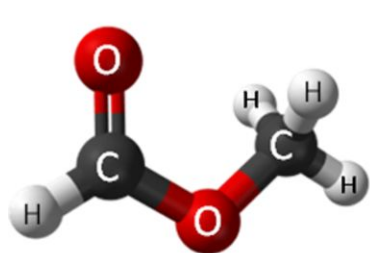


Observations of Complex Organic Molecules

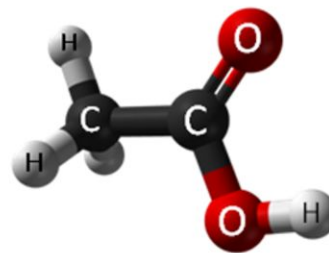
Tom Millar

School of Mathematics and Physics

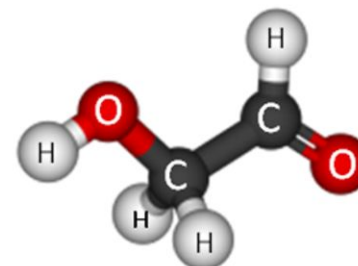
Queen's University Belfast



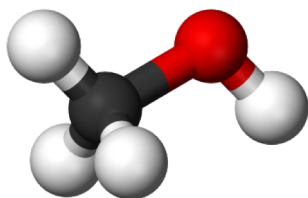
Methyl formate



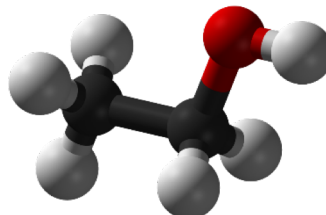
Acetic acid



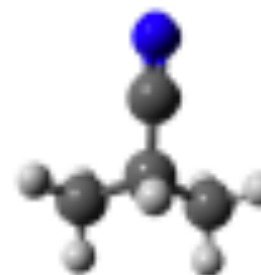
Glycolaldehyde



Methanol



Ethanol

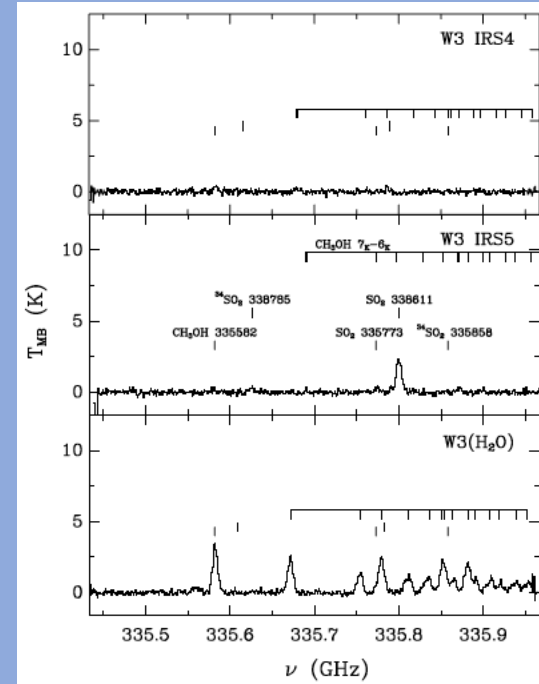
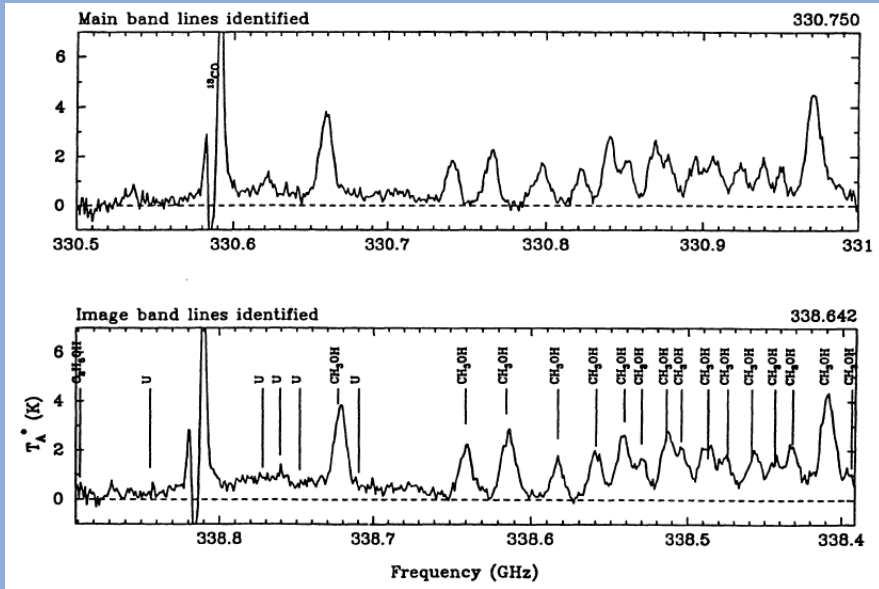


