

# Astrochemistry - a key science driver for a high frequency extension of the SKA

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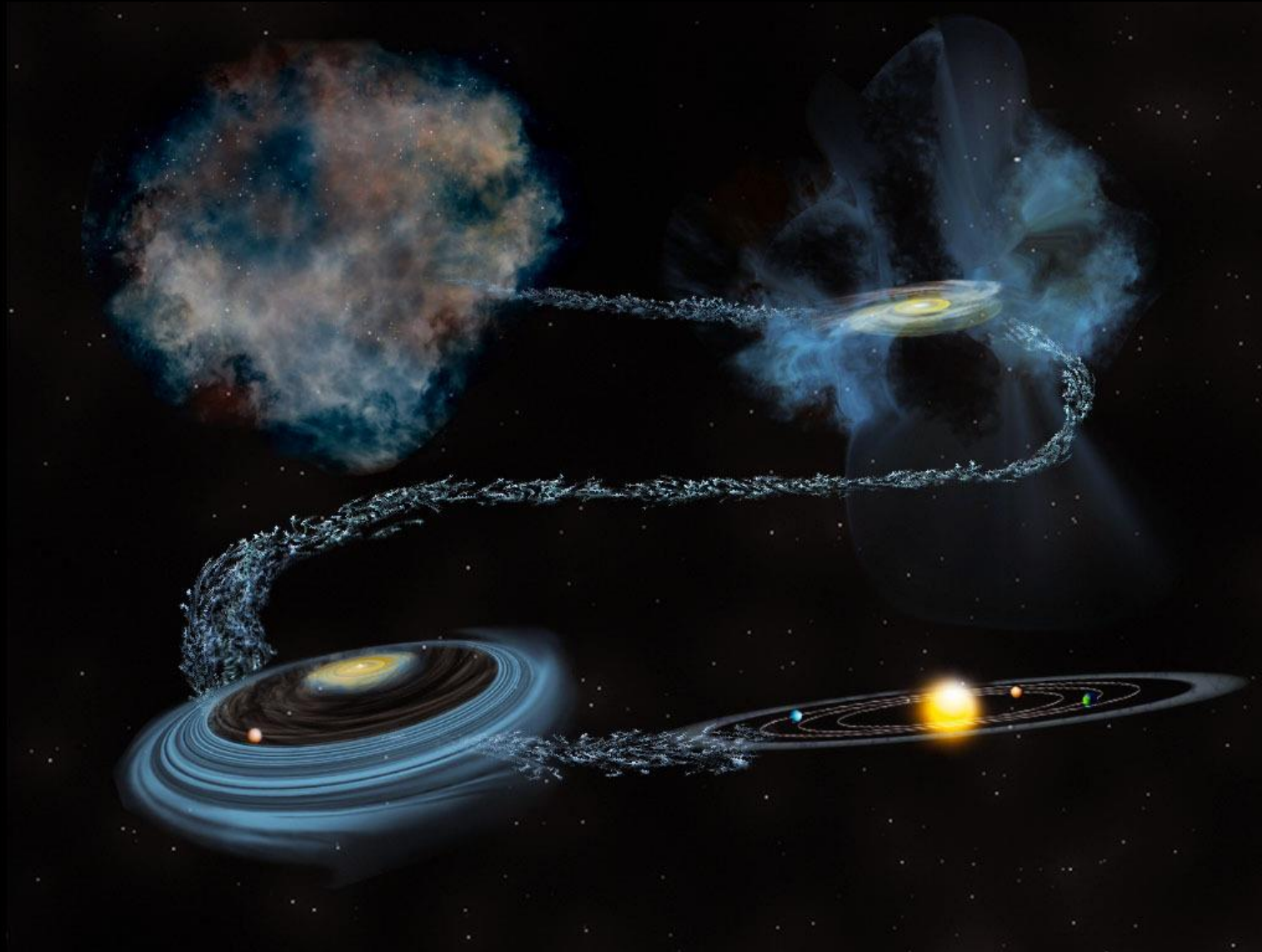
Schweizerischer  
Nationalfonds



