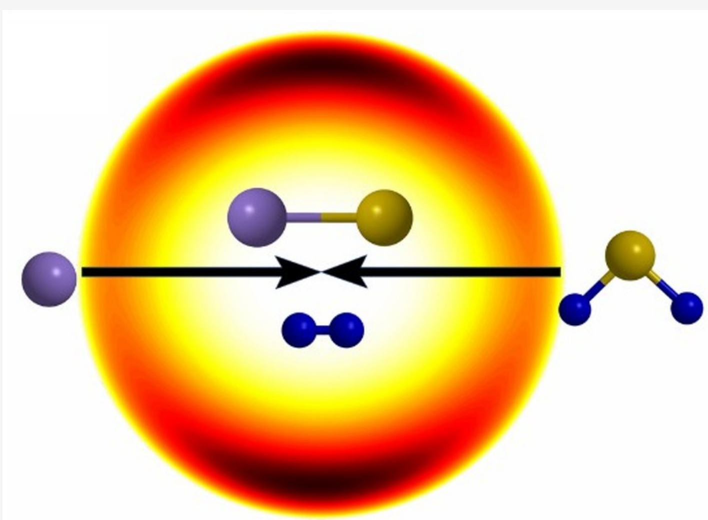
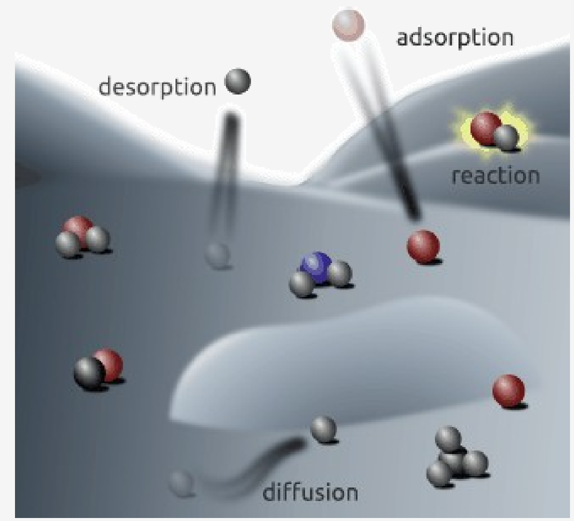
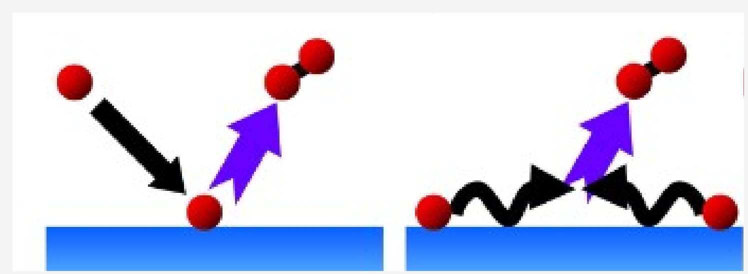
Gas phase reactions





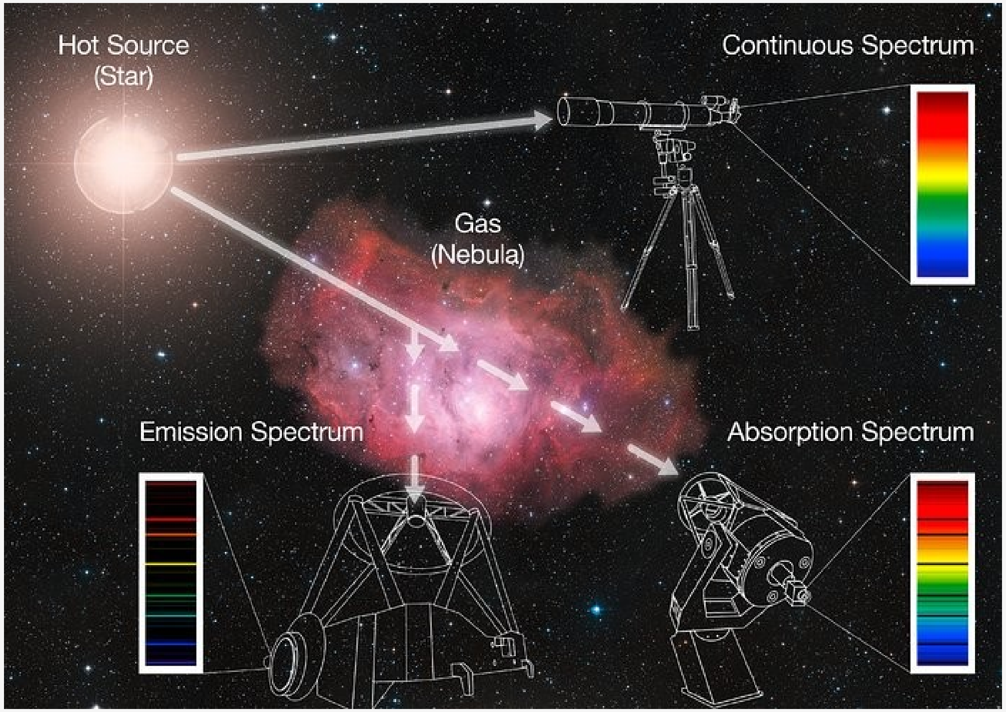
Reactions on grains





How can we understand them?

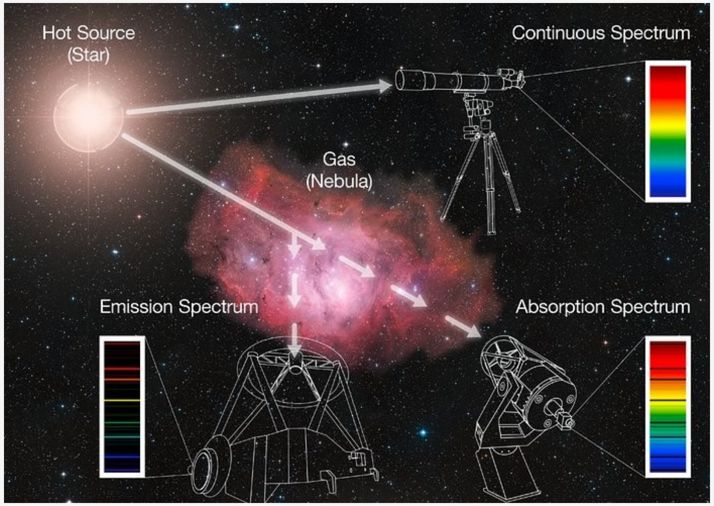
- Observations
- Experiments
- Quantum chemistry



ALMA
Atacama Large Millimeter/submillimeter Array

FAST
Five-hundred-meter Aperture Spherical Radio Telescope

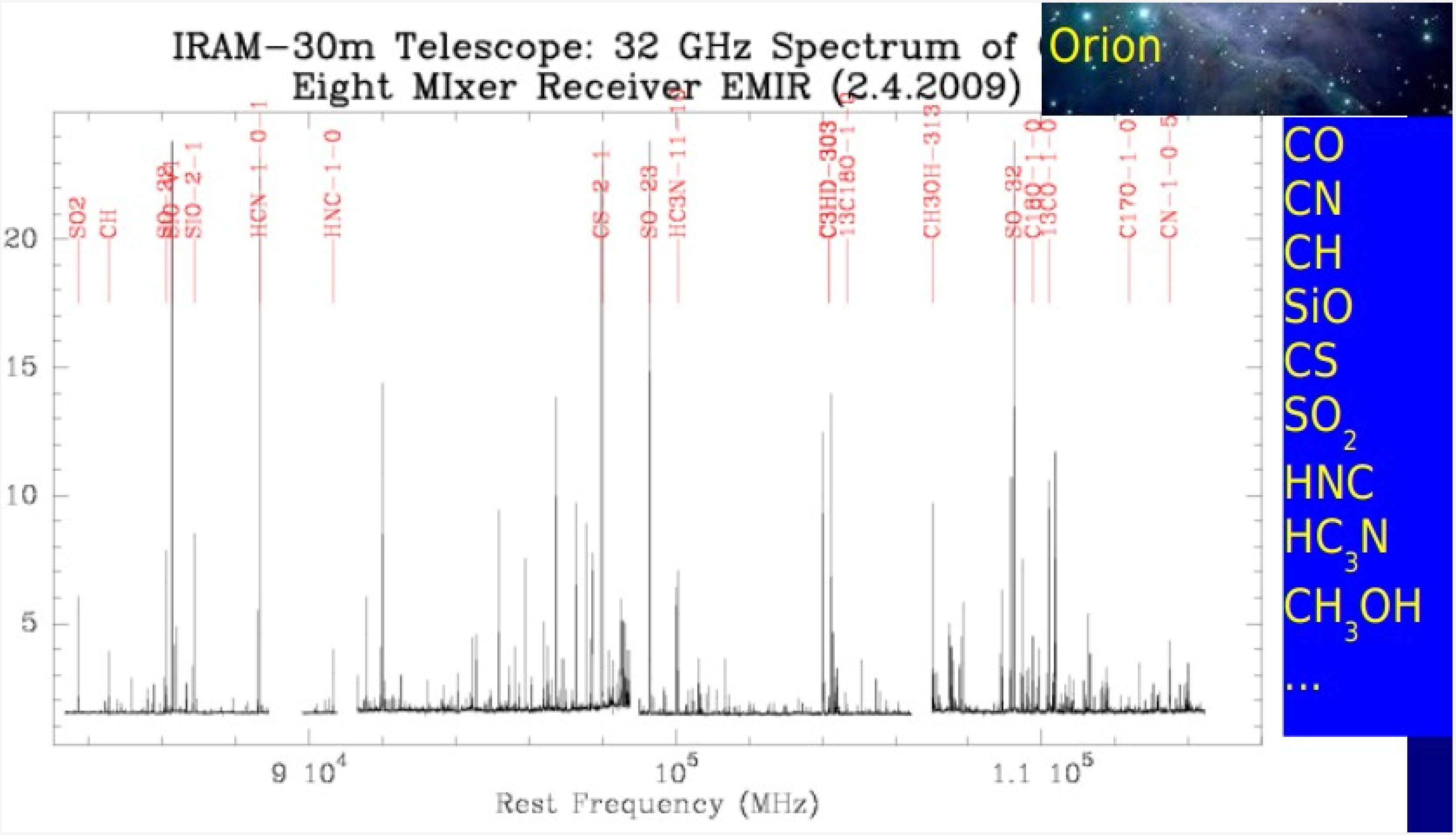
Observations



ALMA
Atacama Large Millimeter/submillimeter Array

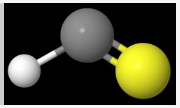
VLA
Very Large Array, NM, USA

FAST
Five-hundred-meter Aperture Spherical Radio Telescope



- CO
- CN
- CH
- SiO
- CS
- SO_2
- HNC
- HC_3N
- CH_3OH
- ...