iso-Propyl Cyanide

Interstellar and Circumstellar Molecules

2-atom		3-atom		4-atom		5-atom	6-atom	7-atom	8-atom	9-atom	10-atom
H2	ArH+	H3+	SiCN	CH3	CNCN	CH4	CH3OH	CH3NH2	HCOOCH3	(CH3)2O	(CH3)2CO
CO	CO+	CH2	SiNC	NH3		CH2NH	CH3SH	CH3CCH	CH3C3N	C2H5OH	CH3C5N
CS	NS+	NH2	c-SiC2	H3O+		H2CCC	C2H4	CH3CHO	HC6H	C2H5CN	CH3CH2CHO
CN	NS	H2O	SiCSI	H2CO		c-C3H2	CH3CN	c-CH2OCH2	C7H	CH3C4H	(CH2OH)2
C2	O2	H2S	AlOH	H2CS		CH2CN	CH3NC	CH2CHCN	HOCH2CHO	C8H	CH3OCH2OH
CH	N2(?)	CCH	AlNC	c-C3H		NH2CN	HC2CHO	HC5N	CH3COOH	HC7N	CH3CHCH2O
CH+	HCl+	HCN	NaCl	l-C3H		CH2CO	NH2CHO	CBH	H2CCCHCN	CH3CONH2	11-atom
HF	AlO	HNC	FeCN	C2H2		HCOOH	HC3NH+	CH2CHOH	H2C6	CH3CHCH2	HC9N
CF+	AlF	HCO	KCN	HCNH+		C4H	H2CCCC	C6H-	CH2CHCHO	C8H-	CH3C6H
SiO	HS	HCO+	CCN	H2CN		HC3N	C5H	CH3NCO	NH2CH2CN	C2H5SH	CH25OCHO
SiS	NaCl	HOC+	CCP	HCCN		HCCNC	HC4H	HC5O	CH3CHNH	HC7O	CH3COOCH3
SiC	FeO(?)	N2H+	HCP	HNCO		HNCCC	HC4N		CH3SiH3	CH3NHCHO(?)	12-atom
SiN	SiH(?)	HNO	HS2	HOCN		H2COH+	c-C3H2O				C6H6
NH	NO+(?)	HCS+	HCS	HCNO		C4H-	CH2CNH				C3H7CN
NO		C3	HSC	HNCS		SiH4	C5N-				C2H5OCH3
SO		C2O		HSCN		C5	C5N				> 12-atom
SO+		C2S		C3N		SiC4	C5S				C60
CP		SO2		C3O		CNCHO	SiH3CN				C70
PO		N2O		C3S		CH3O					C60+
PN		CO2		C3N-		NH3D+					c-C6H5CN
HCl		H2O+		HCO2+		NCCNH+					
KCl		H2Cl+		PH3		H2NCO+(?)					
AlCl		OCS		c-SiC3		CH3Cl					
OH		MgNC		HOOH							
OH+		MgCN		l-C3H+							
SH+		NaCN		HCCO							
CN-		HO2		HMgNC							

204 molecules



W3 – JCMT
 334-365 GHz
 14 species plus 24
 isotopomers
 Helmich & van
 Dishoeck 1997

G34.3+0.15 – JCMT 330-360 GHz
 338 lines, inc. 70 U-lines
 35 species plus 19 isotopomers
 Macdonald et al. 1996