BERN Astrochemistry Research



# What is Astrochemistry?



Credit: Bill Saxton, NSF / AUI / NRAO

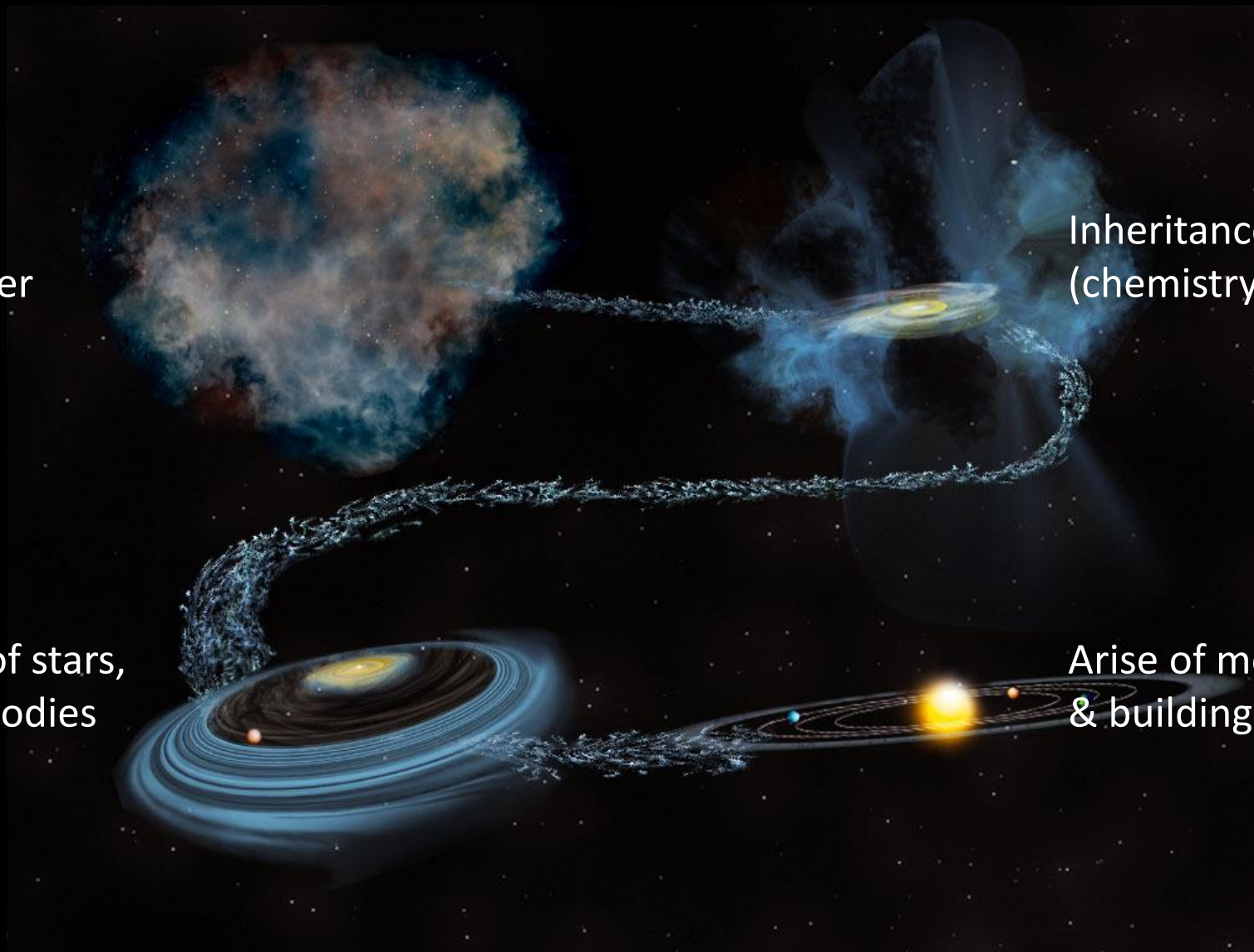
# What is Astrochemistry?

Composition of  
interstellar matter

Inheritance vs. reprocessing  
(chemistry, radiation, heating)

Building blocks of stars,  
planets, minor bodies

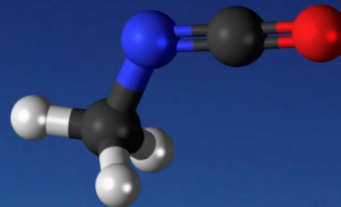
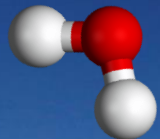
Arise of molecular complexity  
& building blocks of life



Credit: Bill Saxton, NSF / AUI / NRAO

# Census of molecular species in space

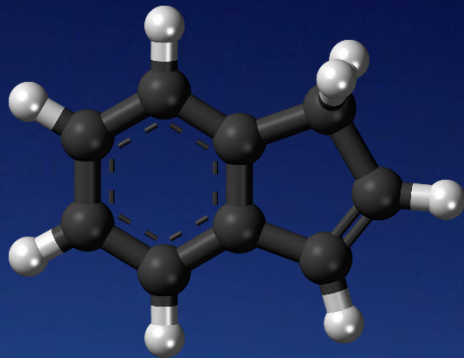
- Around 300 molecules identified in space (McGuire 2022)
- Rotational transitions of larger, heavier molecules (e.g., “building blocks of life”) occur at frequencies  $\leq 70$  GHz
- Less line confusion (number of lines per frequency unit) and line blending (overlapping lines) at those frequencies compared to millimeter regime