Example: HCS



UMIST RATE12
astrochemistry.net

Formation

1	$H_2CS^+ + e^- \rightarrow HCS + H$
2	$SO^+ + C_2H_2 \rightarrow HCO^+ + HCS$
3	$SO^+ + C_2H_4 \rightarrow H_3CO^+ + HCS$
4	$SO^+ + CH_2CCH_2 \rightarrow CH_3CO^+ + HCS$
5	$CH_2 + S \rightarrow HCS + H$

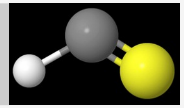
Destruction

1	$HCS + CRPHOT \rightarrow HCS^+ + e^-$
2	$H^+ + HCS \rightarrow CS^+ + H_2$
3	$H_3^+ + HCS \rightarrow H_2CS^+ + H_2$
4	$He^+ + HCS \rightarrow CS^+ + He + H$
5	$He^+ + HCS \rightarrow CS + He + H^+$
6	$H + HCS \rightarrow H_2 + CS$
7	$N + HCS \rightarrow S + HCN$
8	$O + HCS \rightarrow HS + CO$
9	$O + HCS \rightarrow OCS + H$

$$\frac{d[\mathrm{HCS}]}{dt} = k_1^f[\mathrm{CH_2}][\mathrm{S}] + \cdots - k_1^d[\mathrm{O}][\mathrm{HCS}] - \cdots$$

Initial conditions:
- elemental abundances
- temperature
- density

Example: HCS



UMIST RATE12
astrochemistry.net

Initial conditions:
- elemental abundances
- temperature
- density

If we have the rate coefficients:

Formation

1	$H_2CS^+ + e^- \rightarrow HCS + H$
2	$SO^+ + C_2H_2 \rightarrow HCO^+ + HCS$
3	$SO^+ + C_2H_4 \rightarrow H_3CO^+ + HCS$
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Destruction

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4	$He^+ + HCS \rightarrow CS^+ + He + H$
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6	$H + HCS \rightarrow H_2 + CS$
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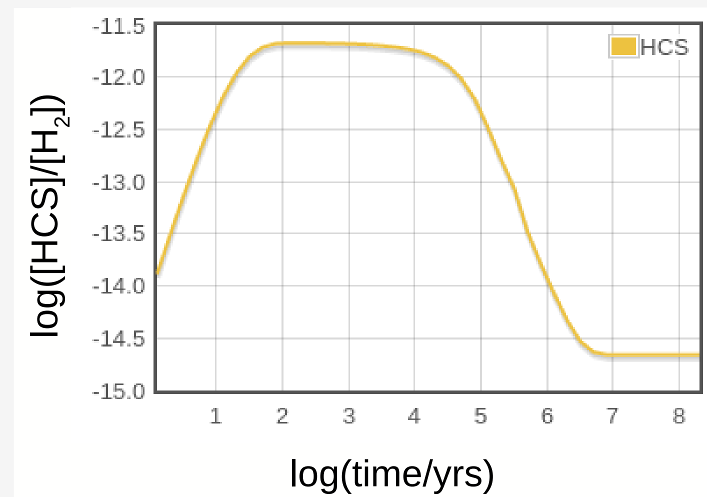
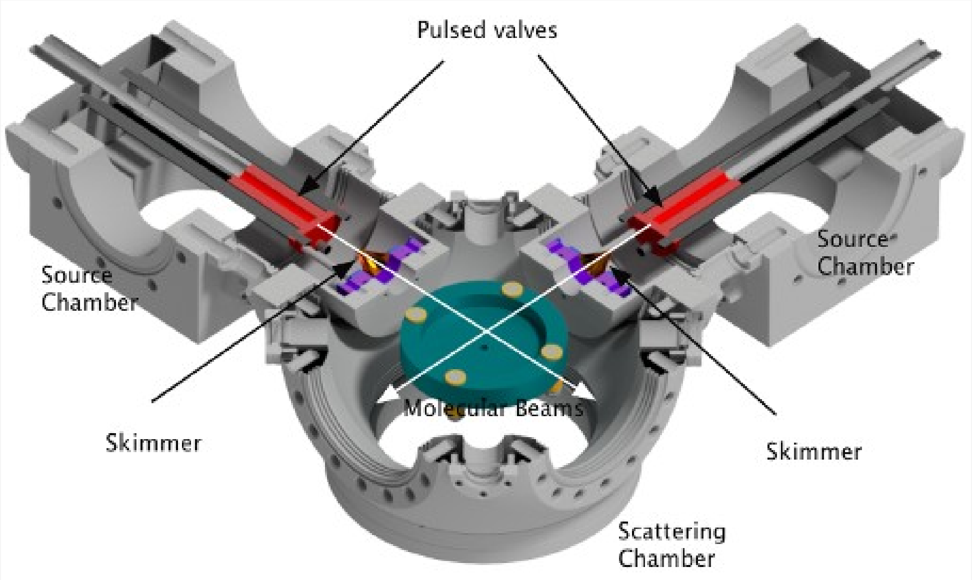
$$\frac{d[\mathrm{HCS}]}{dt} = k_1^f[\mathrm{CH_2}][\mathrm{S}] + \cdots - k_1^d[\mathrm{O}][\mathrm{HCS}] - \cdots$$

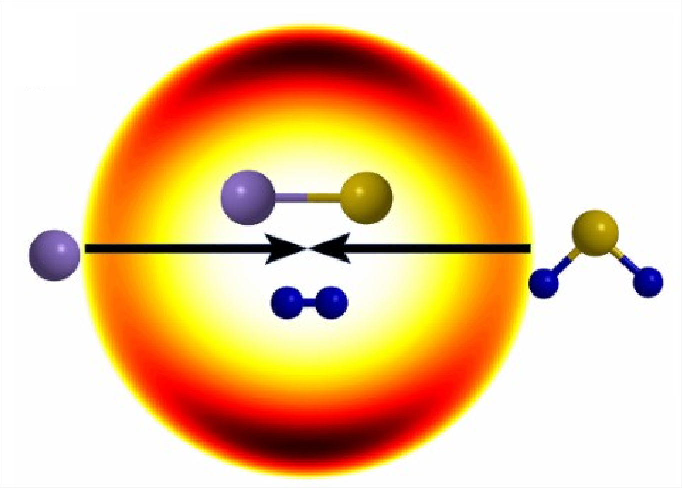
$$\frac{d[\mathrm{CH_2}]}{dt} = \sum_{AB} k^f_{AB}[A][B] - \sum_{CD} k^d_{CD}[C][D]$$



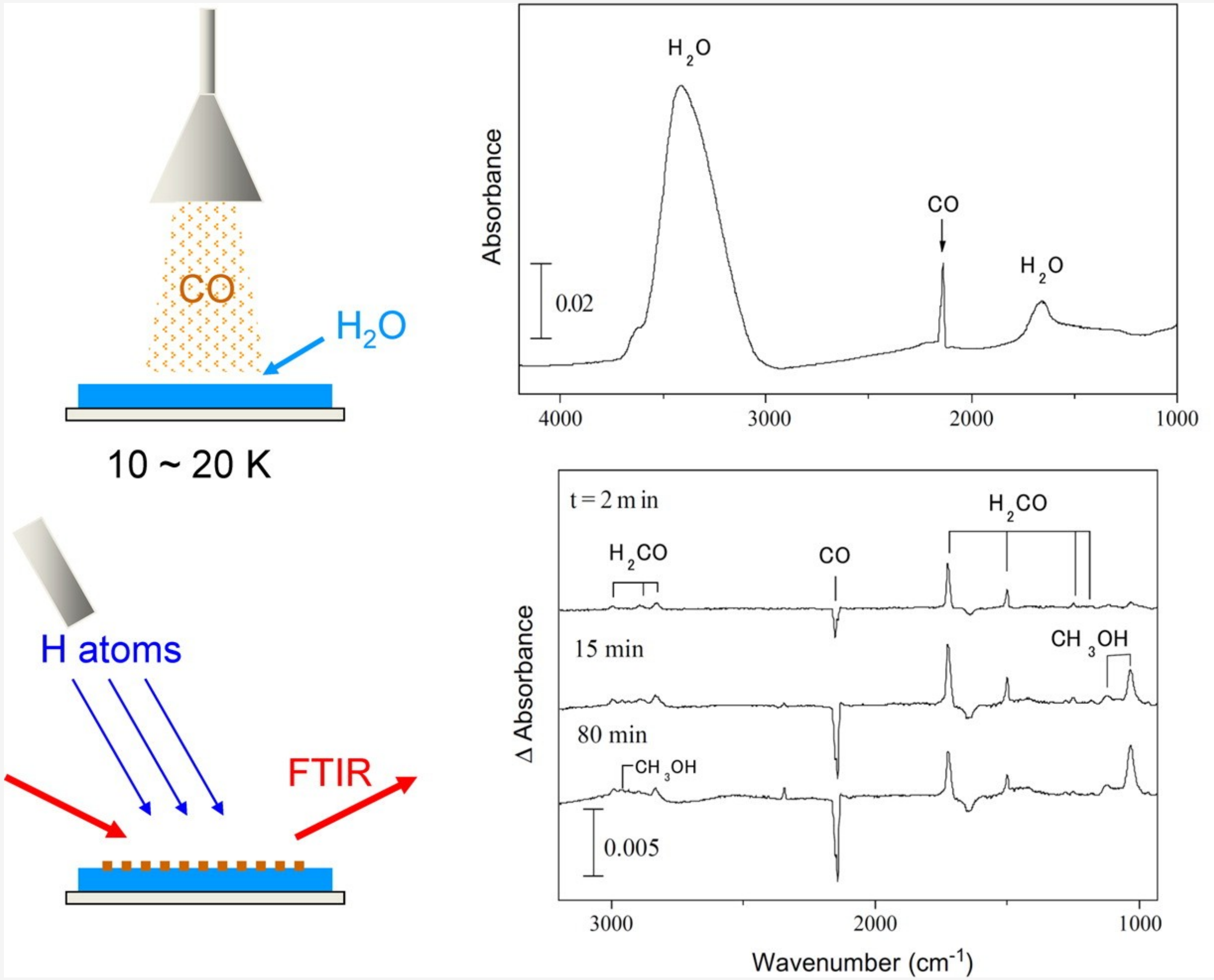
(Should also include, adsorption, photodissociation...)