Rotational diagram analysis – Rotational temperatures, column densities

Radiative transfer calculations – densities, temperature, abundance



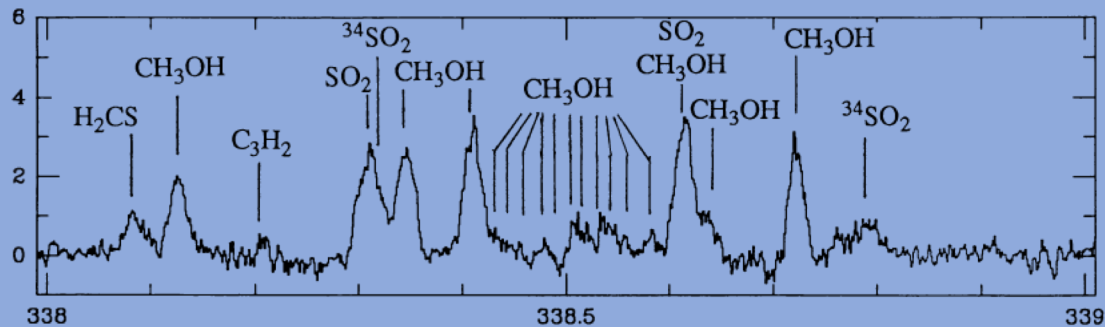
CLOUD STRUCTURES

Sgr B2 Line Surveys

1986 – Bell Labs – Cummins et al – 100GHz, 450 lines, 39 species

1989, 1991 – NRAO – Turner – 100 GHz, 700 lines, 36 species

1991 – CSO – Sutton et al – Sgr B2(M) – 330-355 GHz, 128 lines, 22 species



1998 – SEST – Numellin et al – N, M, NW – 218-264 GHz, 1730, 660, 110 lines

2013 – IRAM – Belloche et al – N, M – 80-116 GHz, 3700, 950 lines, including

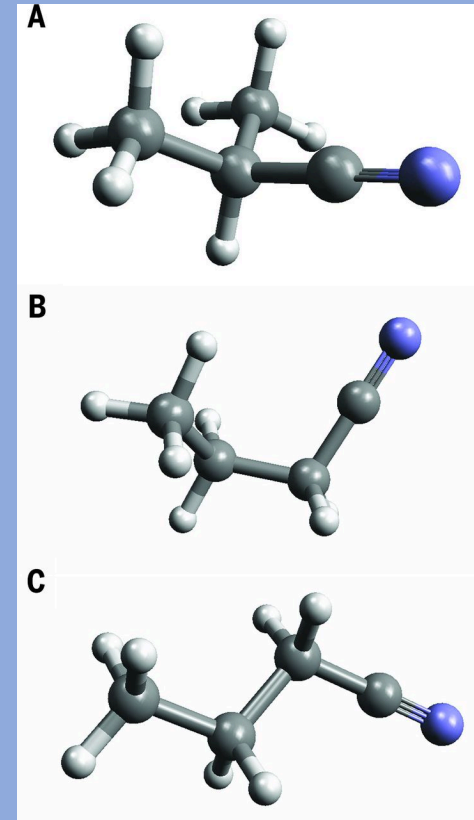
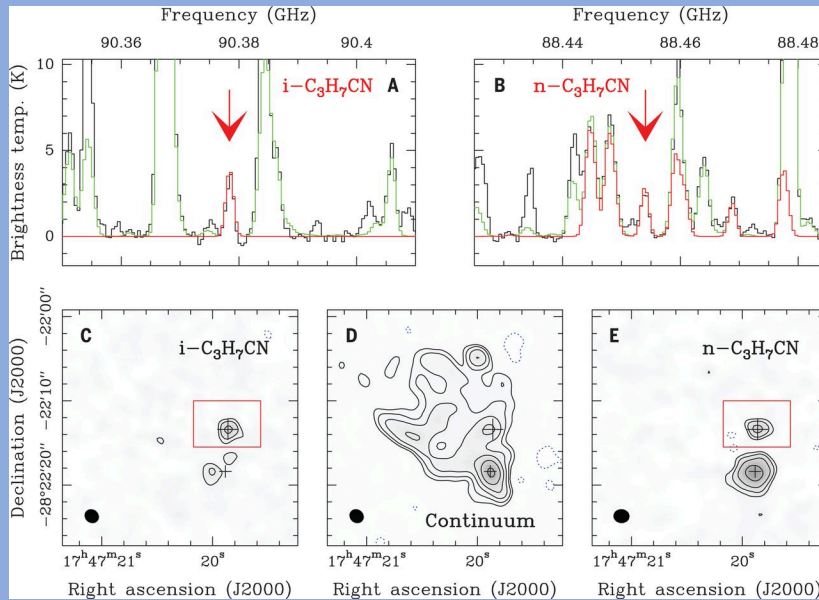
many COMs: amino acetonitrile $\text{NH}_2\text{CH}_2\text{COOH}$, n-propyl cyanide, $\text{C}_3\text{H}_7\text{CN}$, ethyl formate $\text{C}_2\text{H}_5\text{OCHO}$,

