CHEMISTRY WITH ALMA

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OVERVIEW

- (extremely brief) Introduction to astrophysics and astronomy
- Molecular lines in radio-submm astronomy
- ALMA interferometer
- Chemistry of star and planet formation done with ALMA
- Public ALMA data in the ALMA Archive



STAR AND PLANET FORMATION



source: <u>phys.org</u>

ALMA OBSERVATIONS OF HL TAU (SUN-LIKE STAR)



ALMA OBSERVATIONS OF HL TAU (SUN-LIKE STAR)



Stellar disk visible thermal emission from heated dust grains organized in concentric rings with gaps.

As planets and asteroids form in the disk, they reshape this disk, sweeping up the material in their orbit, thus creating a disk structure as observed in HL Tau.

STAR-FORMING CLOUDS IN THE MILKY WAY



Our Sun is located in the Galactic disk, in outer region of the Milky Way.

The Milky Way's disk has a spiral arm structure, a central bar and a massive Black Hole (1E6Msun, 1Msun=2E33 g) in the center.

Dense molecular clouds are formed preferentially on the spiral arms (and bar) where the gravitational potential aids the accumulation of gas and dust.

WE ARE IN THE MILKY WAY DISK...

towards Galactic center



BUT OUR GALAXY IS JUST ONE OF MANY



source: <u>scienceblog.com</u>

LOOKING BACK IN TIME: COSMIC STAR FORMATION HISTORY

Apparent star formation peak at redshift $z\sim2$



Madau et al. 2014

z :

 $\overline{\lambda_0}$

MOLECULAR LINES IN SUBMM ASTRONOMY



ISM ENVIRONMENTS IN THE GALAXY

- cold, dense atomic and molecular gas
 - temperatures from ~10K (at high density, shielded gas) to 5000 K (tenuous gas, not shielded)
 - hydrogen densities from 10 cm⁻³(tenuous gas) to 10⁶ cm⁻³(densest location in molecular clouds)
- warm/hot, ionized gas near hot stars



Herschel dust continuum map showing the cold dense medium in red/yellow, and the dust heated by young stars (blue shells) Image: Henneman et al. 2012, ESA

ISM CONSTITUTION AND MASS OF OUR GALAXY

- ► ~20% of mass is in stars, gas and dust (ISM: 99% gas, 1% dust)
- ► Most gas is HI (atomic) or H₂ (molecular)
- ➤ H₂ radiates inefficiently in cold ISM, because the molecule is light and has no permanent dipole moment: H₂ densities are inferred from dust emission or CO emission.
- ~80% of mass is not visible > dark matter, discovered through HI rotation curves

 Observations

$$\frac{mv^2}{r} = \frac{GmM}{r^2}$$

$$\label{eq:main_stant} \begin{split} M \propto R, v &= constant \\ M &= constant, v \propto r^{-0.5} \end{split}$$



Rotation curve of Galaxy M33, Corbelli et al. 2001

EMISSION PROCESSES IN SPACE OBSERVABLE IN THE CM-SUBMM REGIME

- synchrotron emission
- ► bremsstrahlung
- thermal emission of heated dust
- cosmic microwave background
- spectral line transitions
 - atomic transitions (electronic, radio recombination lines)
 - molecular transitions (rotational, vibrational states)
 - molecular masers (population inversion)
 - electronic nuclear spin transitions (21cm line of Hydrogen)

DUST GRAINS: EXTINCTION AND SURFACE FOR CHEMISTRY

- Dust is very effective at absorbing and scattering high frequency photons, prohibiting to measure signals from the dense regions at optical wavelengths
- ► Radio to FIR frequencies are free of dust extinction
- Dust grain surfaces are important for complex chemistry:
 - Also most of molecular hydrogen formed on grains (in cold temperatures)



EXTINCTION BY DUST DOES NOT AFFECT RADIO & SUBMM

Radio-mm spectral lines are thus ideal probes for the kinematics, temperatures and densities of dense regions with dust extinction







Star-forming regin Barnard 68, Bergin & Tafalla 2007

MOLECULES IN THE MILKY WAY (AS OF APRIL 2016 IN CDMS)