Simulating gas-phase reactions





Simulating reactions on grains



$CO + H \rightarrow HCO$

$HCO + H \rightarrow H_2CO$

$H_2CO + H \rightarrow H_2COH$

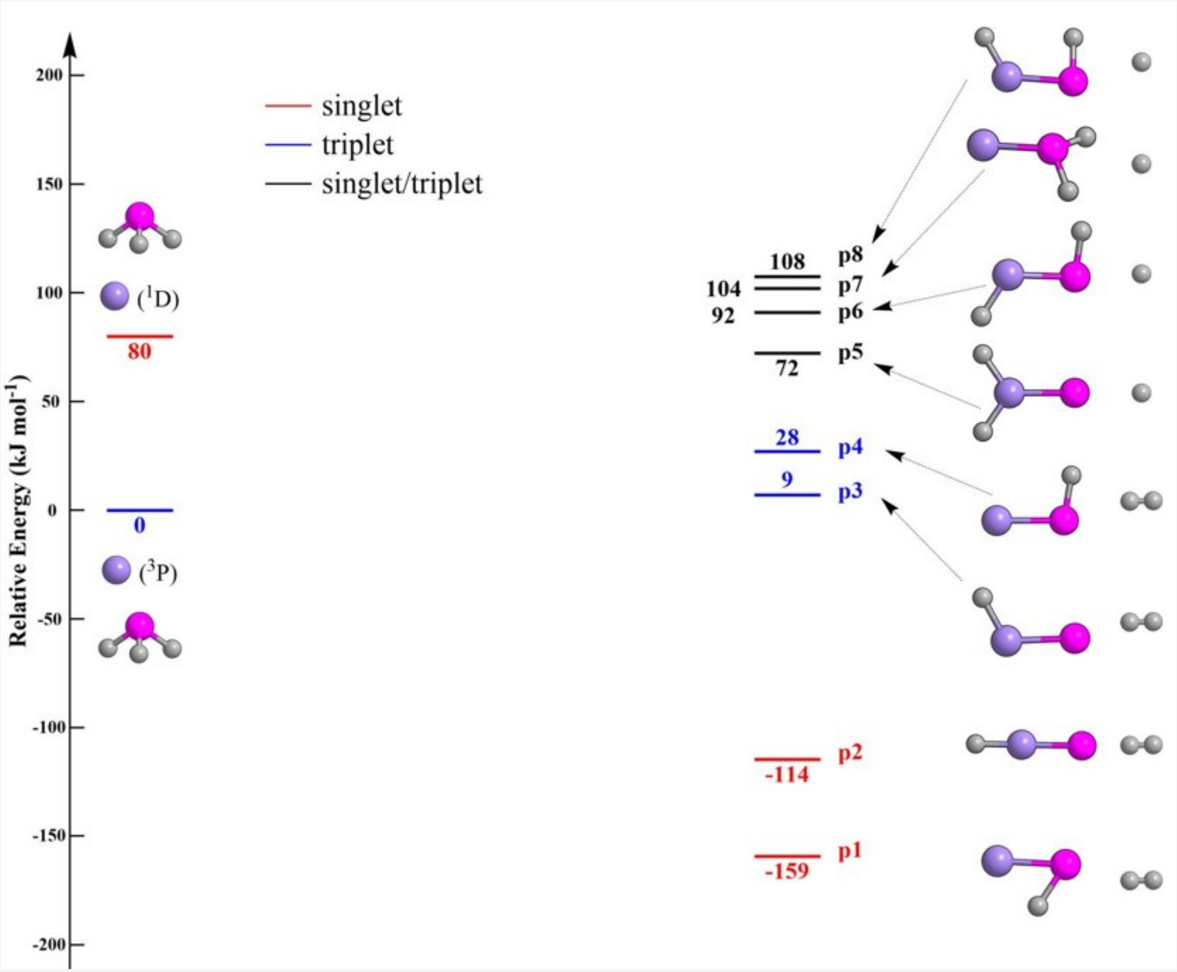
$H_2COH + H \rightarrow CH_3OH$

Lab: 10^{-13} atm, 15 K

ISM: 4. 0×10^{-22} atm

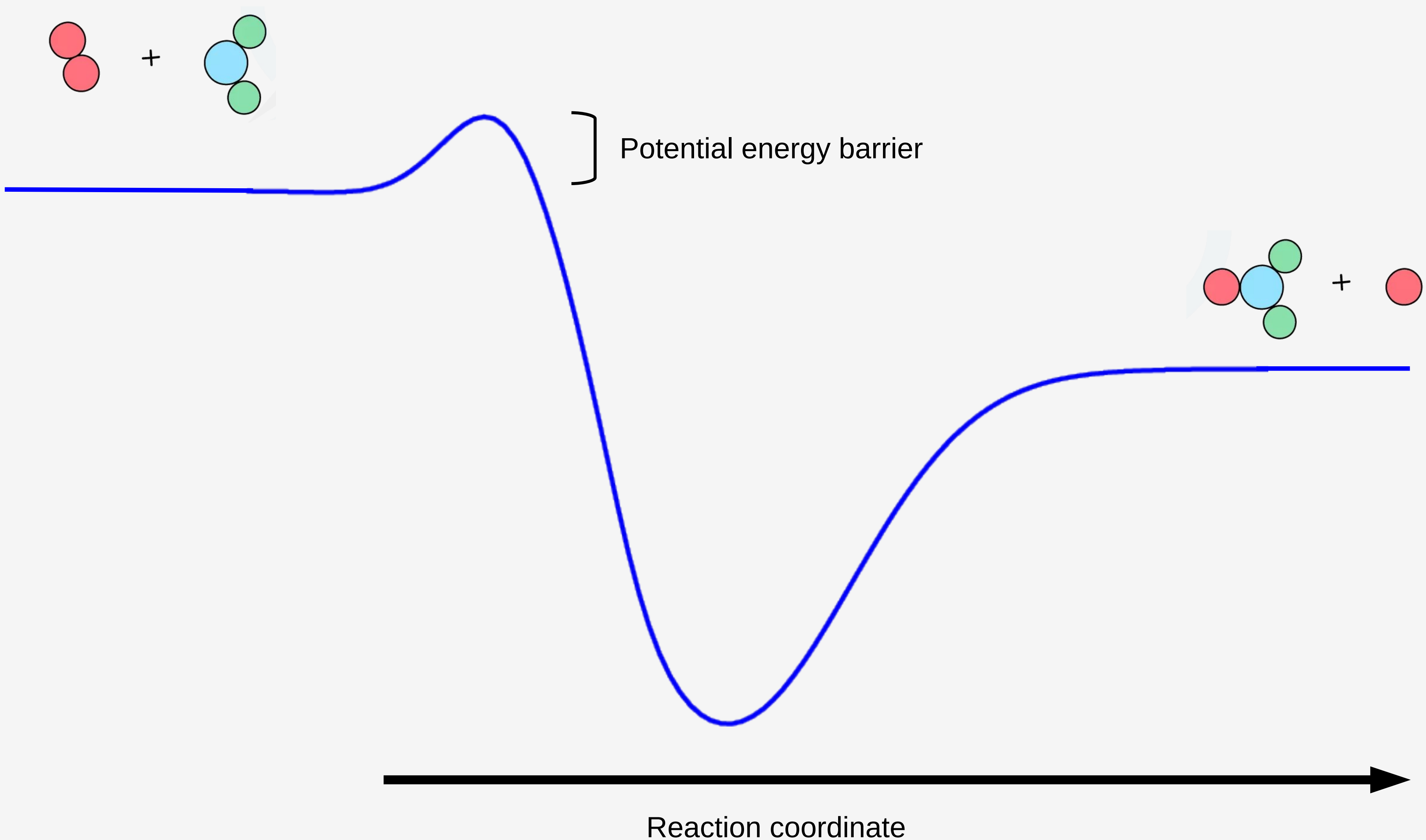
Chem. Rev. **113**, 8783 (2013)

What will happen in Si+PH_3 collisions?