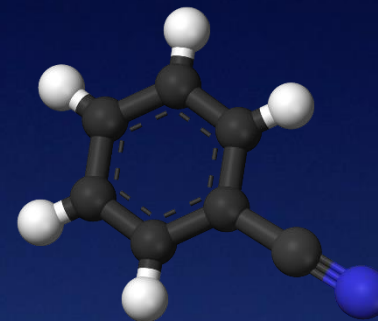
2 Atoms		3 Atoms		4 Atoms		5 Atoms		6 Atoms	7 Atoms		
CH	NH	H <sub>2</sub> O	MgCN	NH <sub>3</sub>	SiC <sub>3</sub>	HC <sub>3</sub> N	C <sub>4</sub> H <sup>-</sup>	CH <sub>3</sub> OH	CH <sub>3</sub> CHO		
CN	SiN	HCO <sup>+</sup>	H <sub>3</sub> <sup>+</sup>	H <sub>2</sub> CO	CH <sub>3</sub>	HCOOH	CNCHO	CH <sub>3</sub> CN	CH <sub>3</sub> CCH		
CH <sup>+</sup>	SO <sup>+</sup>	HCN	SiCN	HNCO	C <sub>3</sub> N <sup>-</sup>	CH <sub>2</sub> NH	HNCNH	NH <sub>2</sub> CHO	CH <sub>3</sub> NH <sub>2</sub>		
OH	CO <sup>+</sup>	OCS	AlNC	H <sub>2</sub> CS	PH <sub>3</sub>	NH <sub>2</sub> CN	CH <sub>3</sub> O	CH <sub>3</sub> SH	CH <sub>2</sub> CHCN		
CO	HF	HNC	SiNC	C <sub>2</sub> H <sub>2</sub>	HCNO	H <sub>2</sub> CCO	NH <sub>3</sub> D <sup>+</sup>	C <sub>2</sub> H <sub>4</sub>	HC <sub>5</sub> N		
H <sub>2</sub>	N <sub>2</sub>	H <sub>2</sub> S	HCP	C <sub>3</sub> N	HOCN	C <sub>4</sub> H	H <sub>2</sub> NCO <sup>+</sup>	C <sub>5</sub> H	C <sub>6</sub> H		
SiO	CF <sup>+</sup>	N <sub>2</sub> H <sup>+</sup>	CCP	HNCS	HSCN	SiH <sub>4</sub>	NCCNH <sup>+</sup>	CH <sub>3</sub> CN	c-C <sub>2</sub> H <sub>4</sub> O		
CS	PO	C <sub>2</sub> H	AlOH	HOCO <sup>+</sup>	HOOH	c-C <sub>3</sub> H <sub>2</sub>	CH <sub>3</sub> Cl	HC <sub>2</sub> CHO	CH <sub>2</sub> CHOH		
SO	O <sub>2</sub>	SO <sub>2</sub>	H <sub>2</sub> O <sup>+</sup>	C <sub>3</sub> O	l-C <sub>3</sub> H <sup>+</sup>	CH <sub>2</sub> CN	MgC <sub>3</sub> N	H <sub>2</sub> C <sub>4</sub>	C <sub>6</sub> H <sup>-</sup>		
SiS	AlO	HCO	H <sub>2</sub> Cl <sup>+</sup>	l-C <sub>3</sub> H	HMgNC	C <sub>5</sub>	HC <sub>3</sub> O <sup>+</sup>	C <sub>5</sub> S	CH <sub>3</sub> NCO		
NS	CN <sup>-</sup>	HNO	KCN	HCNH <sup>+</sup>	HCCO	SiC <sub>4</sub>	NH <sub>2</sub> OH	HC <sub>3</sub> NH <sup>+</sup>	HC <sub>5</sub> O		
C <sub>2</sub>	OH <sup>+</sup>	HCS <sup>+</sup>	FeCN	H <sub>3</sub> O <sup>+</sup>	CNCN	H <sub>2</sub> CCC	HC <sub>3</sub> S <sup>+</sup>	C <sub>5</sub> N	HOCH <sub>2</sub> CN		
NO	SH <sup>+</sup>	HOC <sup>+</sup>	HO <sub>2</sub>	C <sub>3</sub> S	HONO	CH <sub>4</sub>	H <sub>2</sub> CCS	HC <sub>4</sub> H	HC <sub>4</sub> NC		
HCl	HCl <sup>+</sup>	SiC <sub>2</sub>	TiO <sub>2</sub>	c-C <sub>3</sub> H	MgCCH	HCCNC	C <sub>4</sub> S	HC <sub>4</sub> N	HC <sub>3</sub> HNH		
NaCl	SH	C <sub>2</sub> S	CCN	HC <sub>2</sub> N	HCCS	HNCCC	CHOSH	c-H <sub>2</sub> C <sub>3</sub> O	c-C <sub>3</sub> HCCH		
AlCl	TiO	C <sub>3</sub>	SiCSi	H <sub>2</sub> CN		H <sub>2</sub> COH <sup>+</sup>		CH <sub>2</sub> CNH			
KCl	ArH <sup>+</sup>	CO <sub>2</sub>	S <sub>2</sub> H					C <sub>5</sub> N <sup>-</sup>			
AlF	NS <sup>+</sup>	CH <sub>2</sub>	HCS					HNCHCN			
PN	HeH <sup>+</sup>	C <sub>2</sub> O	HSC					SiH <sub>3</sub> CN			
SiC	VO	MgNC	NCO					MgC <sub>4</sub> H			
CP		NH <sub>2</sub>	CaNC					CH <sub>3</sub> CO <sup>+</sup>			
		NaCN	NCS					H <sub>2</sub> CCCS			
		N <sub>2</sub> O						CH <sub>3</sub> CCH			
8 Atoms		9 Atoms		10 Atoms		11 Atoms		12 Atoms	13 Atoms	PAHs	Fullerenes
HCOOCH <sub>3</sub>		CH <sub>3</sub> OCH <sub>3</sub>		CH <sub>3</sub> COCH <sub>3</sub>		HC <sub>9</sub> N		C <sub>6</sub> H <sub>6</sub>	C <sub>6</sub> H <sub>5</sub> CN	1-C <sub>10</sub> H <sub>7</sub> CN	C <sub>60</sub>
CH <sub>3</sub> C <sub>3</sub> N		CH <sub>3</sub> CH <sub>2</sub> OH		HOCH <sub>2</sub> CH <sub>2</sub> OH		CH <sub>3</sub> C <sub>6</sub> H		n-C <sub>3</sub> H <sub>7</sub> CN	HC <sub>11</sub> N	2-C <sub>10</sub> H <sub>7</sub> CN	C <sub>60</sub> <sup>+</sup>
C <sub>7</sub> H		CH <sub>3</sub> CH <sub>2</sub> CN		CH <sub>3</sub> CH <sub>2</sub> CHO		C <sub>2</sub> H <sub>5</sub> OCHO		i-C <sub>3</sub> H <sub>7</sub> CN		C <sub>9</sub> H <sub>8</sub>	C <sub>70</sub>
CH <sub>3</sub> COOH		HC <sub>7</sub> N		CH <sub>3</sub> C <sub>5</sub> N		CH <sub>3</sub> COOCH <sub>3</sub>		1-C <sub>5</sub> H <sub>5</sub> CN			
H <sub>2</sub> C <sub>6</sub>		CH <sub>3</sub> C <sub>4</sub> H		CH <sub>3</sub> CHCH <sub>2</sub> O		CH <sub>3</sub> COCH <sub>2</sub> OH		2-C <sub>5</sub> H <sub>5</sub> CN			
CH <sub>2</sub> OHCHO		C <sub>8</sub> H		CH <sub>3</sub> OCH <sub>2</sub> OH		C <sub>5</sub> H <sub>6</sub>					
HC <sub>6</sub> H		CH <sub>3</sub> CONH <sub>2</sub>									
CH <sub>2</sub> CHCHO		C <sub>8</sub> H <sup>-</sup>									
CH <sub>2</sub> CCHCN		CH <sub>2</sub> CHCH <sub>3</sub>									
NH <sub>2</sub> CH <sub>2</sub> CN		CH <sub>3</sub> CH <sub>2</sub> SH									
CH <sub>3</sub> CHNH		HC <sub>7</sub> O									
CH <sub>3</sub> SiH <sub>3</sub>		CH <sub>3</sub> NHCHO									
NH <sub>2</sub> CONH <sub>2</sub>		H <sub>2</sub> CCCHCCH									
HCCCH <sub>2</sub> CN		HCCCHCHCN									
CH <sub>2</sub> CHCCH		H <sub>2</sub> CCHC <sub>3</sub> N									