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	>12 atom
12	C3*	c-C ₃ H	C5*	C ₅ H	C ₆ H	CH ₃ C ₃ N	CH ₃ C ₄ H	CH ₃ C ₅ N	HC ₉ N	c-C6H6*	HC ₁₁ N
IF	C ₂ H	I-C ₃ H	C4H	<i>I</i> -H ₂ C ₄	CH ₂ CHCN	HC(O)OCH ₃	CH ₃ CH ₂ CN	(CH3)2CO	CH ₃ C ₆ H	n-C3H7CN	C ₆₀ *
ICI	C2O	C ₃ N	C ₄ Si	C2H4*	CH ₃ C ₂ H	CH3COOH	(CH3)2O	(CH ₂ OH) ₂	C ₂ H ₅ OCHO	i-C3H7CN	C70*
2**	C ₂ S	C ₃ O	I-C3H2	CH ₃ CN	HC ₅ N	C7H	CH ₃ CH ₂ OH	CH ₃ CH ₂ CHO	CH3OC(O)CH3	C2H5OCH3 ?	C ₆₀ ⁺ *
н	CH ₂	C ₃ S	c-C3H2	CH ₃ NC	CH ₃ CHO	C ₆ H ₂	HC7N				
e ⁺	HCN	C2H2*	H ₂ CCN	CH ₃ OH	CH ₃ NH ₂	CH ₂ OHCHO	C ₈ H				
N	HCO	NH ₃	CH ₄ *	CH ₃ SH	c-C ₂ H ₄ O	/-HC6H*	CH ₃ C(O)NH ₂				
C	HCO ⁺	HCCN	HC ₃ N	HC ₃ NH ⁺	H ₂ CCHOH	CH ₂ CHCHO (?)	C8H				
o+	HCS ⁺	HCNH ⁺	HC2NC	HC ₂ CHO	С ₆ н [−]	CH2CCHCN	C ₃ H ₆				
P	HOC ⁺	HNCO	нсоон	NH ₂ CHO	CH ₃ NCO 2015	H2NCH2CN	CH ₃ CH ₂ SH (?)				
С	H ₂ O	HNCS	H ₂ CNH	C ₅ N		CH ₃ CHNH					
CI	H ₂ S	HOCO ⁺	H ₂ C ₂ O	/-HC4H*							
CI	HNC	H ₂ CO	H ₂ NCN	I-HC4N							
н	HNO	H ₂ CN	HNC ₃	c-H ₂ C ₃ O			2 atoms	3_atoms	continued	1)	
C	MgCN	H ₂ CS	SiH ₄ *	H ₂ CCNH (?)			02	HCP	continucu		
S	MgNC	H ₃ O ⁺	H ₂ COH ⁺	C ₅ N			CF ⁺	CCP			
CI	N ₂ H ⁺	c-SiC3	C4H	HNCHCN			SiH?	AIOH			
н	N ₂ O	CH3*	HC(O)CN				PO	H ₂ O ⁺			
N	NaCN	C ₃ N ⁻	HNCNH				AIO				
0	OCS	PH ₃	CH ₃ O				710	H201			
o ⁺	SO ₂	HCNO	NH4 ⁺				OHT	KCN			
N	c-SiC2	HOCN	H_2NCO^+ (?)				CN	FeCN			
	- 	110001	NCCNH ⁺				SH ⁺	HO ₂			
0	002	HSCN	2015				SH	TiO ₂			
S	NH ₂	H ₂ O ₂					HCI ⁺	C ₂ N		Source (
S	H3 ^{+ (*)}	C ₃ H ⁺					TiO	Si ₂ C			• 1
F	SICN	HMgNC						2015		<u>www.astr</u>	<u>o.uni-ko</u>
D	AINC	2015					ArH				<u>cdms/m</u>
90?	SiNC						NO ⁺ ?				