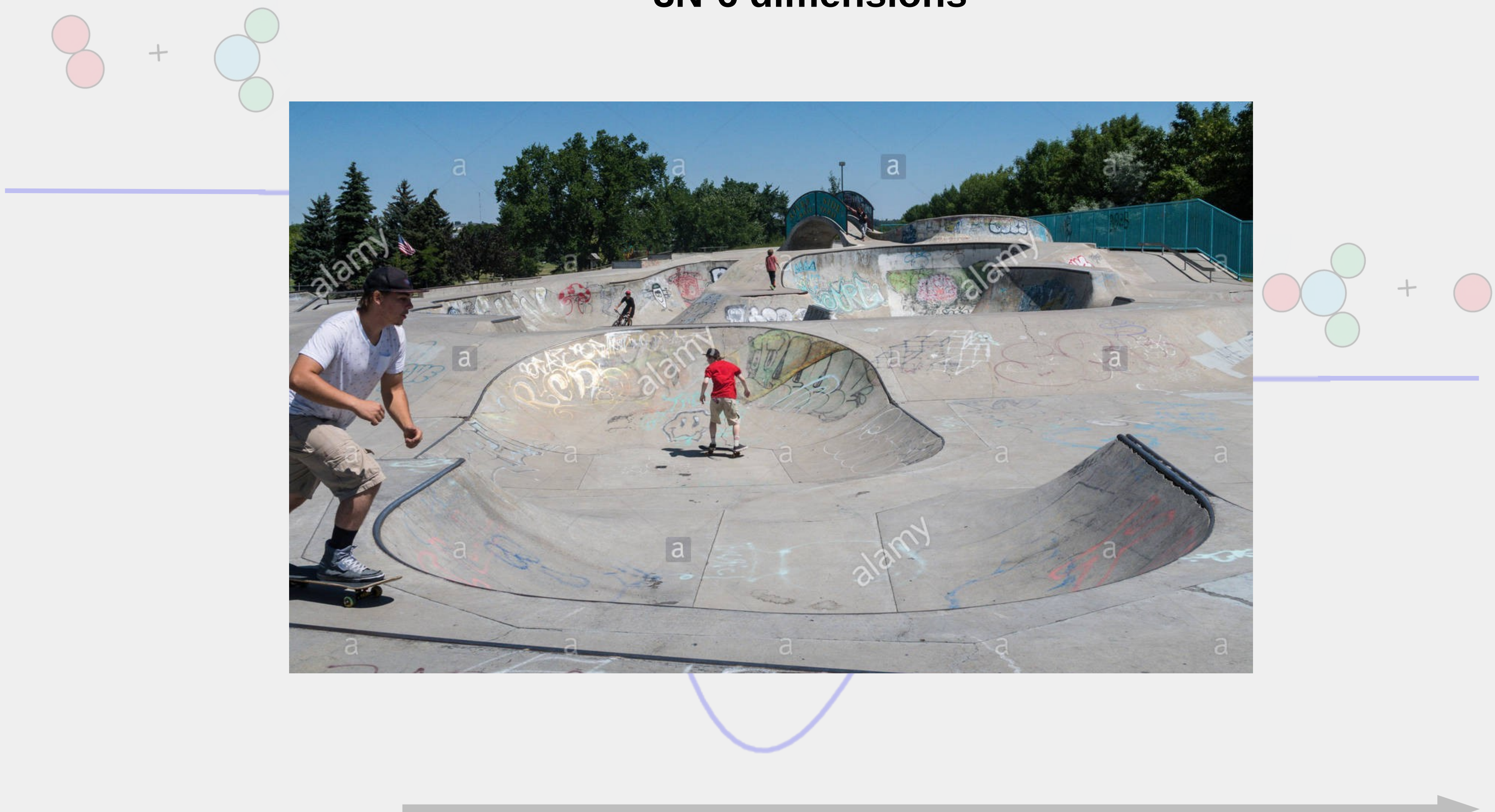


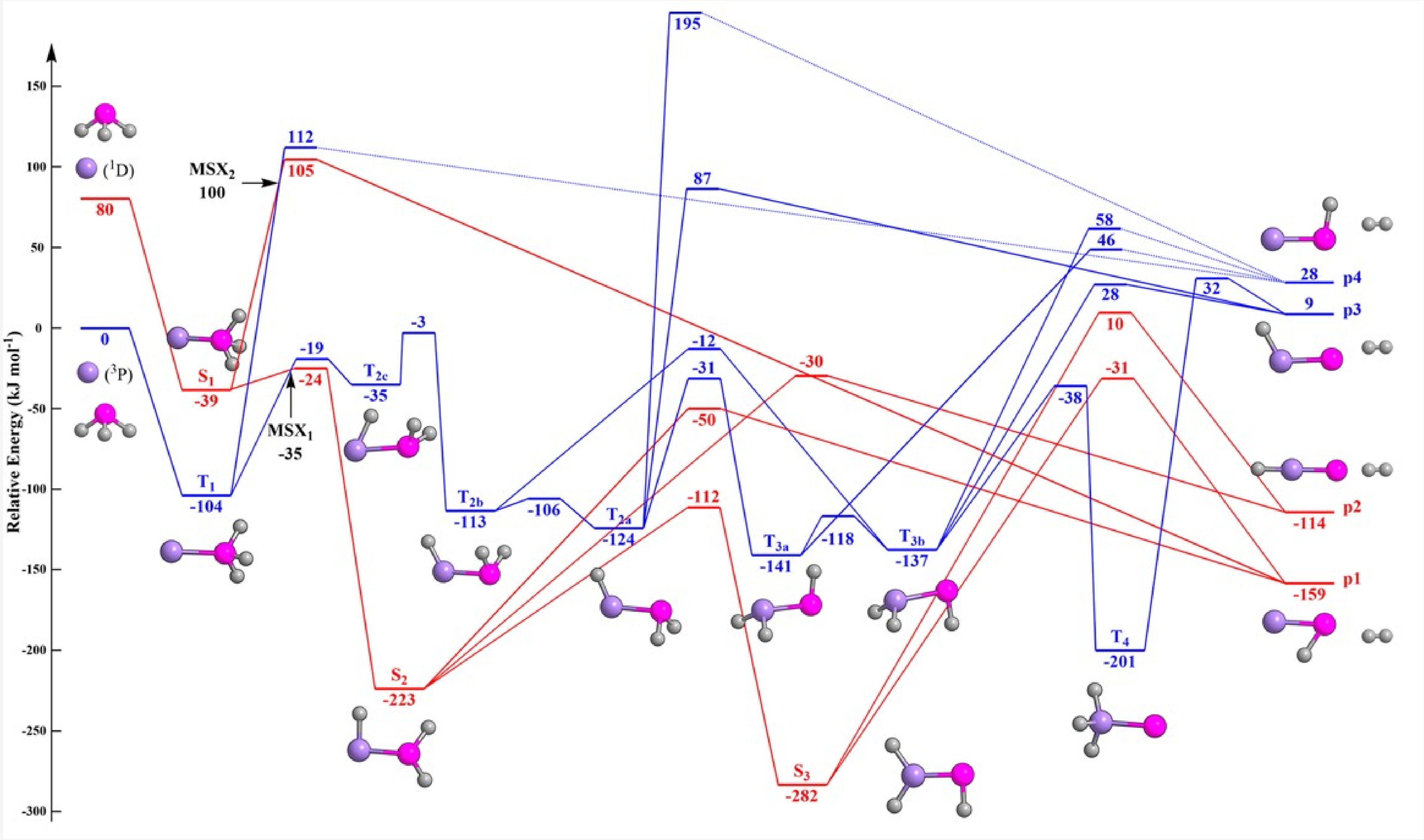
CCSD(T)-F12/aug-cc-pV(T+d)Z // M06-2X/cc-pV(T+d)Z

J. Phys. Chem. Lett. **12**, 2489 (2021)


+
Potential energy barrier
+
Reaction coordinate

3N-6 dimensions





J. Phys. Chem. Lett. **12**, 2489 (2021)

Recent work in our group

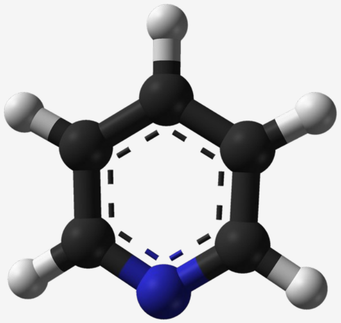
Reactants	Main product	Reference
C/C_2+NH_3 $C_4H_3+H_2CN$ // $C_3H_3+H_2C_2N$	isoquinoline	Nat. Astron. **8**, 856 (2024)
$H_2CO+HCO$ @ice	$HOCH_2CHO$	MNRAS **519**, 2518 (2023)
N+PH / P+NH	PN	PASA 40, e011 (2023)
N+PN	N_2	MNRAS **518**, 5996 (2023)
$CN+SiH_4$	SiH3CN	JACS **144**, 8649 (2022)
$Si+SO_2$	SiO+SO	MNRAS **515**, 369 (2022)
$P+O_2$	PO	J. Mol. Model **28**, 259 (2022)
O+PN & N+PO	NO	MNRAS **493**, 229 (2021)
Si+SH	SiS	Astrophys. J. **920,** 37 (2021)
$Si+PH_3$	HPSi	J. Phys. Chem. Lett. **12**, 2489 (2021)
$Si+H_2S$	SiS	Sci. Adv. **7**, eabg7003 (2021)
$SiH+H_2S$	HSiS	Phys. Chem. Chem. Phys., **23**, 13647 (2021)
$SiH+PH_3$	H_2SiP	Phys. Chem. Chem. Phys., ***23***, 18506 (2021)
$Si+CH_3SH$	HSiS	J. Phys. Chem. Lett. **12**, 5979 (2021)
$Si+SH/SH_2$	SiS	MNRAS **493**, 299 (2020)
SiS+O	SiO	MNRAS **481**, 1858 (2018)

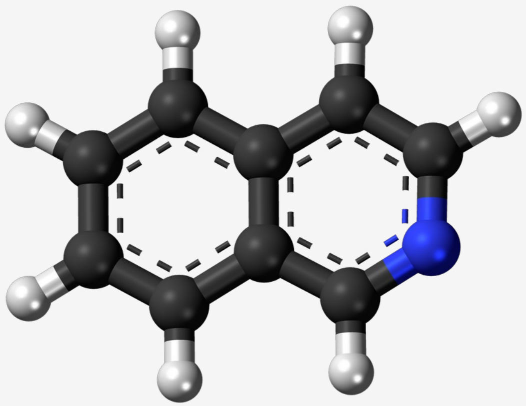
Collaborations

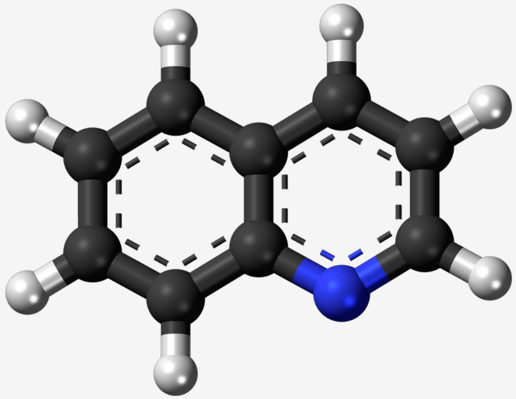
Astronomers:
- Valentine Wakelam (Univ. Bordeaux)
- Bertrand Lefloch (Univ. Grenoble)
- Edgar Mendoza (Univ. Huelva)


Experimentalist:
- Ralf Kaiser (Univ. of Hawaii)

Case 1:
Aromatic molecules containing nitrogen







Aromatic molecules containing nitrogen

nature astronomy

Article https://doi.org/10.1038/s41550-024-02267-y

Low-temperature formation of pyridine and (iso)quinoline via neutral–neutral reactions

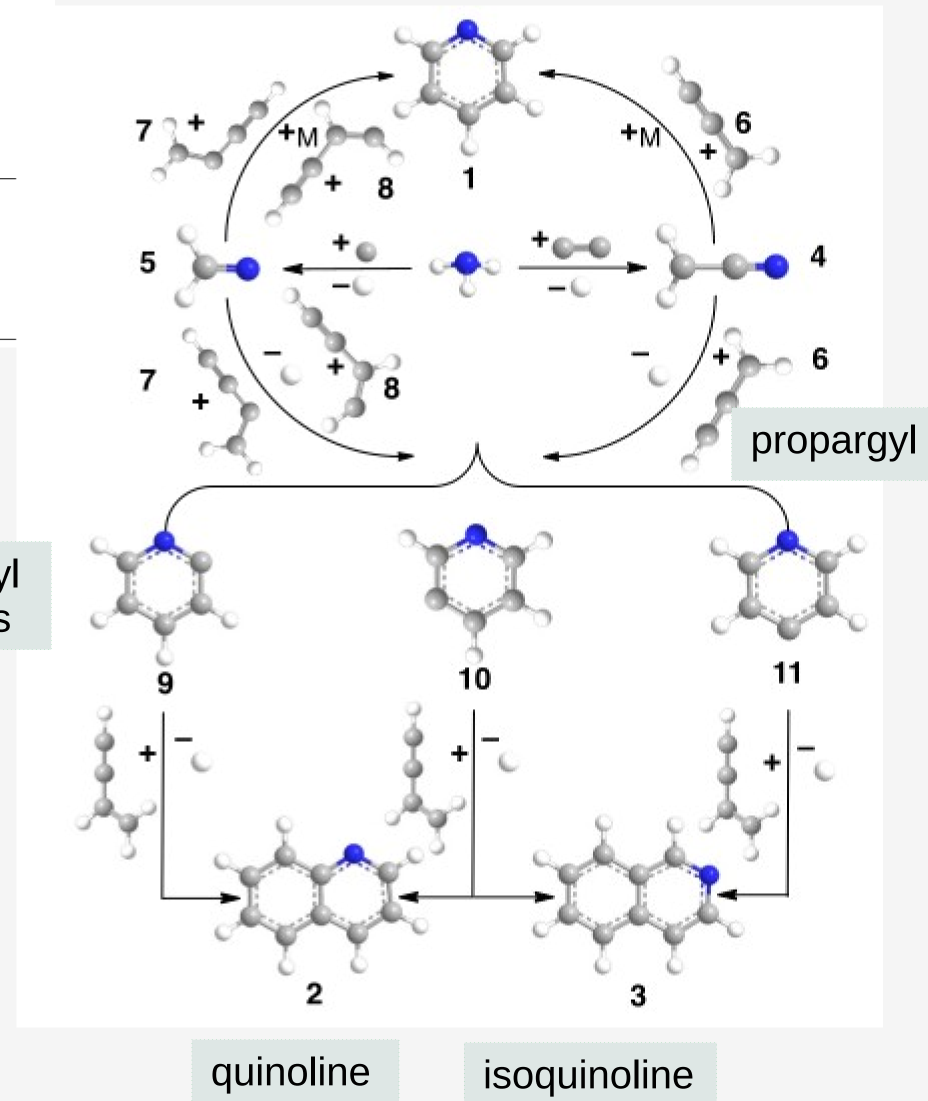
Received: 21 February 2023

Accepted: 9 April 2024

Published online: 13 May 2024

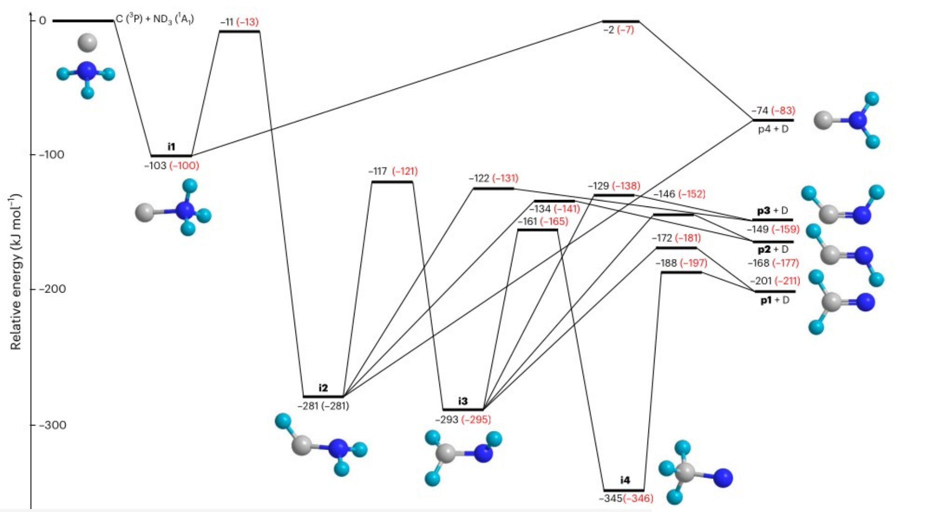
Check for updates

Zhenghai Yang[1], Chao He[1], Shane J. Goettl[1], Alexander M. Mebel[2], Paulo F. G. Velloso[3], Márcio O. Alves[3], Breno R. L. Galvão[3], Jean-Christophe Loison[4], Kevin M. Hickson[4], Michel Dobrijevic[5], Xiaohu Li[6,7] & Ralf I. Kaiser[1]



