The Hot Molecular Core G331.512-0.103: Detection of CH_2NH and its implications for NH_2CH_2COOH

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ALLAM 2019

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Outline and Themes

- Introduction
  Elements and molecules
- Scientific case
  'The penultimate step'
- Method
  Observations and calculations
- Results
  Detection and formation
- Future

The vicuña and the antenna.
(Credit: Jaime Guarda/ESO)

A Production of Amino Acids Under Possible Primitive Earth Conditions

Stanley L. Miller[1, 2]

G. H. Jones Chemical Laboratory, University of Chicago, Chicago, Illinois

The idea that the organic compounds that serve as the basis of life were formed when the earth had an atmosphere of methane, ammonia, water, and hydrogen instead of carbon dioxide, nitrogen, oxygen, and water was suggested by Oparin (*1*) and has been given emphasis recently by Urey (*2*) and Bernal (*3*).

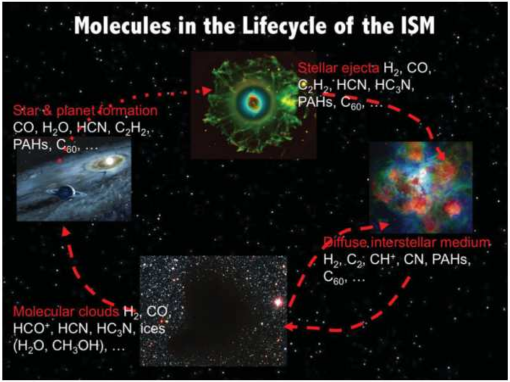
[1] National Science Foundation Fellow, 1952–53.
[2] Thanks are due Harold C. Urey for many helpful suggestions and guidance in the course of this investigation.

Science 1953.

Vol. 117, Issue 3046, pp. 528-529

Lazcano & Bada 2003. Origins of Life and Evolution of the Biosphere.

Vol 33, pp. 235-242



- Molecular formation include bottom-up and top-down routes;
- The whole cycle takes few billion years, with each phase characterized by distinctive molecules.

Tielens A. G. G. M. 2013. The Molecular Universe.
Rev. Mod. Phys. 85, 1021.

Elements and molecules

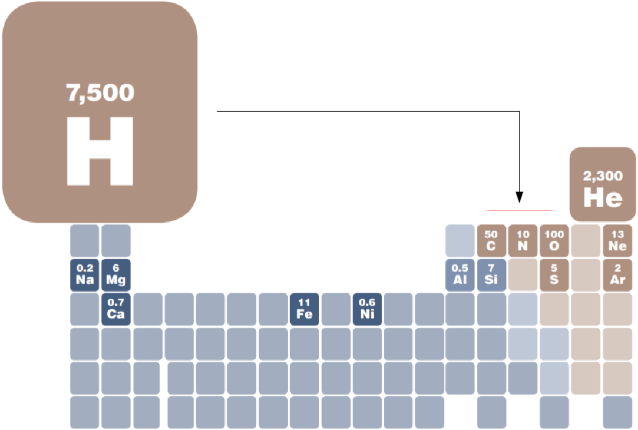
✓ **The Chemical Universe**

CHANDRA X-ray Observatory.

http://chandra.harvard.edu/resources/illustrations/chemistry_universe.html

✓ The Molecular Universe

McCarthy & Thaddeus 2001. Chem. Soc. Rev., 30, 177.



Elements and molecules

✓ The Chemical Universe

CHANDRA X-ray Observatory.

http://chandra.harvard.edu/resources/illustrations/chemistry_universe.html

✓ The Molecular Universe

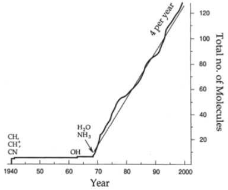
McCarthy & Thaddeus 2001. Chem. Soc. Rev., 30, 177.