EXTRAGALACTIC MOLECULES (APRIL 2016, CDMS)

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	>8 atoms
ОН	H ₂ O	H ₂ CO	c-C ₃ H ₂	CH ₃ OH	CH ₃ CCH	HC ₆ H	c-C ₆ H ₆ *
со	HCN	NH ₃	HC ₃ N	CH ₃ CN	CH ₃ NH ₂		C ₆₀ * (?)
H ₂ *	HCO ⁺	HNCO	CH ₂ NH	HC ₄ H*	CH ₃ CHO		
СН	C ₂ H	C ₂ H ₂ *	NH ₂ CN	HC(O)NH ₂			
CS	HNC	H ₂ CS?	/-C ₃ H ₂				
CH+ **	N_2H^+	HOCO ⁺	H ₂ CCN				
CN	OCS	с-С ₃ Н	H ₂ CCO				
SO	HCO	H ₃ O⁺	C ₄ H				
SiO	H ₂ S	<i>I-</i> C ₃ H					
CO ⁺	SO ₂						
NO	HOC ⁺						
NS	C ₂ S						
NH	H ₂ O ⁺						
OH ⁺	HCS ⁺						
HF	H ₂ Cl ⁺						
SO ⁺	NH ₂						
ArH ⁺ 2015							
CF ⁺ 2016							

Source: Cologne Database for Molecular Spectroscopy, <u>https://www.astro.uni-</u> <u>koeln.de/cdms/molecules</u>

LINE RICHNESS

- ALMA observations of a star-forming core show a line forest
- To identify these molecular lines, knowledge of their rest frequencies, and upper (or lower) state energy is extremely important
- Spectral line identification in astronomy thus depends heavily on laboratory experiments



Beltran et al. 2014

SPLATOLOGUE: ONLINE MOLECULAR DATABASE

http://www.cv.nrao.edu/php/splat/



 $h\nu = E_U - E_L$

	Species	Chemical Name	Ordered Freq (GHz) (rest frame, redshifted)	Resolved QNs	CDMS/JPL Intensity	Lovas/AST Intensity	E _L (cm ⁻¹)	E _L (K)	Linelist
1	H ₂ O v=0	Water	247.44010, 247.44010	14(4,10) - 15(3,13)	-9.00970		2872.5806	4133.0296	JPL
2	H ₂ O v=0	Water	259.95218, 259.95218	13(6,8) - 14(3,11)	-8.66900		2739.4286	3941.4523	JPL
3	H ₂ O v=0	Water	266.57410, 266.57410	21(4,17) - 20(7,14)	-14.10890		5739.2279	8257.5225	JPL
4	HCO [±] v=0	Formylium	267.55763, 267.55763	3-2	-0.85420	12.	8.9250	12.8410	CDMS

Found 4 lines in ALMA Band 6 (211-275 GHz), showing 1 - 4

RADIATIVE TRANSPORT



At radio-submm frequencies (hv/kT is small) the measured brightness temperature with the radio antenna can be approximated by $au_{
u} \propto N/T$

 $T_{A} = (T_{ex} - T_{bg})(1 - \exp(-\tau_{\nu}))$ $\tau_{\nu} < 1 \text{ optically thin: measure column density: } T_{A} \sim T$ $\tau_{\nu} > 1 \text{ optically thick: measure temperature } T_{A} \sim T$