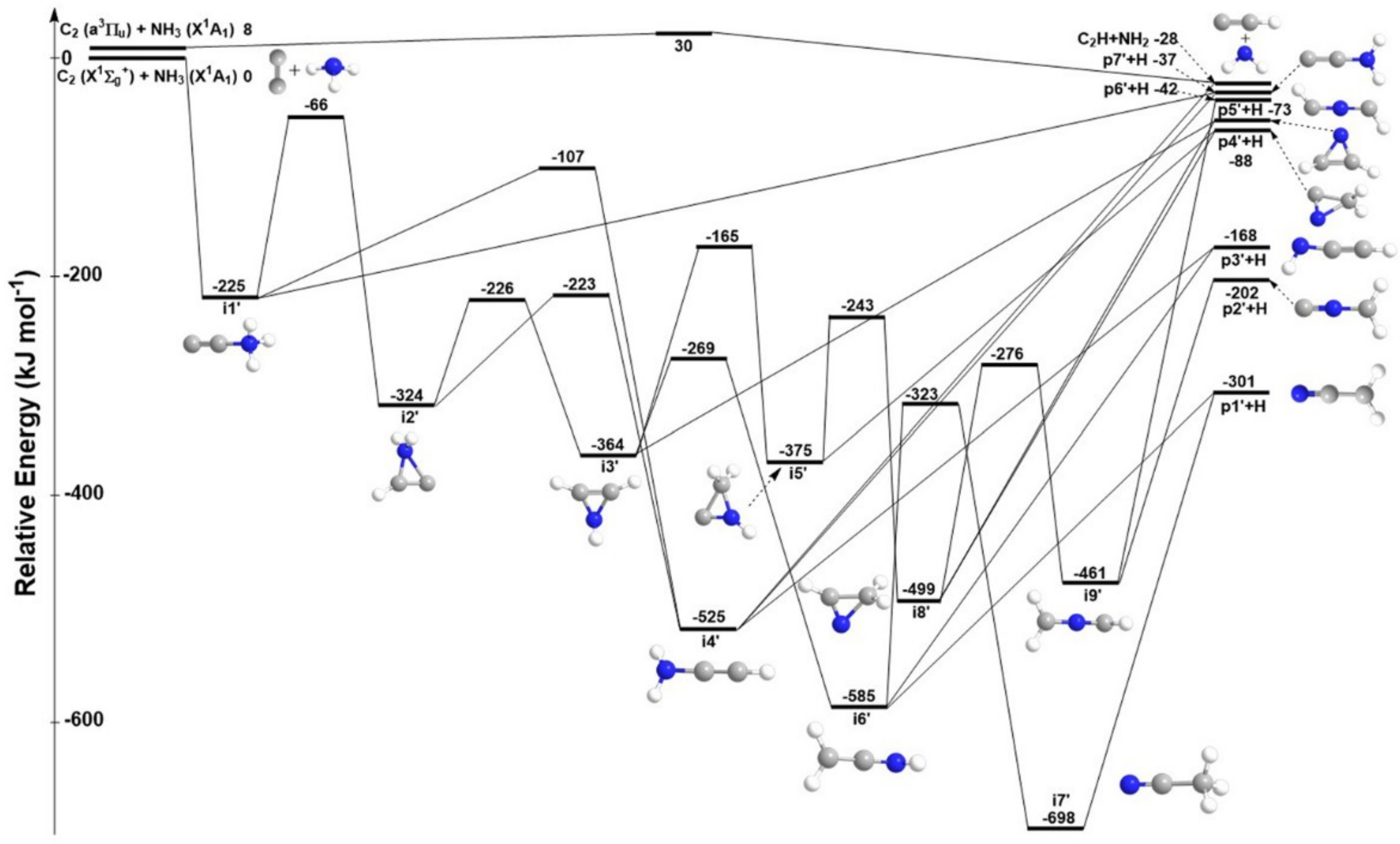
Potential route to nitrogenous bases (building blocks of DNA)

Formation of CH_2N and C_2H_2N



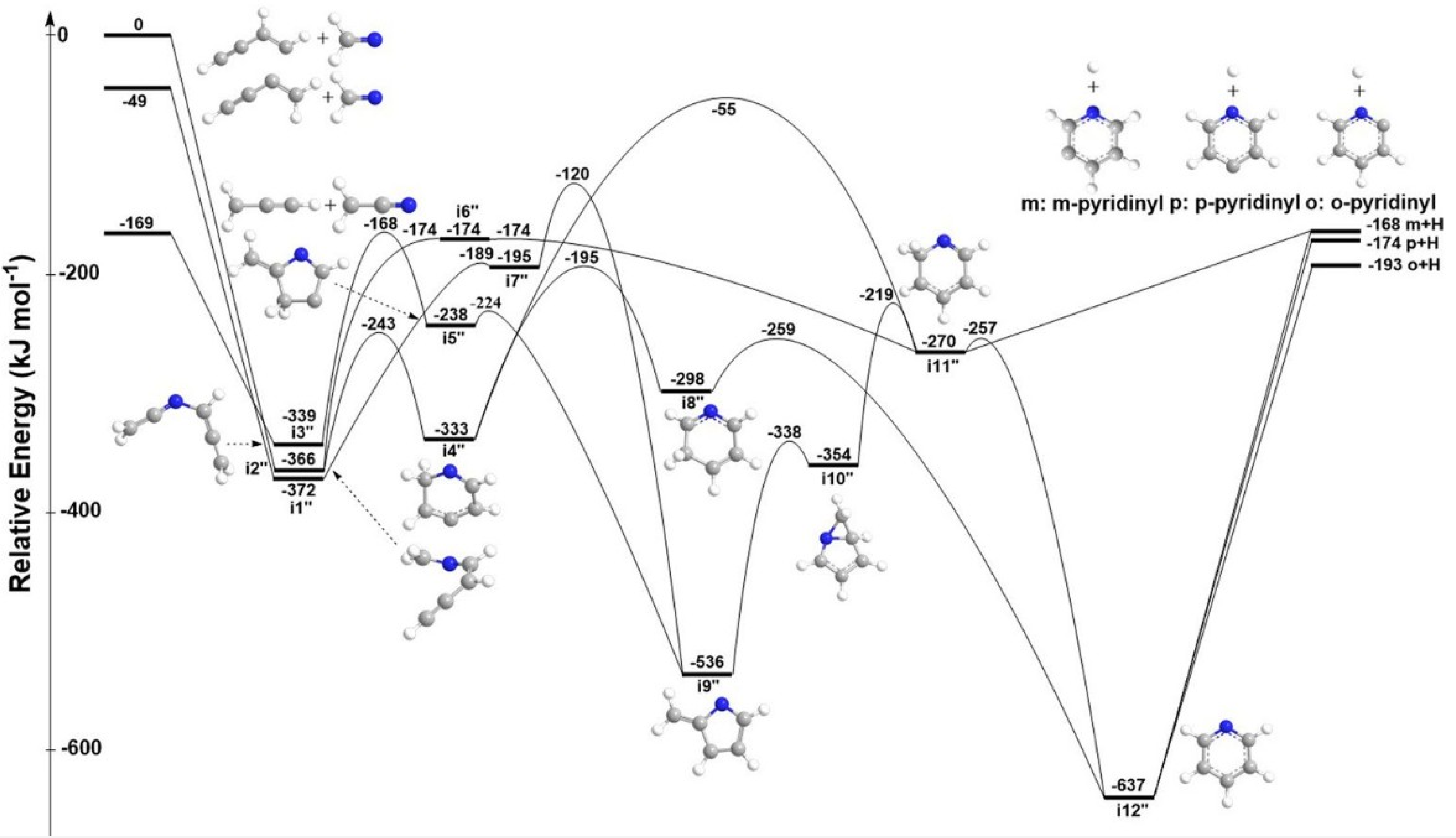
Experiment:
209 ± 26 kJ mol^{-1}

Calculations:
201 kJ mol^{-1}

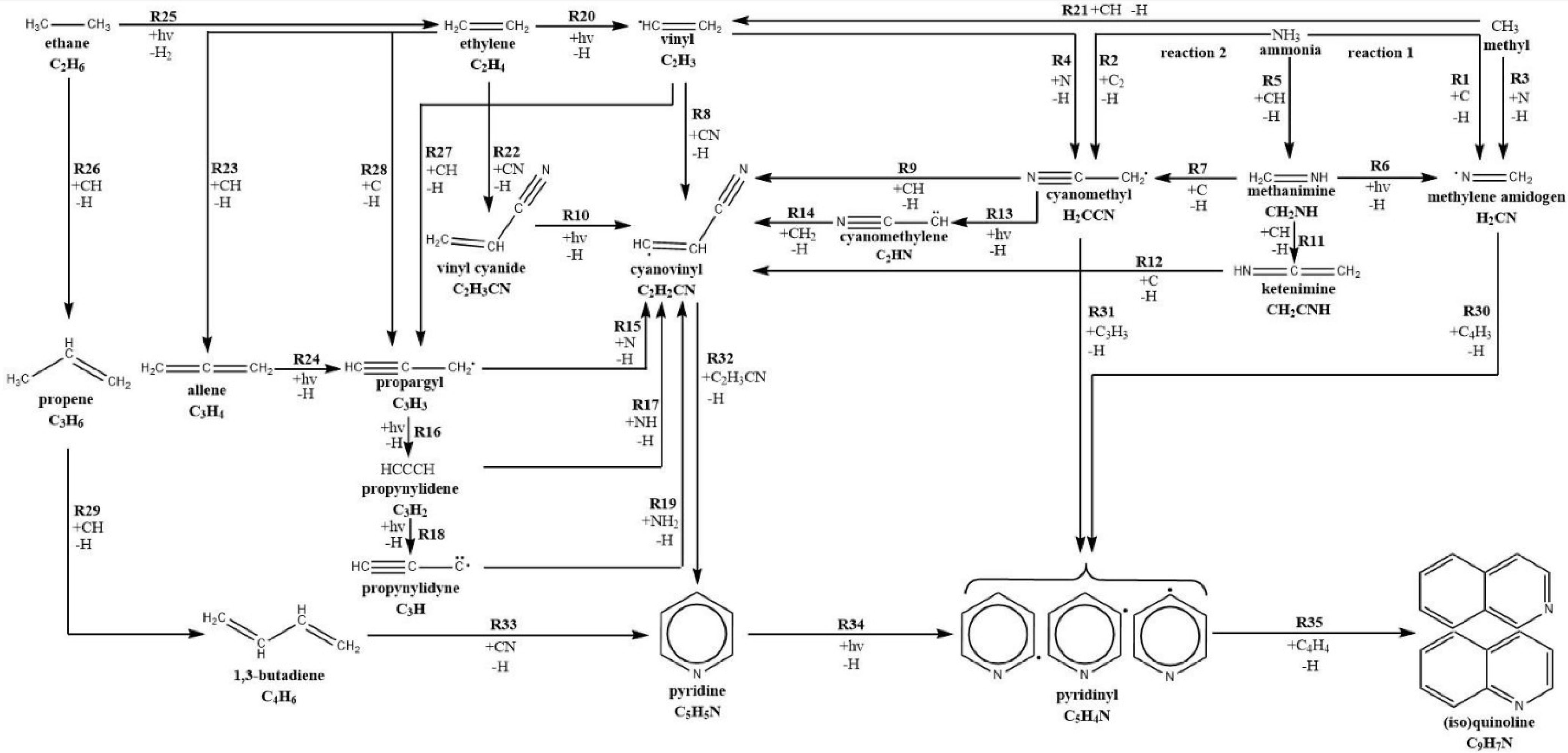


Experiment:
310 ± 26 kJ mol^{-1}

Calculations:
301 kJ mol^{-1}



Relative Energy (kJ mol-1)
0
-200
-400
-600
0
-49
-169
-168
-174
i6''
-174
-174
-189
-195
i7''
-120
-195
-55
-238
i5''
-224
-243
-339
i3''
-366
i2''
-372
i1''
-333
i4''
-298
i8''
-259
-536
i9''
-338
-354
i10''
-219
-270
i11''
-257
-637
i12''
m: m-pyridinyl p: p-pyridinyl o: o-pyridinyl
-168 m+H
-174 p+H
-193 o+H



Supplementary Fig. 3. **Updated reaction network in TMC-1.** Compilation of key bimolecular reactions and photodissociation processes newly introduced into the astrochemical model for TMC-1 leading to pyridine, pyridinyl, and (iso)quinoline.