Known Interstellar and Circumstellar Molecules (July 2000)

Number of Atoms

2	3	4	5	6	7	8	9
H_2	H_2O	NH_3	SiH_4	CH_3OH	CH_3CHO	CH_3CO_2H	CH_3CH_2OH
OH	H_2S	H_3O^+	CH_4	NH_2CHO	CH_3NH_2	HCO_2CH_3	$(CH_3)_2O$
SO	SO_2	H_2CO	CHOOH	CH_3CN	CH_3CCH	CH_3C_2CN	CH_3CH_2CN
SO^+	HN_2^+	H_2CS	HC≡CCN	CH_3NC	CH_2CHCN	C_7H	$H(C{\equiv}C)_3CN$
SiO	HNO	HNCO	CH_2NH	CH_3SH	HC_4CN	H_2C_6	$H(C{\equiv}C)_2CH_3$
SiS	SiH_2?	HNCS	NH_2CN	C_5H	C_6H		C_8H
NO	NH_2	CCCN	H_2CCO	HC_2CHO	c-CH_2OCH_2		
NS	H_3^+	HCO_2^+	C_4H	$CH_2=CH_2$	C_7^-?		
HCl	NNO	CCCH	c-C_3H_2	H_2CCCC			
NaCl	HCO	c-CCCH	CH_2CN	HC_3NH^+			
KCl	HCO^+	CCCO	C_5	C_5N			
AlCl	OCS	CCCS	SiC_4	C_5S?			
AlF	CCH	HCCH	H_2CCC				
PN	HCS^+	$HCNH^+$	HCCNC				
SiN	c-SiCC	HCCN	HNCCC				
NH	CCO	H_2CN	H_3CO^+				
CH	CCS	c-SiC_3					
CH^+	C_3	CH_3					
CN	MgNC	CH_2D^+?					
CO	NaCN						
CS	CH_2						
C_2	MgCN						
SiC	HOC^+						
CP	HCN						
CO^+	HNC						
HF	SiCN						
	KCN?						

— Carbon chains
— Complex Organic Molecules
— Tracers of shocks and UV-irradiation



Cometary Glycine: Comet 81P/Wild 2

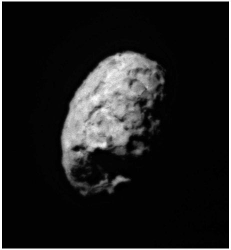


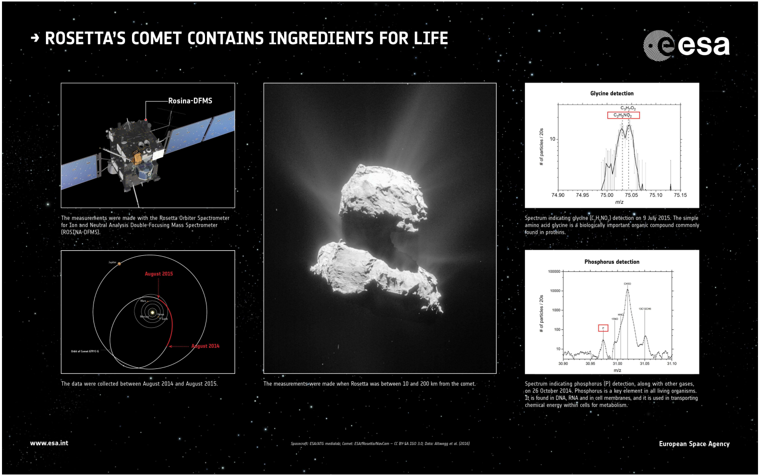
Table 1. Summary of the amino acid concentrations in water extracts of Stardust flight foils[a].

Amino acid	This study						Previous study[b]	
	C2103N,0	C2016N,2	C2017N,0	C2078N,0	C2125N,2		C2092S,0	
	Both sides (total)				Aerogel side (total)	Metal side (total)	Both sides (free)	Both sides (total)
Glycine	34	2	13	19	21	<3	27	68
β-alanine	2	1	1	3	<2	<2	1	7
D-alanine	<3	<3	<3	<3	<3	<3	<3	<4
L-alanine	2	<1	1	1	1	<3	6	12
EACA[c]	326	51	66	327	186	126	11	1,413

Elsila, Glavin & Dworkin 2009.
Meteoritics & Planetary Science 44, 9, 1323
Mission: Stardust. Target: Wild 2. Spacecraft: Stardust.