MOLECULAR SPECTROSCOPY

Typical medium Temperature

Table 2. Parameters of the commonly observed short cm/mm molecular lines

Chemical ^a formula	Molecule name	Transition	ν/GHz	E_{μ}/K^{b}	$A_{ij}/\mathrm{s}^{-1^{c}}$	
H ₂ O	ortho-water*	$J_{K_aK_c} = 6_{16} - 5_{23}$	22.235253	640	1.9×10^{-9}	
NH ₃	para-ammonia	(J, K) = (1, 1) - (1, 1)	23.694506	23	1.7×10^{-7}	
NH ₃	para-ammonia	(J, K) = (2, 2) - (2, 2)	23.722634	64	2.2×10^{-7}	K
NH ₃	ortho-ammonia	(J, K) = (3, 3) - (3, 3)	23.870130	122	2.5×10^{-7}	
SiO	silicon monoxide*	J = 1 - 0, v = 2	42.820587	3512	3.0×10^{-6}	
SiO	silicon monoxide*	J = 1 - 0, v = 1	43.122080	1770	3.0×10^{-6}	
SiO	silicon monoxide	J = 1 - 0, v = 0	43.423858	2.1	3.0×10^{-6}	
CS	carbon monosulfide	J = 1 - 0	48.990964	2.4	1.8×10^{-6}	
DCO ⁺	deuterated formylium	J = 1 - 0	72.039331	3.5	2.2×10^{-5}	
SiO	silicon monoxide*	J = 2 - 1, v = 2	85.640456	3516	2.0×10^{-5}	
SiO	silicon monoxide*	J = 2 - 1, v = 1	86.243442	1774	2.0×10^{-5}	
$H^{13}CO^+$	formylium	J = 1 - 0	86.754294	4.2	3.9×10^{-5}	
SiO	silicon monoxide	J = 2 - 1, v = 0	86.846998	6.2	2.0×10^{-5}	
HCN	hydrogen cyanide	J = 1 - 0, F = 2 - 1	88.631847	4.3	2.4×10^{-5}	
HCO^+	formylium	J = 1 - 0	89.188518	4.3	4.2×10^{-5}	
HNC	hydrogen isocyanide	J = 1 - 0, F = 2 - 1	90.663574	4.3	2.7×10^{-5}	
N_2H^+	diazenylium	$J = 1 - 0, F_1 = 2 - 1,$				
		F = 3 - 2	93.173809	4.3	3.8×10^{-5}	
CS	carbon monosulfide	J = 2 - 1	97.980968	7.1	2.2×10^{-5}	
C18O	carbon monoxide	J = 1 - 0	109.782182	5.3	6.5×10^{-8}	
¹³ CO	carbon monoxide	J = 1 - 0	110.201370	5.3	6.5×10^{-8}	
CO	carbon monoxide	J = 1 - 0	115.271203	5.5	7.4×10^{-8}	
H ₂ ¹³ CO	ortho-formaldehyde	$J_{K_{c}K_{c}} = 2_{12} - 1_{11}$	137.449959	22	5.3×10^{-5}	
H ₂ CO	ortho-formaldehyde	$J_{K_{0}K_{0}} = 2_{12} - 1_{11}$	140.839518	22	5.3×10^{-5}	
CS	carbon monosulfide	J = 3 - 2	146.969049	14.2	6.1×10^{-5}	
C18O	carbon monoxide	J = 2 - 1	219.560319	15.9	6.2×10^{-7}	
¹³ CO	carbon monoxide	J = 2 - 1	220.398714	15.9	6.2×10^{-7}	
CO	carbon monoxide	J = 2 - 1	230.538001	16.6	7.1×10^{-7}	
CS	carbon monosulfide	J = 5 - 4	244.935606	33.9	3.0×10^{-4}	
HCN	hydrogen cyanide	J = 3 - 2	265.886432	25.5	8.5×10^{-4}	
HCO^+	formylium	J = 3 - 2	267.557625	25.7	1.4×10^{-3}	
HNC	hydrogen isocyanide	J = 3 - 2	271.981067	26.1	9.2×10^{-4}	

density proportional to A Choose molecular species depending on n, T of gas you want to probe. Also must consider expected strength of line, depends on intrinsic strength (prop to A) +chemical abundance. Must be strong enough to detect, but may want to avoid being optically thick

Critical

n> ncrit - collision dominated and the excitation temperature will close to the kinetic temperature of the gas

PHYSICAL PROPERTIES FROM MOLECULAR LINES



1000

200

400

*E*_ (K)

600

Rotational diagram method:

using several level populations under the assumption that they all come from the same region, are characterized by one temperature and are optically thin allow to obtain the temperature and column density simultaneously

Herbst & van Dishoek 2009

COMPARE WITH CHEMICAL MODELS



Measurements of molecular lines, especially if more transitions or species are involved can than be compared with chemical models (formation pathways) that predict abundances.

Figure 11

Comparison of fractional abundances calculated with gas-phase (*a*) and gas-grain (*b*) models for a cold core with oxygen-rich abundances (C/O = 0.4). The Ohio State networks were used without anions. The model parameters are T = 10 K, $n_{\rm H} = 2 \times 10^4$ cm⁻³, and the cosmic ray ionization rate per H₂ molecule of $\zeta = 1.3 \times 10^{-17}$ s⁻¹. Horizontal lines represent observed species in TMC-1. Provided by D. Quan.