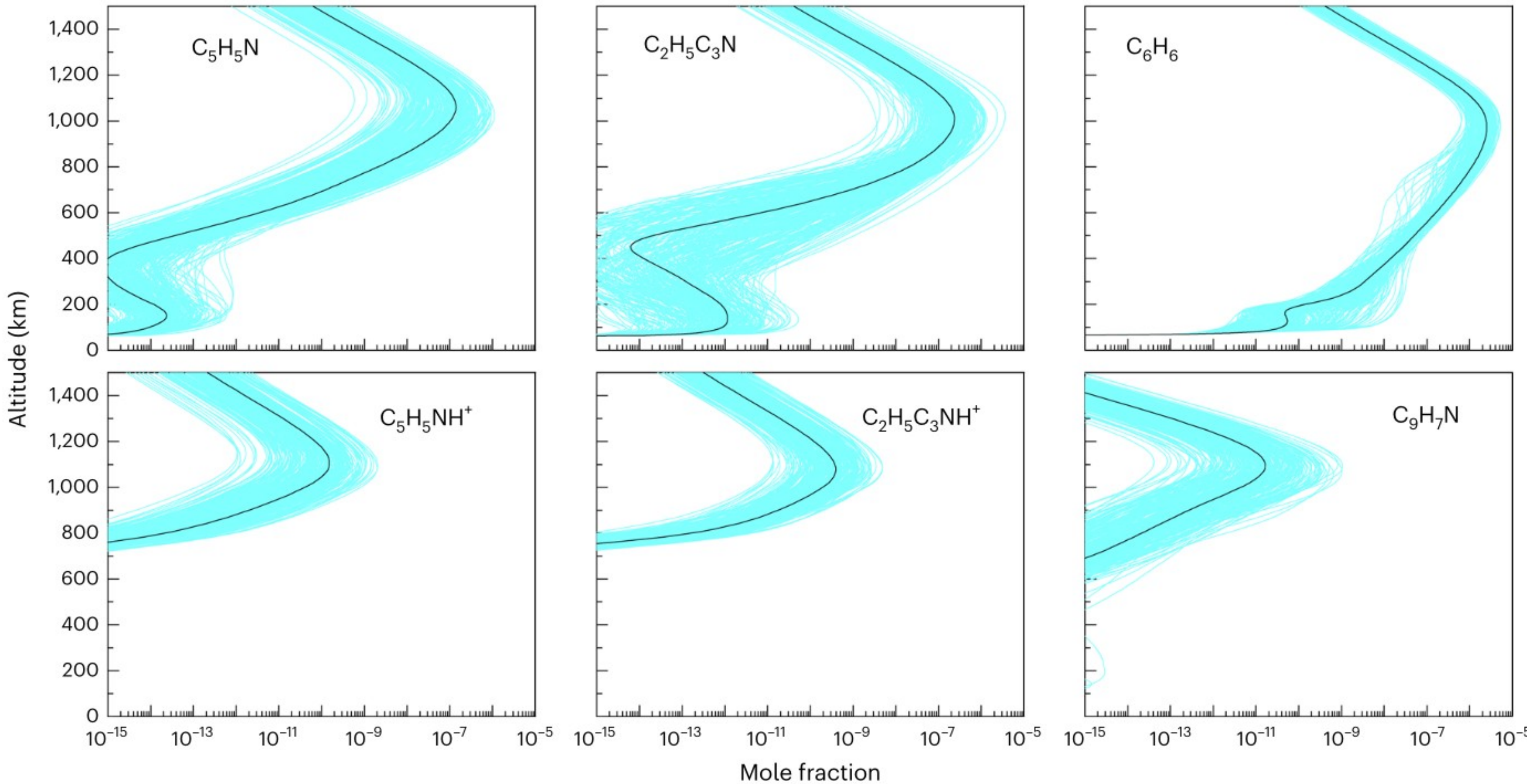
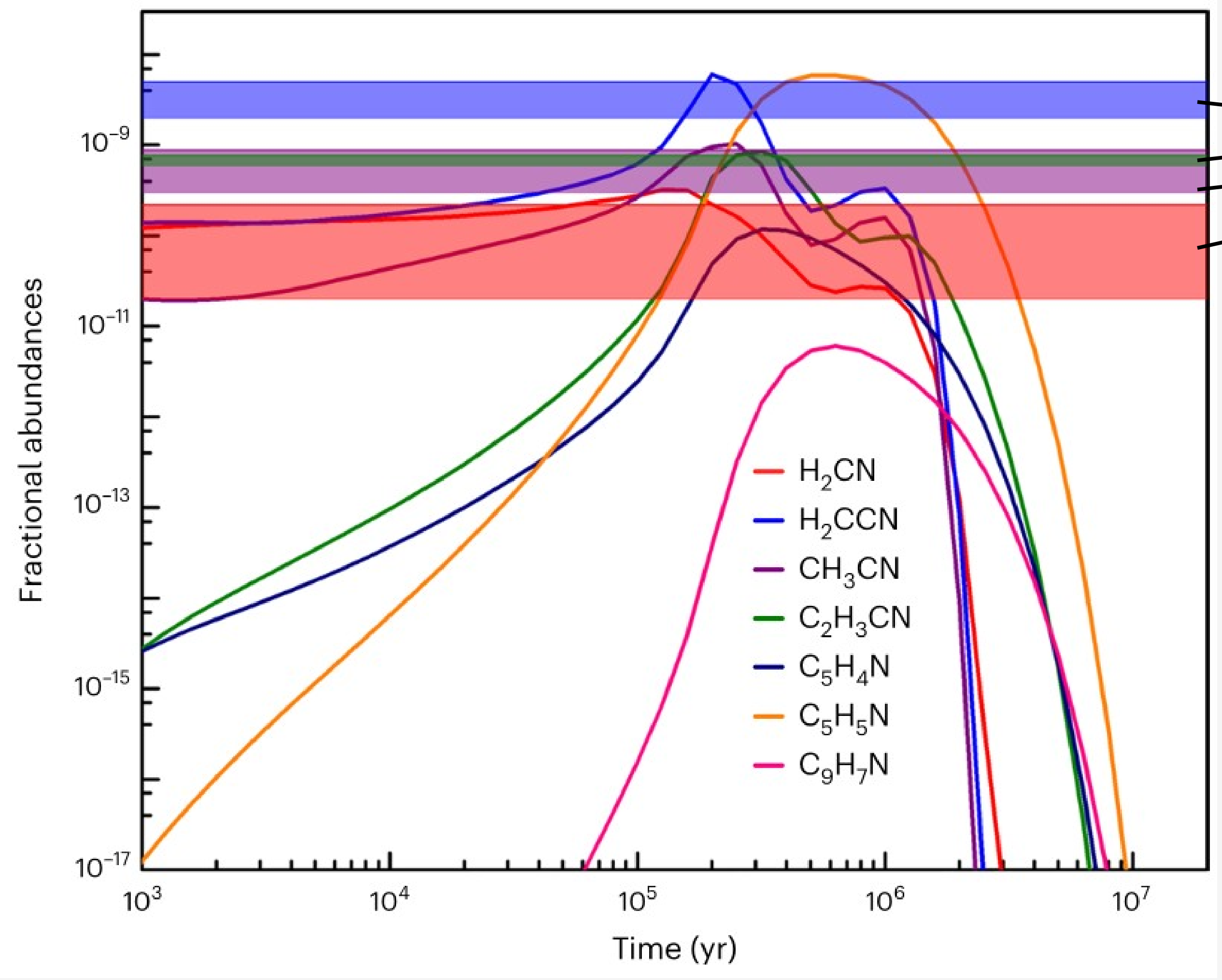


Fig. 5 | Results of the astrochemical model for Titan’s atmosphere. Mole fraction profiles for six species obtained from a one-dimensional photochemical model of Titan’s atmosphere. The solid black lines represent the nominal model results, with 280 runs of the Monte Carlo analysis shown as cyan lines. Please refer to the text for details on the error analysis and the assignment of the species.

Mole fraction of $(1.5\pm0.3)\times10^{-9}$ at m/z=80 ($C_5H_5NH^+$) derived from the Cassini INMS data agrees well with the sum of $C_5H_5NH^+$ and $C_2H_5C_3NH^+$ of the atmospheric models ranging between 2.5×10^{-9} and 5.4×10^{-10}

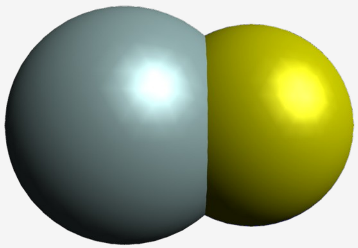
Taurus molecular cloud



Observed abundances for H_2CN, H_2CCN, CH_3CN C_2H_3CN,

We predict
pyridine (C_5H_5N), pyridinyl ($C_5H_4N\cdot$) and (iso)quinoline (C_9H_7N)
to be present in amounts detectable by radio telescopes

Case 2:
Silicon monosulfide
SiS



Case: Formation of SiS

- Interstellar grains should be more quickly destroyed than formed

- How come grains are so common in the ISM?

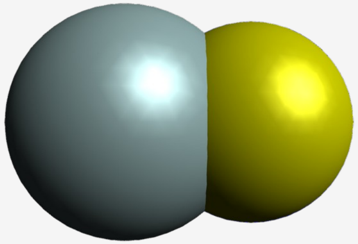
- Better understanding of molecular mass growth processes

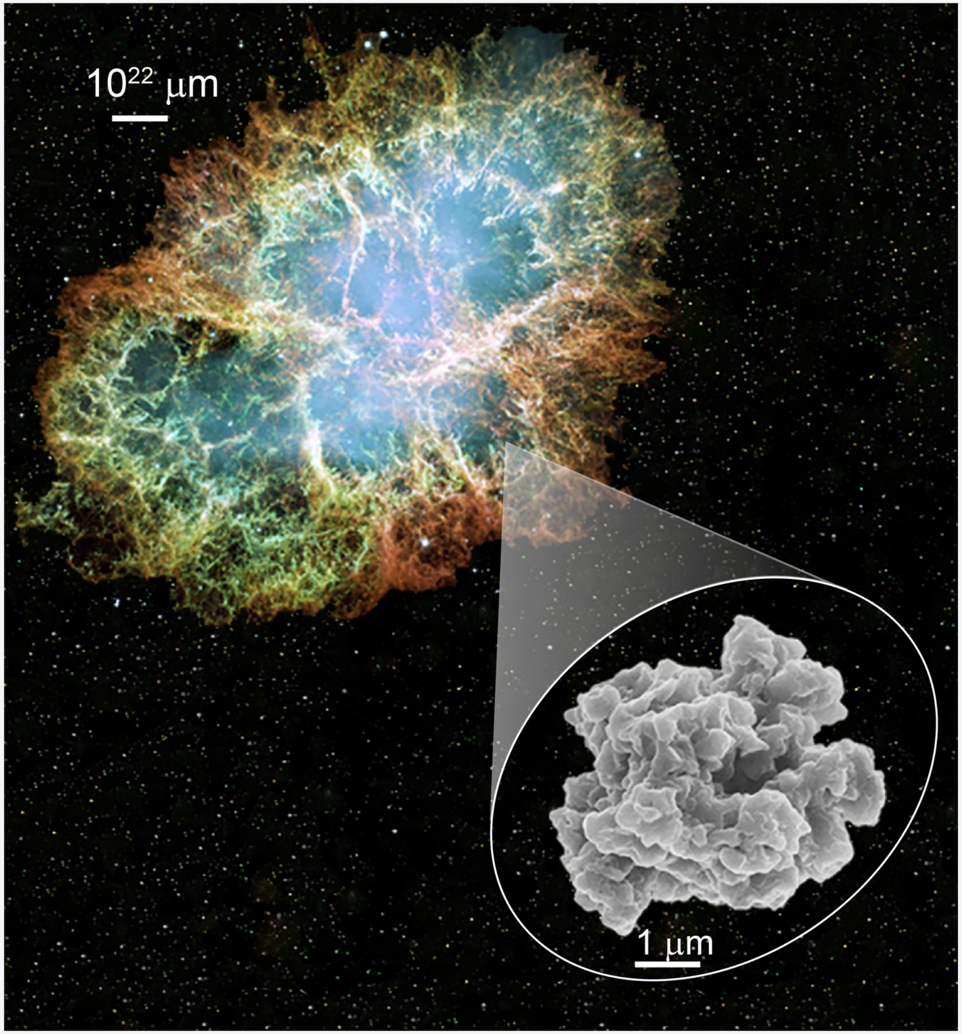
- Carbonaceous and silicates are begining to be understood.