Image credit: NASA/JPL-Caltech

Cometary Glycine: Comet 67P/Churyumov-Gerasimenko



Altwegg, Balsiger, Bar-Nun et al. 2016. Science Advances, Vol 2., no. 5
Mission: Rosetta. Comet 67P/Churyumov-Gerasimenko

Image Credit: ESA/Rosetta/NAVCAM CC BY-SA IGO 3.0

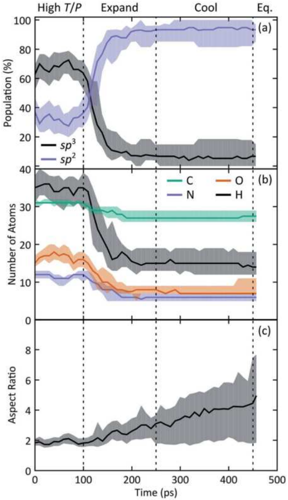
Shock synthesis: Impact events on early Earth

Chemistry in shock

* (T) 298 K $\longrightarrow$ 3000 K
* (ρ) 1.0 g cm^{-3} $\longrightarrow$ 2.5 g cm^{-3}
* (P) 48 GPa

Comet of the century: A horizon special

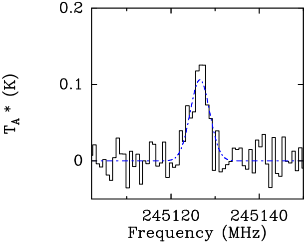
Graphic image: Weave VFX/BBC



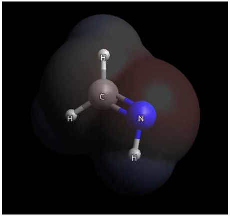
Kroonblawd, Lindsey & Goldman 2019.

Chem. Sci., 10, 6091-6098

Spectral survey Methanimine



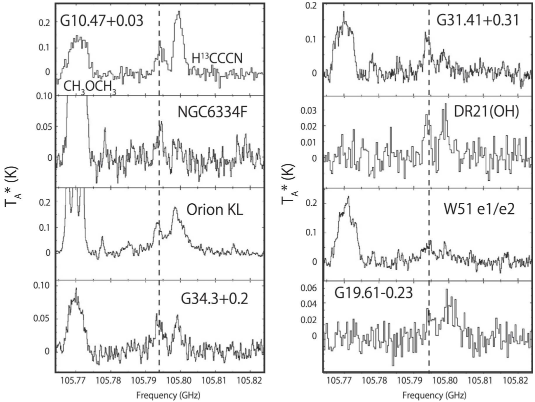
CH_2NH in G331.512-0.103: $4_{1,4}$-$3_{1,3}$ at 245126.014 MHz.



Pic credits: ALMA, APEX gallery http://www.almaobservatory.org/en/images/

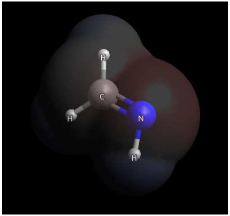
Formation path for glycine

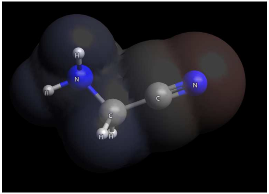
Suzuki et al. 2016 ApJ 825 79:
CH_2NH in 12 high-mass and 2 low-mass star forming regions

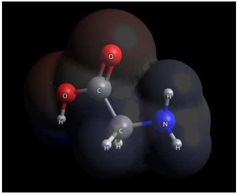


- e.g. Kim & Kaiser 2011; Theule et al. 2011 and Woon 2002; Holtom et al. 2005; Peltzer et al. 1984; Danger et al. 2011.