Herbst & van Dishoek 2009

KINEMATICS FROM DOPPLER SHIFTS OF LINES

redshift of the galaxy

°40'36'8

°40'36!D

5(J2000)

(a)

- Rotational curves of Galaxies
- In our own Milky Way, most of the distances are based on their spectral line velocity under the assumption of a rotational model

35

30

V_{LSR} (km,

Collapsing motions, rotating disks around stars

(b)





 ν_0

 Δv

VERY COLD CHEMISTRY: DEPLETION & DEUTERATION

To study the prestellar cores, which centers are very cold <10K and dense (>10⁵ cm⁻³) one need to resort to deuterated molecules because common Cbearing molecules will be depleted



From Ceccarelli & Caselli, PPVI

THE ALMA INTERFEROMETER

ALMA

high sensitivity in radio-submm regime

Iocated at the driest site on Earth: the Chilean Atacama desert



APERTURE SYNTHESIS

- An interferometer measures per each antenna pair (baseline) the source brightness distribution (visibility) at the spatial scale to which the baseline is sensitive.
- With a sufficient number of visibilities measured, one can reconstruct an image by Fourier inversion.
- The interferometer is filters out emission from structures bigger than the shortest baseline and cannot recover structures smaller than then the longest baseline





Images: APSYNSIM

EXAMPLE: OBSERVING 5 GAUSSIANS WITH

V (MN)

V (M.N)

V (M)



E-W offset (km)



with 6 antennas 20min

ALMA 12m array baseline to ~2km 20min

ALMA 12m array, baselines to ~8km 20min

ALMA: HIGH RESOLUTION IMAGING

► antennas are movable, allowing to change the angular resolution, which is proportional to the inverse of the antenna separation, baseline $FOV \propto \frac{\lambda}{D}$ $\theta_{res} \propto \frac{\lambda}{b_{max}}$ $\theta_{max} \propto \frac{\lambda}{b_{min}}$



► the largest angular scale measurable with an interferometer $dependent he short et baseline b_{res} baseline b_{max} \qquad \theta_{max} \propto \frac{\lambda}{b_{min}}$

ALMA SPECTROSCOPY

- ► ALMA will have 10 bands between 30 to 900 GHz
- ➤ can have up to 8GHz of instantaneous bandwidth, and allows high spectral resolution (up to 0.03MHz) $\theta_{\rm synth}$
- full polarization measurements possible



SCIENCE WITH ALMA

CHEMISTRY WITH ALMA: STAR AND PLANET FORMATION



- branched alkyl molecules present in ISM
- cold gas reservoir from ice desorption in protostellar disk
- studying the Titan atmosphere

BRANCHED ALKYL MOLECULES IN ISM

Amino acids have been found in meteorites. It is not known whether the amino acids have been present in the ISM from which the meteorite formed (protostellar disk), or if they formed on the meteoroid/asteroid.



X-axis: various meteorites (Burton et al. 2012)

CM2: Murchinson meteorite



BRANCHED ALKYL MOLECULES WITH ALMA

Branched propyl cyanide detected in Sgr B2 (star-forming region near the Galactic Center) by Belloche et al. (2015). Due to the very high column density of Sgr B2 allowed the detection of this low-abundance species.



BRANCHED ALKYL MOLECULES WITH ALMA

The abundance of i- (branched) and n- (straight chain) propyl cyanide in Sgr B2 is 0.4:1. In meteorites the branched amino acids dominate over their straight chain isomers.



Belloche et al. 2015

BRANCHED ALKYL MOLECULES WITH ALMA

Chemical models favor a bias toward branched propyl cyanide (2.2:1), however there are several uncertainties regarding the chemistry on the surface of icy dust grains.

fractional chemical abundances of alkyl cyanides with respect to molecular hydrogen, H₂. These abundances represent the warm-up phase of hot-core evolution. Solid lines indicate gas-phase species; dotted lines of the same color indicate the same species in the solid phase. The main phase change from solid to gas for each molecule is caused by thermal desorption from the grain surfaces, according to speciesspecific binding energies.