# Census of molecular species in space

- Recent detections achieved at wavelengths  $\geq 4\text{mm}$ /frequencies  $\leq 80\text{ GHz}$  with Yebes and Green Bank telescopes by QUIJOTE (PI: Cernicharo) and GOTHAM (PI: McGuire) molecular line surveys
- Line stacking for some detections  $\rightarrow$  need higher sensitivity
- Single point observations  $\rightarrow$  require high angular resolution and sensitivity for spatial information (crucial for understanding chemical links!)



Indene



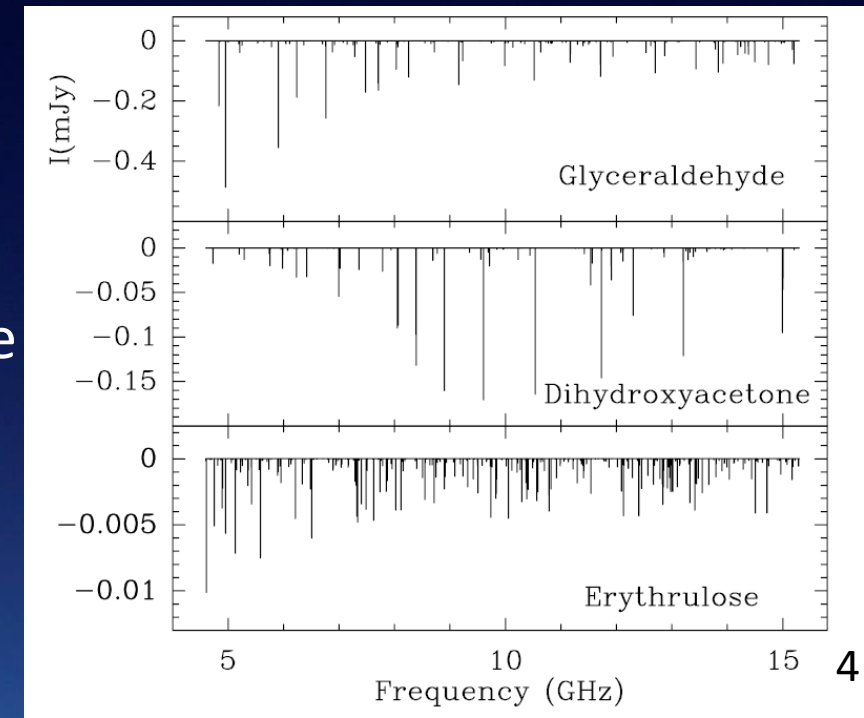
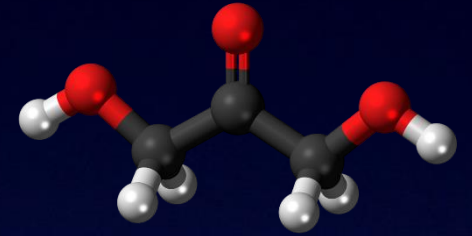
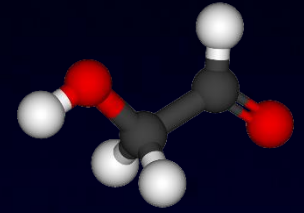
Benzonitrile