56, 46 species detected

30, 50% of all lines are U-lines

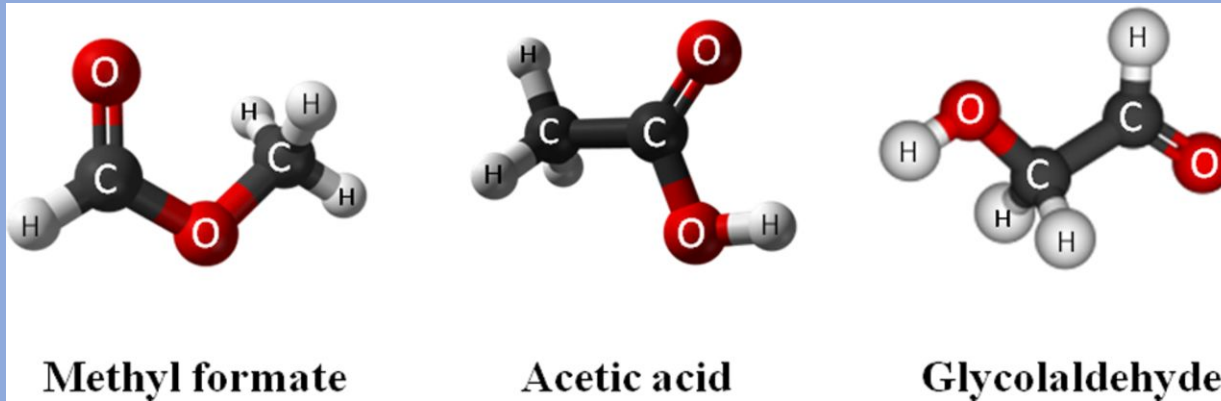
Sgr B2 Line Surveys

2014 – ALMA – Belloche et al – iso-propyl cyanide

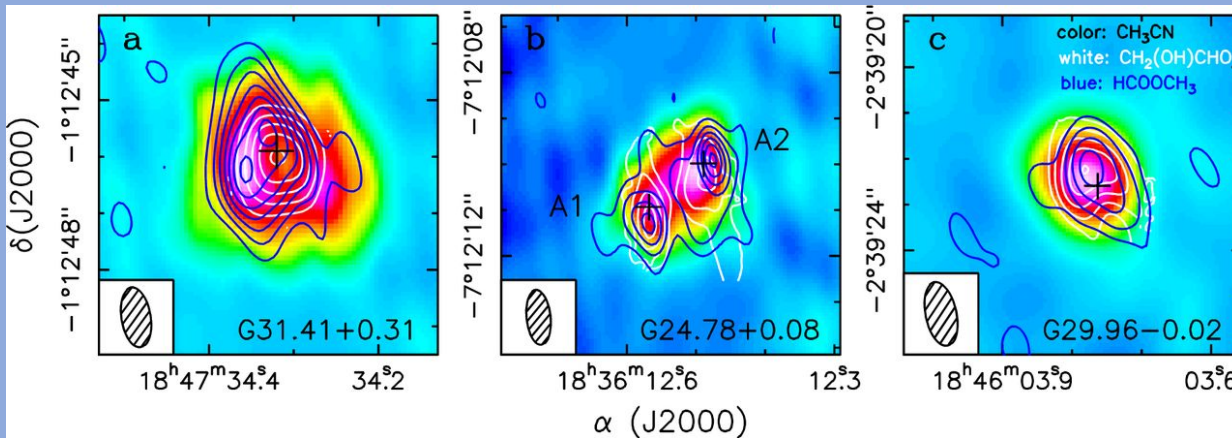


Identify new molecules by fitting LTE calculated spectra of **ALL** identified molecules