Fig. 3. Simulated



The detection of this branched iso-propyl cyanide suggests that there is a link between interstellar chemistry in star-forming regions and the molecular composition of meteors.

Corrected 3 October, 2014; see full text.

Belloche et al. 2015

GAS/DUST DISTRIBUTION IN PROTOSTELLAR DISKS

- Planet formation occurs in the protostellar disk from the refractionary dust, volatile (chemical compounds with low boiling points, e.g. CO, CO₂, NH₃,H₂O) ice, and gas
- spatial distribution of volatile abundances helps to determine the composition of nascent planets at different disk radii



EVOLUTION OF A PROTOSTELLAR DISK



DISK TEMPERATURE AND MOLECULAR EMISSION



desorption of CO back to gas phase by interaction with high energy photons due to decrease of density

COLD GAS RESERVOIR IN PROTOSTELLAR DISK VIA ICE DESORPTION

DCO⁺ is found in two concentric rings, an inner ring (warm CO, small dust grains present) and an outer ring (cold CO, no small dust grains)



COLD GAS RESERVOIR IN PROTOSTELLAR DISK VIA ICE DESORPTION





- inner ring: in balance with CO thermal desorption due to radial decrease in disk temperature
- outer ring: evidence of non-thermal desorption of CO and the efficient formation of DCO⁺ via :

 $H2D^+ + CO \rightarrow H_2 + DCO$

• outer ring is not coincident with dust continuum emission, meaning that the density of small dust grain have decreased - also grain growth would explain the decrease in dust continuum emission and UV shielding.

Oeberg et al. 2015

TITAN ATMOSPHERE

- Titan (Mass~2M_{moon}) is the only moon with a dense atmosphere in our Solar system and the only other body which has a liquid surface (Stofan et al. 2007)
- Atmosphere: 98% Nitrogen, 2% methane (earth: 78% nitrogen, 21% oxigen, 0.9 argon)



ETHYL CYANIDE (C₂H₅CN) TO CONSTRAIN TITAN CHEMISTRY

- From lab plasma-discharge experiments expected to be highly abundant (e.a. Thomson et al. 1991)
- C₂H₅CNH⁺ found by Cassini satellite (Vuitton et al. 2007)
- Measures of C2H5CN necessary to constrain formation pathways, and constrain models for for the formation of nitriles and other large organic molecules



ETHYL CYANIDE (C₂H₅CN) WITH ALMA

ALMA's four spectral windows:



Cordiner et al. 2015

ETHYL CYANIDE (C₂H₅CN) WITH ALMA



Southern hemisphere ethyl cyanide peak

Titans seasons cause a reversal (N-S) of the atmospheric circulation: the disappearance of ethyl cyanide in the north implicates a shorter chemical lifetime than that of the CH3CN, HC3N, and CH3CCH

color: Titan continuum emission, contours: molecular line emission

ETHYL CYANIDE (C₂H₅CN) WITH ALMA

Table 2 Best-fitting C2H5CN Model Abundances and Vertical Column Densities								
Model	Abundance (ppb)	z_r^a (km)	χ^2	$N (\mathrm{cm}^{-2})$				
Step (100 km)	0.79	100	1.43	1.3×10^{15}				
Step (200 km)	3.24	200	1.01	4.6×10^{14}				
Step (300 km)	9.25	300	0.97	1.7×10^{14}				
Step (400 km)	73.1	400	0.98	2.1×10^{14}				
Gradient	1.30	292	0.97	3.6×10^{14}				

^a Reference altitude for abundance.



Comparing various radiative transfer models with ALMA measure of ethyl cyanide it can be deduced that methyl cyanide is most concentrated at altitudes of 200km and higher.

Cordiner et al. 2015

CALIBRATED ALMA DATA IN ARCHIVE

- ► 1 year after delivery to PI, data are publicly available on the ALMA archive
- You can download raw data with a reduction script in CASA (ALMA data reduction software)
- ➤ You can always ask help to the Italian ARC @ IRA :)