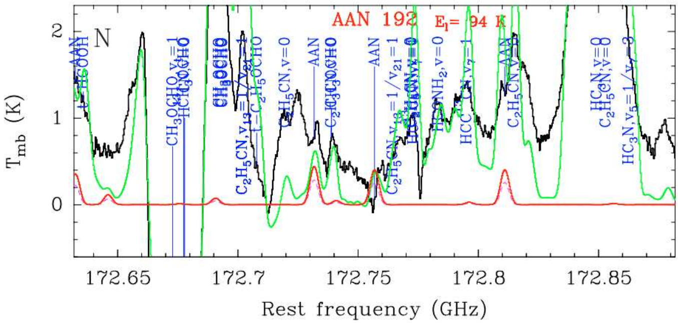
CH_2NH, NH_2CH_2CN and NH_2CH_2COOH







Amino acetonitrile in Sgr B2(N)



Belloche et al. 2008 A&A 482, 179

(also Belloche et al. 2008. A&A 492, 769)

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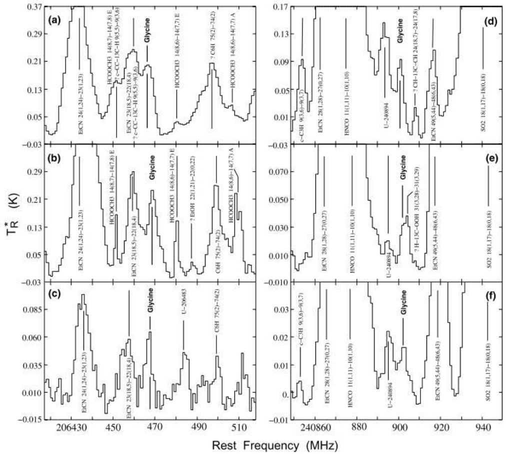
Search for interstellar glycine

Kuan et al. 2003. ApJ, 593, 848



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Observations

Instruments: APEX-I, -II, -III and SEPIA-B5 (around 50 hs)

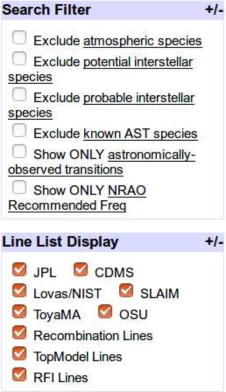
- **(2019)** Cyanoacetylene and their isotopologues in G331.512-0.103;
- **(2018–2019)** Hot molecular core candidates across the southern Milky Way;
- **(2016–2019)** Glycolaldehyde and pre-biotic molecules in the powerful outflow/hot core G331.512-0.103 (I, II, III)

(Bronfman et al. 2008; Merello et al. 2014; Mendoza et al. 2018; Hervías-Caimapo et al. 2019; Duronea et al. 2019)

Pic credits: ALMA, APEX gallery http://www.almaobservatory.org/en/images/

Making a detection: databases

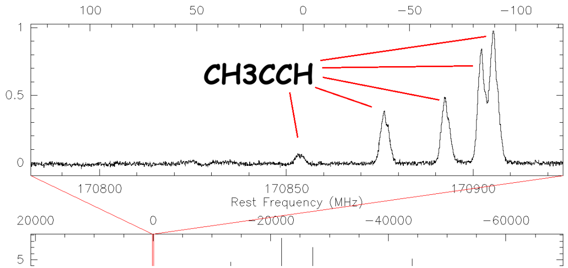
Without considering the spectroscopy, the filter by databases



- Splatalogue: https://www.cv.nrao.edu/php/splat
- https://spec.jpl.nasa.gov
- https://cdms.astro.uni-koeln.de
- https://physics.nist.gov/cgi-bin/micro/table5/start.pl

Essential criteria for (new) detections

1) First of all, think in contamination
2) Rest frequencies ⟶ Laboratory work, high-precision Hamiltonian models
3) Frequency agreement ⟶ Agreement between the rest frequency and the LSR velocity of the source
4) Beam dilution effects
5) Relative intensities ⟶ Consistency of dipole moments, line strengths, frequencies, energy levels, rotational temperatures

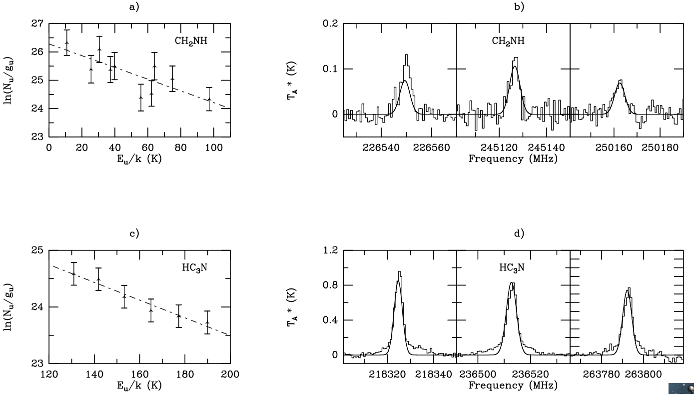


(e.g. Snyder, Lovas & Hollis et al. 2005. ApJ, 619:914-930)