# Detection of new species: sugars

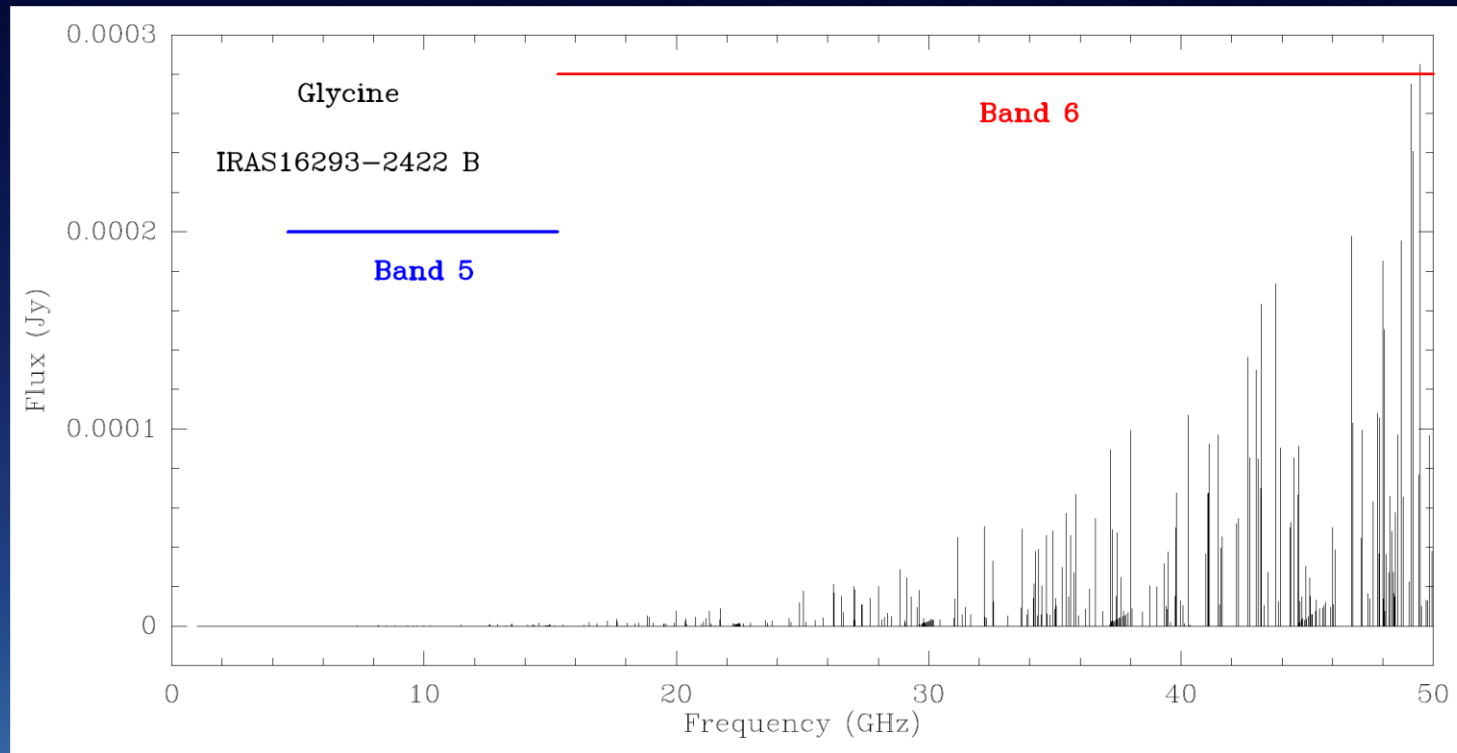
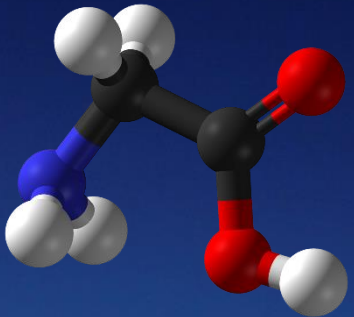
- C2-“sugar” glycolaldehyde  $\text{CH}_2\text{OHCHO}$  detected (e.g., Hollis et al. 2000, Halfen et al. 2006, Jørgensen et al. 2012)
- Unsuccessful searches for C3 sugars like glyceraldehyde ( $\text{CHOCHOHCH}_2\text{OH}$ ) or dihydroxyacetone ( $\text{CH}_2\text{OHCOCH}_2\text{OH}$ ) Present in meteorites!
- SKA band 5 and 6 well suited for observing prebiotic species (strength of rotational transitions for high dipole moment molecules drops dramatically at lower freq.)

Predicted absorption spectra for prebiotic species  
Jiménez-Serra et al. 2022, FSPAS 9, 843766

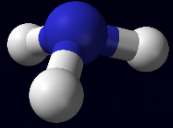


# Glycine – the simplest amino acid

- The holy grail in astrochemistry
- Detected in meteorites and comet 67P/Churyumov–Gerasimenko
- Sub-/Millimeter detections not confirmed – best observed in SKA band 6 (too faint in band 5!)