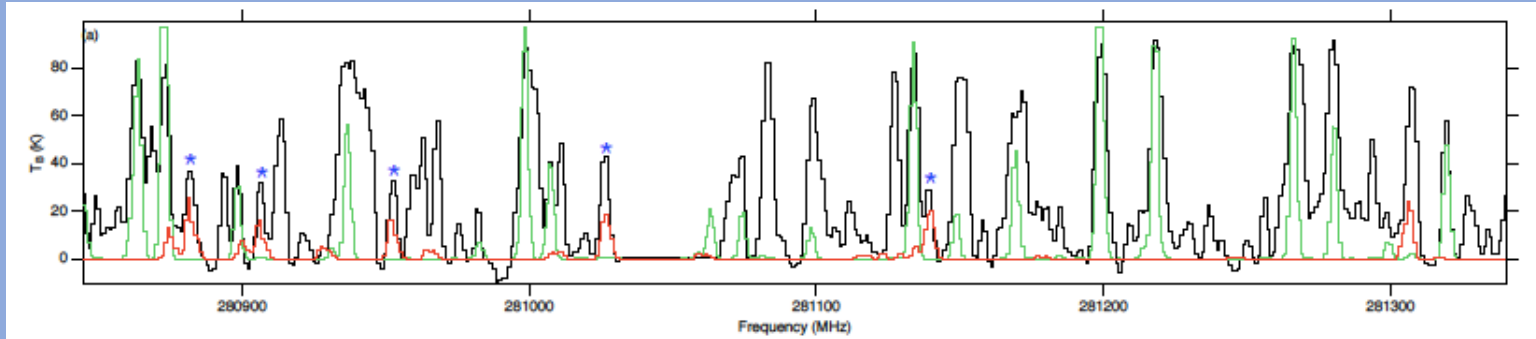
COMs in Hot Molecular Cores



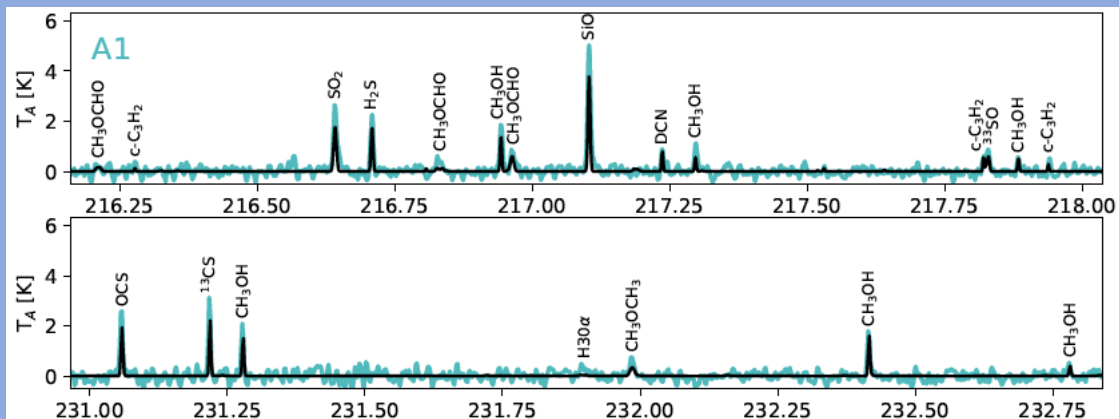
PdBI Maps: Methyl formate (blue), glycolaldehyde (white), CH₃CN (colours) Calcutt et al. 2014 MNRAS, 443, 3157



Complex Chemistry – Hot IS Clouds



ALMA detection of methoxymethanol, $\text{CH}_3\text{OCH}_2\text{OH}$, in NGC 6334I MM1, $T_{\text{rot}} = 200\text{K}$
 Formation: $\text{CH}_3\text{O} + \text{CH}_2\text{OH}$ on ice
 McGuire et al ApJL, 851, L46 (2017)



ALMA: COMs in the LMC
 CH_3OH , CH_3OCHO , CH_3OCH_3
 $T_{\text{rot}} = 130\text{K}$
 Sewilo et al ApJ, 853, L19 (2018)

Solar mass protostars

Ophiuchus d=125 pc low-mass star-forming region



IRAS16293-2422

Rich source of organic and deuterated molecules

(van Dishoeck+ 1995, Cazaux+2003)

NASA/WISE

IRAS 16293-2422

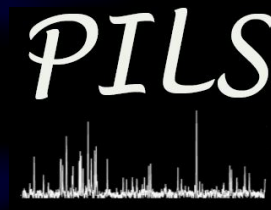
ALMA: 0.4-3 mm

Source B
Face-on disk

Source A
Inclined disk

Pineda et al. 2012
Oya et al. 2016

Protostellar Interferometric Line Survey (PILS)