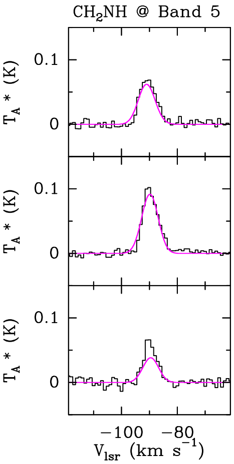
The case of G331.512-0.103: CH_2NH and HC_3N

Prediction and observation: APEX/Sepia band 5 (Mendoza et al. in prep)

- a) and b): CH_2NH
  $T_{exc} \approx 40$ K and $N \approx 1.2 \times 10^{14}$ cm^{-2}
- c) and d): HC3N
  $T_{exc} \approx 85$ K and $N \approx 6.9 \times 10^{14}$ cm^{-2}



CH_2NH in G331 as seen with APEX/Band5



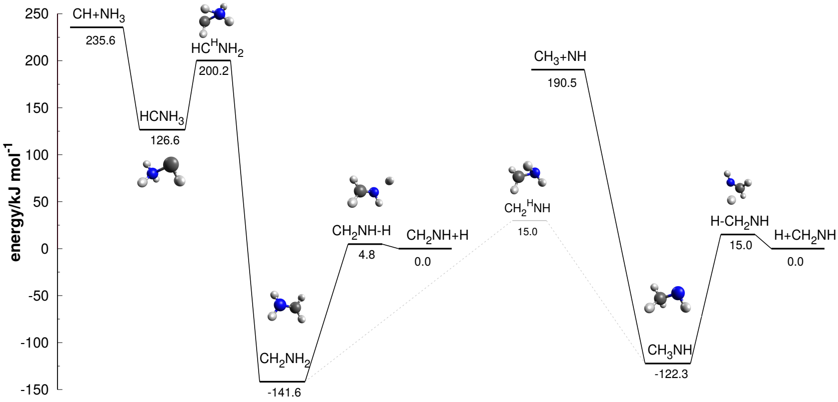
Spectral analysis

- ∗ 16 lines of CH_2NH between 160 - 352 GHz;
- ∗ Excitation components $10 < E_u(\mathrm{K}) < 200$;
- ∗ Emission origin in discussion $T < 70$ K. $N \simeq 10^{14}$ cm^{-2};

Frequency (MHz)	E_u (K)	A_{ij} ($1 \times 10^{-5} \mathrm{s}^{-1}$)
166852.248	11.0789	21.1
172267.519	17.4749	10.3
178073.945	45.8521	31.4

Theoretical studies on the CH_2NH formation

- Precursors: CH, NH_3, CH_3 and NH
- Reaction: CH + NH_3 $\longrightarrow$ CH_2NH + H



Mendoza et al. in prep

e.g. Mallard et al. 1994. Bocherel et al. 1996. Blitz et al. 2012. Suzuki et al. 2016

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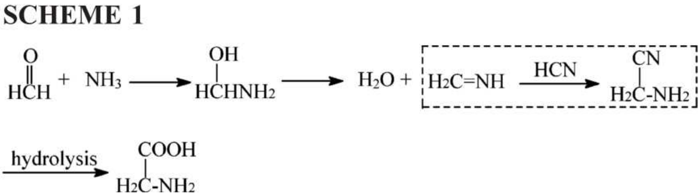
The penultimate step: Strecker synthesis

- The role of CH_2NH, H_2O, HCN and HNC in a Strecker synthesis to produce glycine (Koch et al. 2008. J. Phys. Chem. C, 112, 2972-2980)