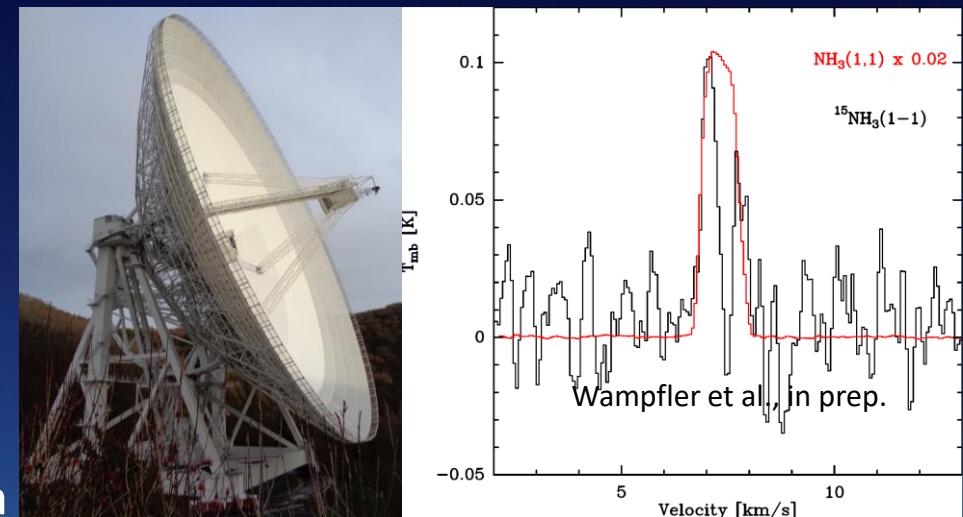
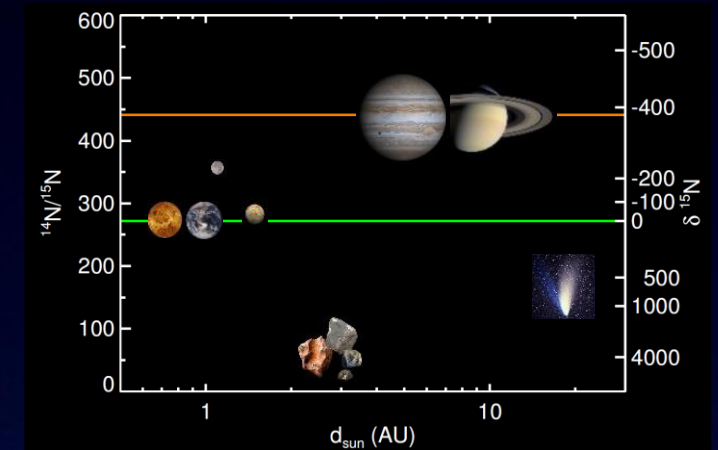
SKA Memo 20-01  
Conway et al. (2020)



# Volatiles: Ammonia



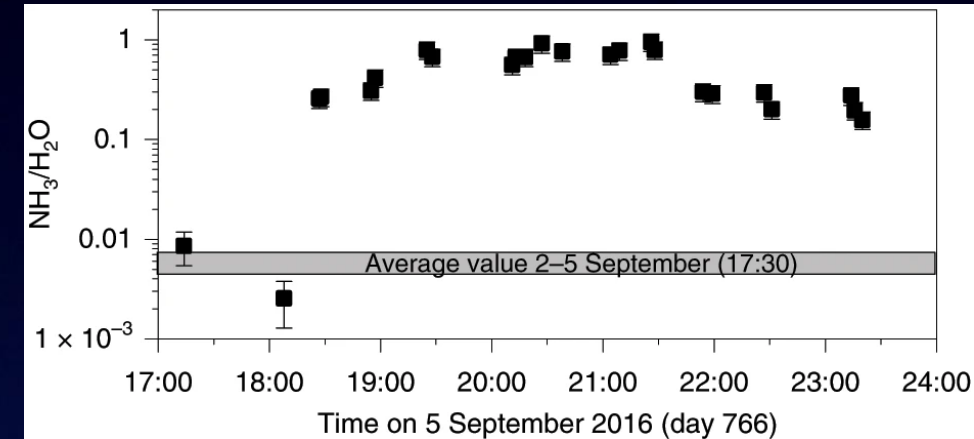
- Motivation:
  - Important nitrogen reservoir
  - „Missing nitrogen problem“
  - Isotopic ratios as fingerprints for evolutionary history
- Nitrogen inversion transitions in band 6
  - $\text{NH}_3$  at 23.7 GHz
  - $^{15}\text{NH}_3$  at 22.6 GHz (potential issue: frequency protection!)
- Band 6 opportunities:
  - mapping
  - higher sensitivity & angular resolution for faint sources
  - increasing chances of detection for comets (ammonia photo-dissociated on short scale)



Effelsberg 100m

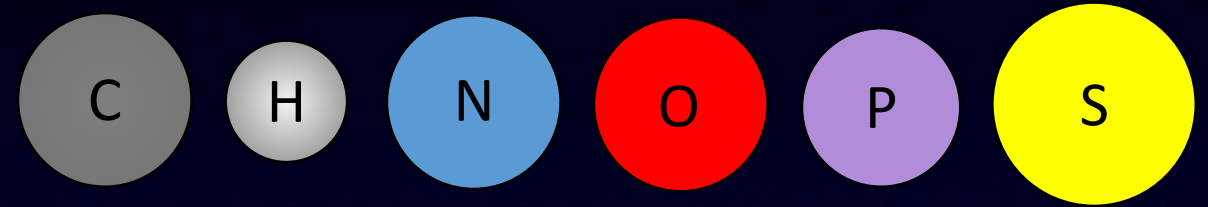
# Semi-volatiles: ammonium salts

- 6 different ammonium salts detected in comet 67P (Altwegg et al. 2020 & 2022, Poch et al. 2020)
- Spectroscopy limited but frequencies available from literature fall in C, X, and Ku band (8-18 GHz)
- Attempts for detection with GBT and Effelsberg were not successful (lack of sensitivity or angular resolution, unstable nature?)
- SKA could provide better sensitivity and angular resolution for ammonium salts, but also other salts (NaCl, NaCN, KCl etc.), e.g. for constraining carriers of sodium