What about sulfides grains?

SiS: possibly sets the initial stage

$SiS+Mg \rightarrow MgS_{(s)}+Si$





Formation

UMIST RATE12
astrochemistry.net

e Downloads Species Search...

	Reaction
1	$C^+ + SiS \rightarrow SiS^+ + C$
2	$H^+ + SiS \rightarrow SiS^+ + H$
3	$S^+ + SiS \rightarrow SiS^+ + S$
4	$SiS + CRPHOT \rightarrow S + Si$
5	$C^+ + SiS \rightarrow SiC^+ + S$
6	$H_3^+ + SiS \rightarrow HSiS^+ + H_2$
7	$HCO^+ + SiS \rightarrow HSiS^+ + CO$
8	$He^+ + SiS \rightarrow S^+ + Si + He$
9	$He^+ + SiS \rightarrow S + Si^+ + He$
10	$SiS + PHOTON \rightarrow S + Si$

Destruction

1	$HSiS^+ + e^- \rightarrow SiS + H$
2	$H_2S + HSiS^+ \rightarrow H_3S^+ + SiS$
3	$HCN + HSiS^+ \rightarrow HCNH^+ + SiS$
4	$NH_3 + HSiS^+ \rightarrow NH_4^+ + SiS$
5	$C^- + SiS^+ \rightarrow C + SiS$
6	$C_{10}^- + SiS^+ \rightarrow C_{10} + SiS$
7	$C_{10}H^- + SiS^+ \rightarrow C_{10}H + SiS$
8	$C_2^- + SiS^+ \rightarrow C_2 + SiS$
9	$C_2H^- + SiS^+ \rightarrow C_2H + SiS$
10	$C_3^- + SiS^+ \rightarrow C_3 + SiS$
11	$C_3H^- + SiS^+ \rightarrow C_3H + SiS$
12	$C_3N^- + SiS^+ \rightarrow C_3N + SiS$
13	$C_4^- + SiS^+ \rightarrow C_4 + SiS$
14	$C_4H^- + SiS^+ \rightarrow C_4H + SiS$
15	$C_5^- + SiS^+ \rightarrow C_5 + SiS$
16	$C_5H^- + SiS^+ \rightarrow C_5H + SiS$
17	$C_5N^- + SiS^+ \rightarrow C_5N + SiS$
18	$C_6^- + SiS^+ \rightarrow C_6 + SiS$
19	$C_6H^- + SiS^+ \rightarrow C_6H + SiS$
20	$C_7^- + SiS^+ \rightarrow C_7 + SiS$
21	$C_7H^- + SiS^+ \rightarrow C_7H + SiS$
22	$C_8^- + SiS^+ \rightarrow C_8 + SiS$
23	$C_8H^- + SiS^+ \rightarrow C_8H + SiS$
24	$C_9^- + SiS^+ \rightarrow C_9 + SiS$
25	$C_9H^- + SiS^+ \rightarrow C_9H + SiS$
26	$CH^- + SiS^+ \rightarrow CH + SiS$
27	$CN^- + SiS^+ \rightarrow CN + SiS$
28	$H^- + SiS^+ \rightarrow H + SiS$
29	$O^- + SiS^+ \rightarrow O + SiS$
30	$O_2^- + SiS^+ \rightarrow O_2 + SiS$
31	$OH^- + SiS^+ \rightarrow OH + SiS$
32	$S^- + SiS^+ \rightarrow S + SiS$

Models differ from observation by two orders of magnitude

Silicon monosulfide (SiS)

THE ASTROPHYSICAL JOURNAL, 920:37 (7pp), 2021 October 10
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SiS Formation in the Interstellar Medium through Si+SH Gas-phase Reactions

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MNRAS **493,** 299–304 (2020) doi:10.1093/mnras/staa269
Advance Access publication 2020 January 29

SiS formation via gas phase reactions between atomic silicon and sulphur-bearing species

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Astronomy & Astrophysics

New SiS destruction and formation routes via neutral-neutral reactions and their fundamental role in interstellar clouds at low- and high-metallicity values

Edgar Mendoza[1], Samuel F. M. Costa[2], Miguel Carvajal[1,3], Sérgio Pilling[4], Márcio O. Alves[2], and Breno R. L. Galvão[2,5]

$$k(T) = \alpha\,(T/300)^{\beta}\,\exp\left(-\gamma/T\right).$$

Index [(a)]	Reaction	α(cm^{-3}s^{-1})	β	γ(K)	Description [(b)]
1	$C + SiS \rightarrow S + SiC$	1.20×10^{-9}	0.020	23 261	This work
–1	$S + SiC \rightarrow C + SiS$	2.81×10^{-10}	–0.171	–0.383	This work
2	$C + SiS \rightarrow Si + CS$	1.59×10^{-9}	0.0277	29.25	This work
–2	$Si + CS \rightarrow C + SiS$	5.74×10^{-9}	0.389	12174	This work
3	$S + SiC \rightarrow Si + CS$	3.20×10^{-10}	–0.152	2.073	This work
–3	$Si + CS \rightarrow S + SiC$	3.84×10^{-9}	0.143	35 604	This work
4	$Si + HS \rightarrow SiS + H$	0.916×10^{-10}	–0.6433	11.525	QCT
–4	$SiS + H \rightarrow Si + HS$	0	0	0	Endo.
5	$Si + H_2S \rightarrow SiS + H_2$	1×10^{-10}	0	0	Exp
–5	$SiS + H_2 \rightarrow Si + H_2S$	0	0	0	Endo.
6	$Si + SO \rightarrow SiS + O$	1.77×10^{-11}	0.16	–20	QCT
7	$Si + SO \rightarrow SiO + S$	1.53×10^{-10}	–0.11	32	QCT
8	$SiS + O \rightarrow SiO + S$	9.53×10^{-11}	0.29	–32	QCT
9	$SiH + S \rightarrow SiS + H$	0.63×10^{-10}	–0.11	11.6	QCT
9b	$SiH + S \rightarrow SH + Si$	0.025×10^{-10}	–0.13	9.38	QCT
10	$SiH + S_2 \rightarrow SiS + SH$	1×10^{-10}	0	0	PES
11	$Si + SO_2 \rightarrow SiO + SO$	1×10^{-10}	0	0	PES
12	$SiS + O_2$	0	0	0	Endo

Destruction

$SiS+C \rightarrow SiC+S$

$SiS+O \rightarrow SiO+S$

$SiS+H \rightarrow$ nothing

$SiS+H_2 \rightarrow$ nothing

Formation

$SH+Si \rightarrow SiS+H$

$H_2S+Si \rightarrow SiS+H_2$

Kinetic & models

The Astrophysical Journal. **920,** 37 (2021).

Experiments & astrochemical models

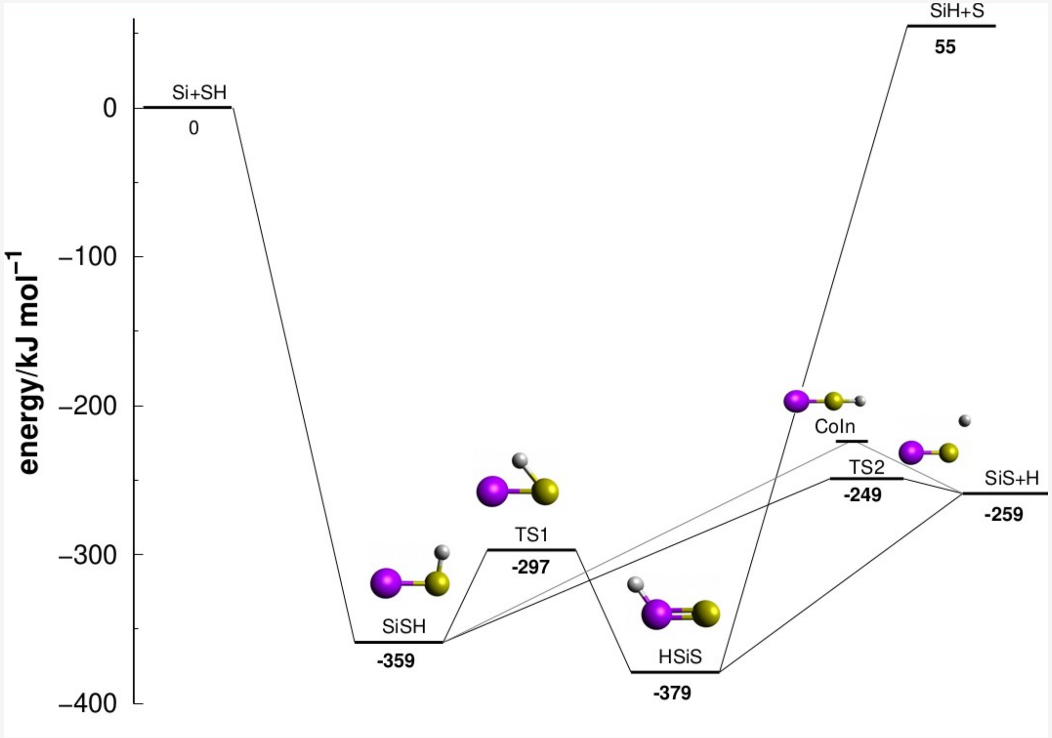
Science Advances **7**, eabg7003 (2021).