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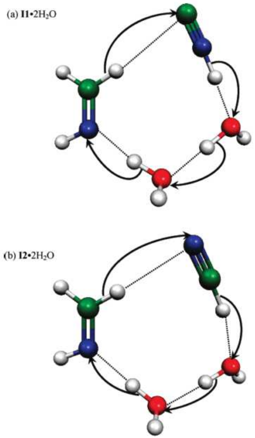
The penultimate step: Strecker synthesis



Interstellar ice models

- Reaction between CH_2NH and HCN and HNC to produce NH_2CH_2CN
- Isomerization HCN $\rightarrow$ HNC vs HNC $\rightarrow$ HCN

✓ The reaction with HNC is sufficiently low in comparison with HCN

Of course: observations and simulations suppose (diverse) complex systems
H_2O, HCN, HNC, CH_2NH...

Koch et al. 2008. J. Phys. Chem. C, 112, 2972-2980

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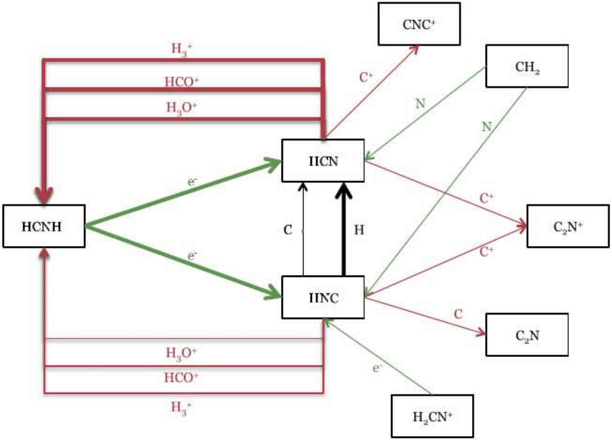
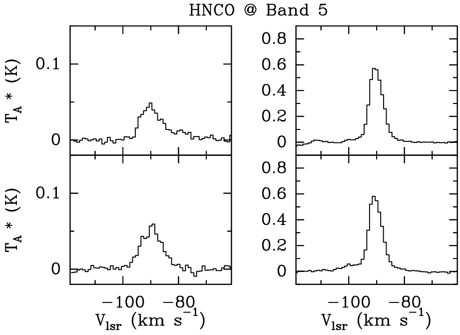
The importance of HCN and HNC in Star-Forming Regions



Loison, Wakelam & Hickson 2014. MNRAS, 443, Issue 1,
Graninger, Herbst, Öberg, Vasyunin 2014. ApJ, 787:74

HNCO in G331 as seen with APEX/Band5



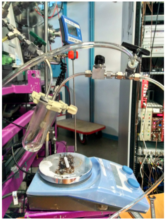
Frequency (MHz)	E_u (K)	A_{ij} (1 × $10^{-5}s^{-1}$)
175792.3332(±0.014)	211.07	0.127
175843.701(±0.03)	37.98	7.64
197764.7327(±0.0167)	220.56	0.144
197821.39(±0.03)	47.47	10.8

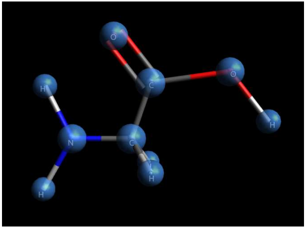
Mendoza et al. in prep

Summarizing

(Partial) conclusions

- CH_2NH: Prediction and confirmation in G331
- CH_2NH: as an key building block for pre-biotic chemistry
- $N(CH_2NH) \simeq 10^{14}$ cm^{-2}, $T < 70$K
- CH_2NH lines comparable with those observed in other HMCs



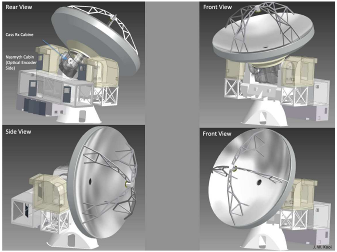


observations + experiments + models

Perspectives

LLAMA Project
Interesting science with the band 5

- Maser of HCN at 177 GHz
- Maser of H2O at 183 GHz
- Typical spectral tracers as CH_3CN, CH_3OH, CH_3CCH and HC_3N
- Pre-biotic chemistry: NH_2CHO and HNCO



www.llamaobservatory.org/english.html

thank you!