Altwegg et al. 2020, Nat. As. 4, 533

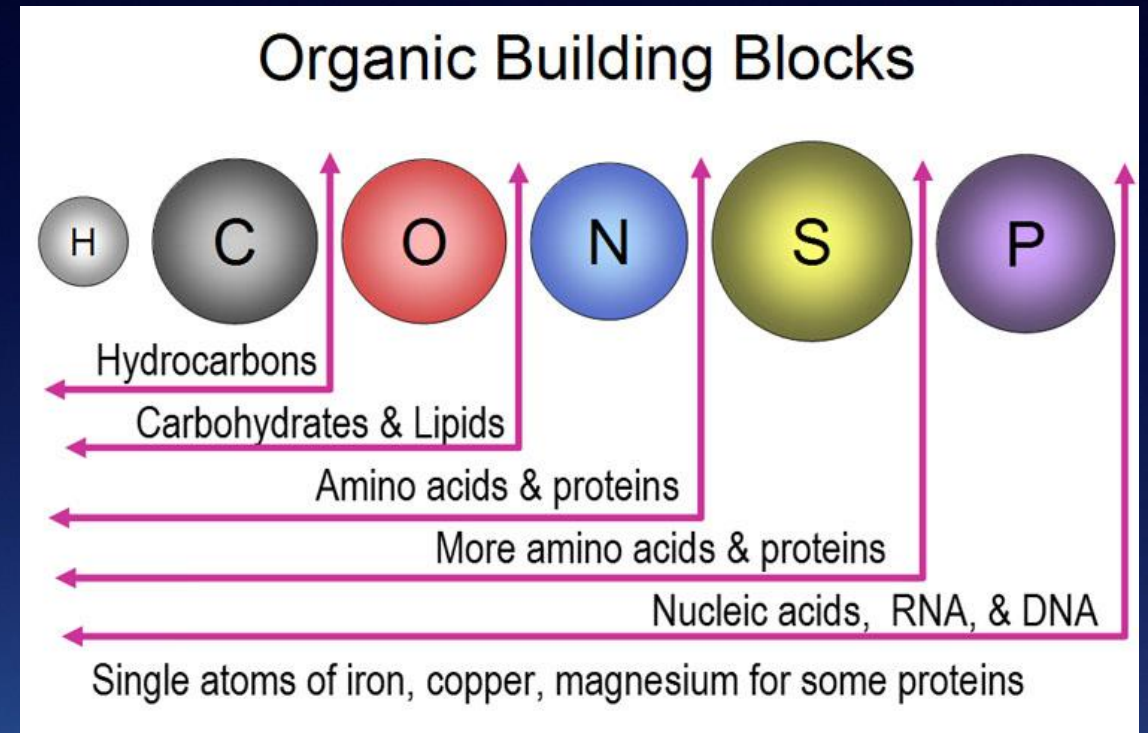
# Carriers of Phosphorus

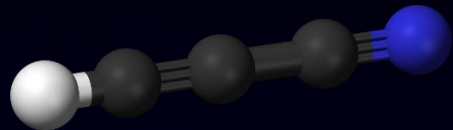


- Phosphorus is a key element for life
- Fundamental rotational transitions of PN at around 46.9 GHz, P<sup>15</sup>N at 44.5 GHz

PH<sub>3</sub> (phosphine) also has transitions in this frequency range

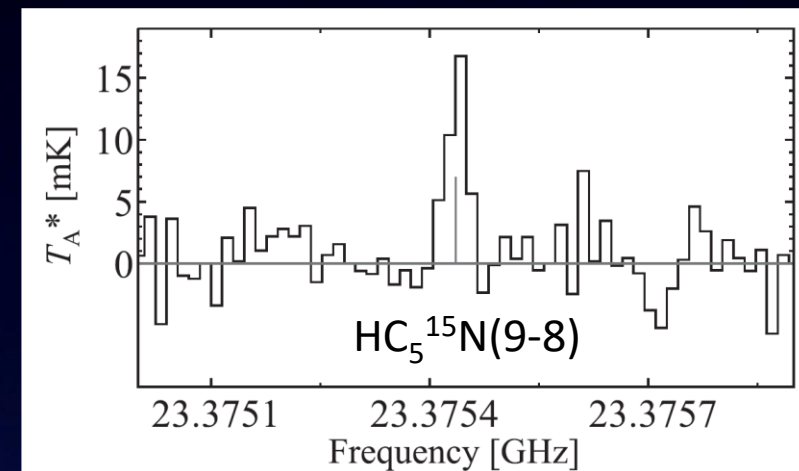
- Band 6 could allow for better constraints on origin and carriers of phosphorus and other essential elements like nitrogen