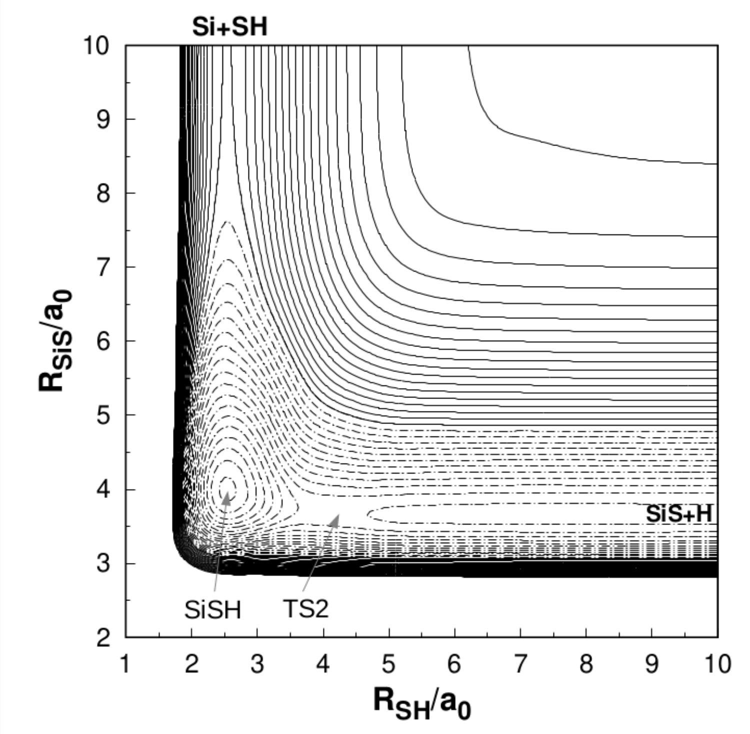
Si+SH → SiS+H - Energies

Energies: MRCI(Q)/CBS
aug-cc-pV(Q + d)Z & aug-cc-pV(5 + d)Z

2267 single point energies

Fitted full dimensional PES:
DMBE method



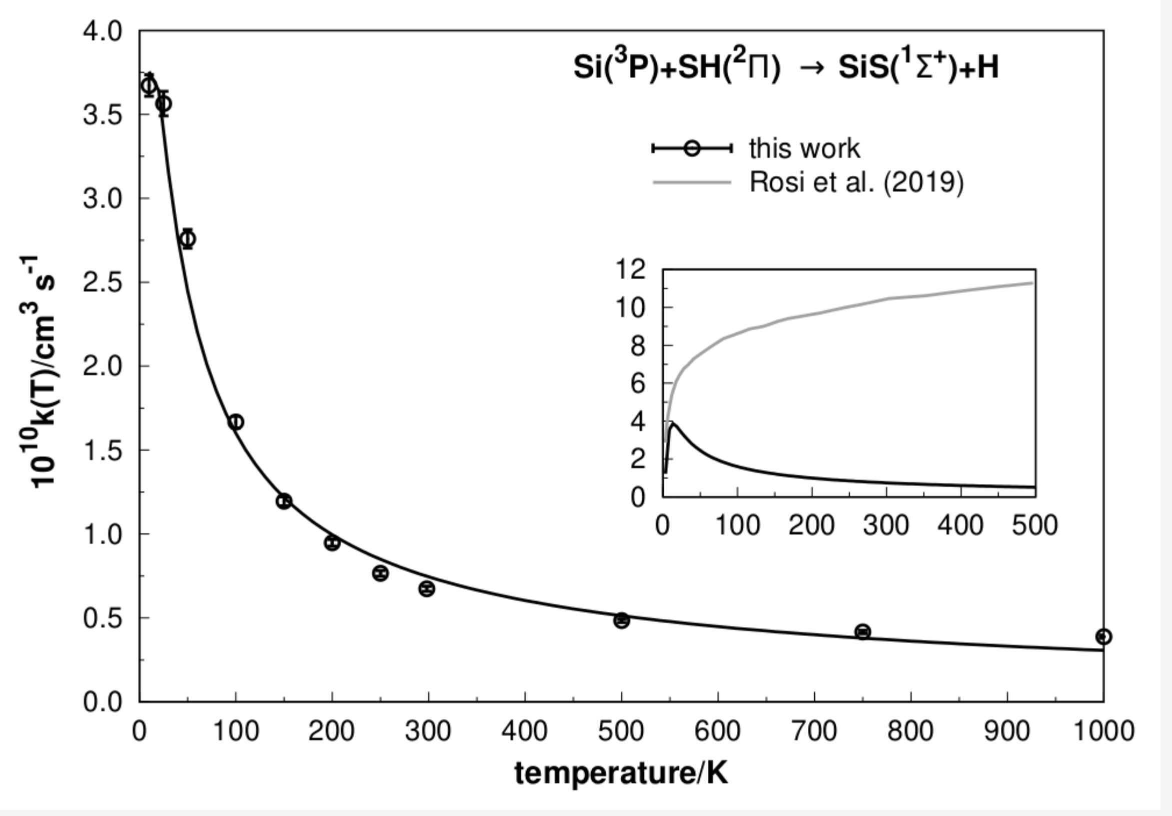


Astrophys. J. **920,** 37 (2021)

Rate coefficients:
Quasiclassical trajectories

10000 trajectories for each Temp.

$$k(T) = g_e(T)\left(\frac{8k_BT}{\pi\mu}\right)^{1/2}\pi b_{max}^2\frac{N^r}{N}$$



Astrophys. J. **920,** 37 (2021)

Gas-grain Astrochemical modeling
Nautilus / KIDA database

Valentine Wakelam
(Univ. Bordeaux)

Edgar Mendoza
(Univ. de Huelva)

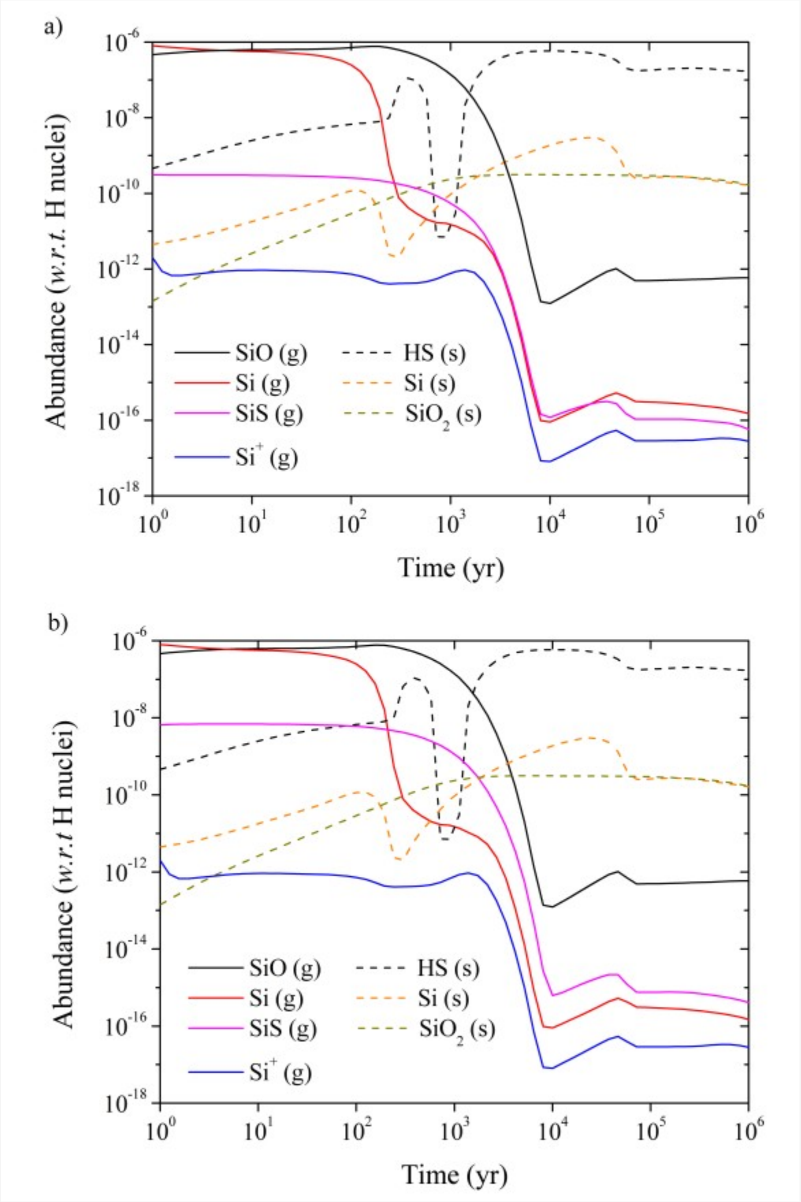
3 phases model:
- cold molecular cloud
- shock phase
- gas and dust cools down

Observed abundance:
[SiS/H] ∼ 1 × 10^{-8}

Model: 0.7 × 10^{-8}

Observations in the shock L1157-B1
MNRAS. **470**, L16 (2017).

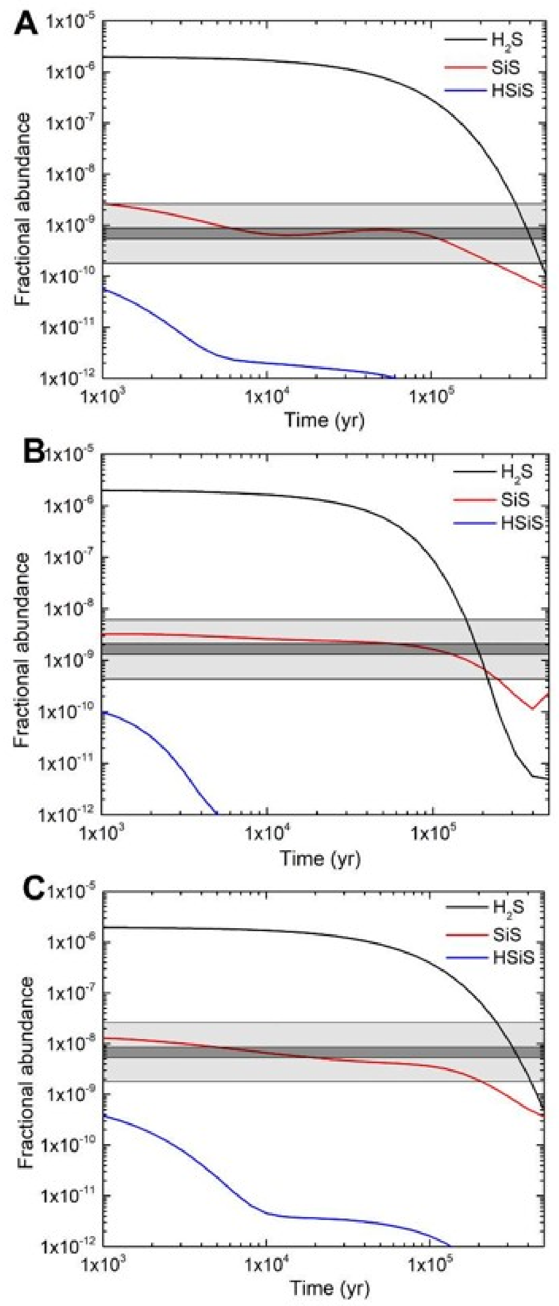
Our model:
Astrophys. J. **920,** 37 (2021)



Experiments
Ralf Kaiser
(University of Hawai'i)

Models (UMIST)

Tom Millar
(Queen's Univ. Belfast)



Abundance:
$[SiS]/[H_2]$

Orion hot core

Orion Plateau

Orion 15.5 km s -1

Sci. Adv. **7**, eabg7003

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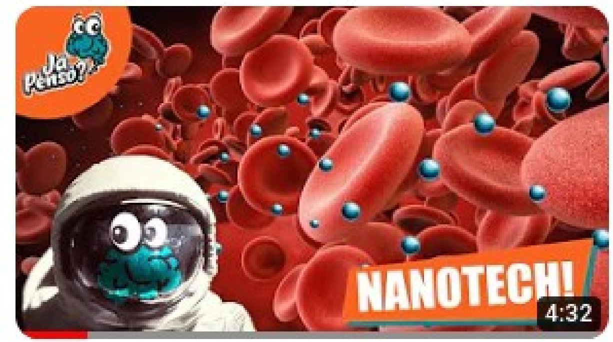

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