# Cyanopolyynes

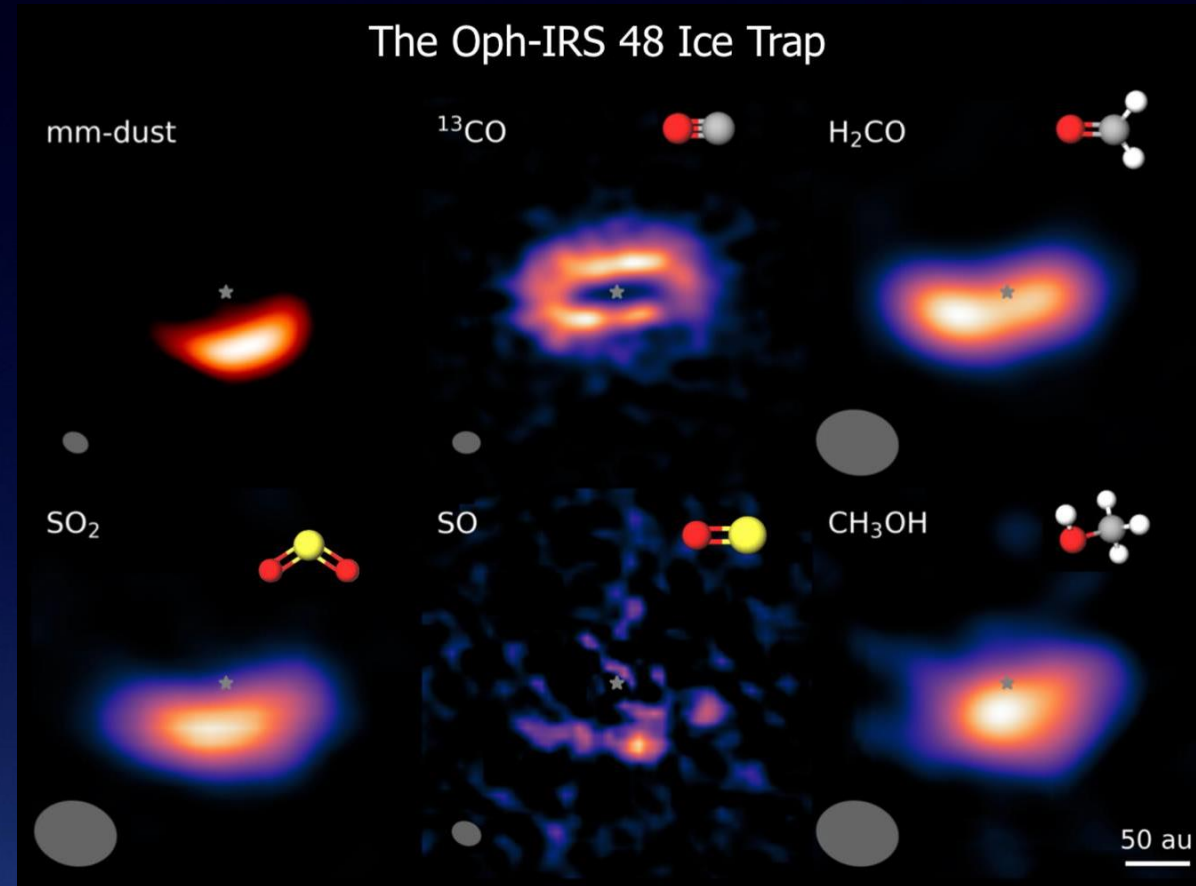
- Cyanopolyynes (e.g.  $\text{HC}_3\text{N}$ ,  $\text{HC}_5\text{N}$ , ...) commonly observed in star-forming regions (irradiated environments)
- Peak of emission for many occurs in band 6 (e.g.  $\text{HC}_5\text{N}$  around 40 GHz at 10 K)
- Studying isotopic fractionation which can provide insight into formation routes and chemistry (requires high sensitivity)
- Mapping is key for understanding chemical links between different species
- Band 6 offers opportunities for surveys and isotopologues



Taniguchi et al. (2017), PASJ, 69, L7

# Synergies with ALMA – multiscale probing

- Complex physical and chemical structures of star-forming regions and disks
- Ability to probe different scales crucial for understanding evolution of disks (e.g. dust traps vs. rings for  $\mu\text{m}$ , mm, (and cm?) dust, different temperature regimes for molecular transitions at different wavelengths)
- Band 6 – especially if frequencies extend beyond 24 GHz – would close the gap between ALMA band 1 and SKA band 5.



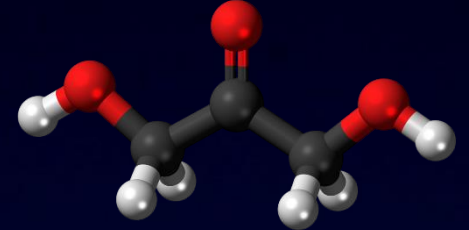
Credit: Nienke van der Marel

# Solar system/star and planet formation

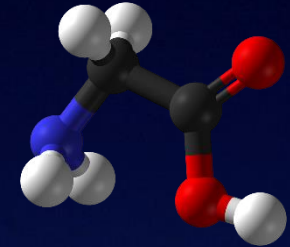
- Protoplanetary disk structure from continuum emission at cm wavelengths as constraints for planet formation models and pebble accretion scenarios, and peering into the terrestrial planet forming zone that may be opaque at higher frequencies
- Study youngest embedded exoplanets and star-planet interactions (aurorae from magnetic interactions, e.g. Pineda & Villadsen 2023)
- Solar system bodies (comets, moons (in particular Enceladus and Titan, planets) – higher angular resolution at shorter wavelengths – in support of space missions and centered around origin of life questions

# High frequencies (band 6) crucial for Astrochemistry!

- Detection of large prebiotic species including building blocks of life like sugars heavily relies on availability of band 5 and 6 frequencies



- Detection of simplest amino acid glycine only feasible in band 6 (too faint in band 5)



- Closing frequency gap with ALMA indispensable for complete picture of chemistry (inventory of species/spectral surveys, constraining excitation conditions, spatial distribution) and understanding link between chemical composition and dust structure in planet-forming regions of disks

→ SKA can only exploit its full potential for astrochemistry with band 6!