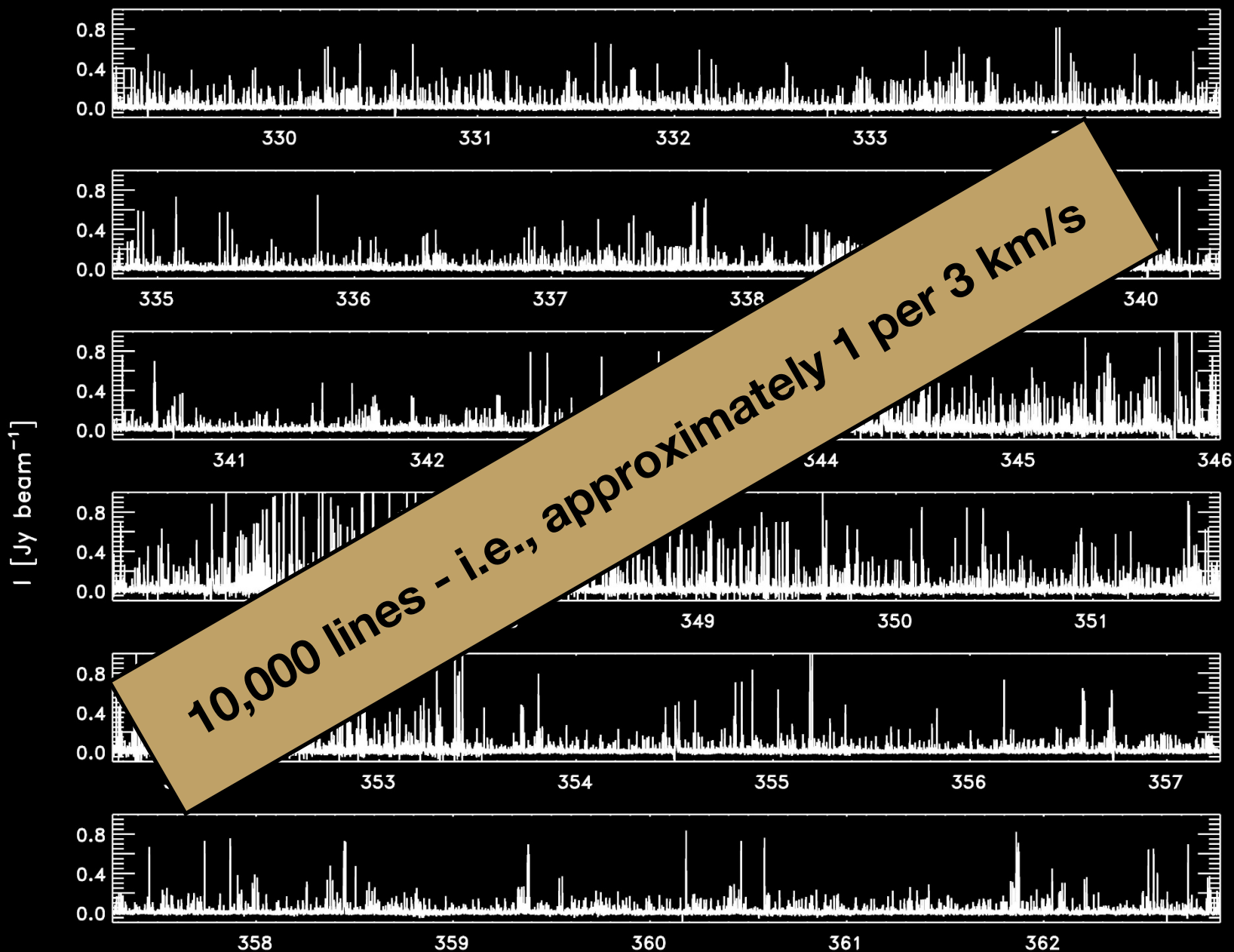
329-363 GHz
0.5 acsec res
Sensitivity 100x

Jørgensen et al. 2016

60 AU



PILS survey: Full spectral survey of IRAS 16293–2422



Freq [GHz]

Jørgensen et al. 2016, 2018

PILS – Deuterated COMs

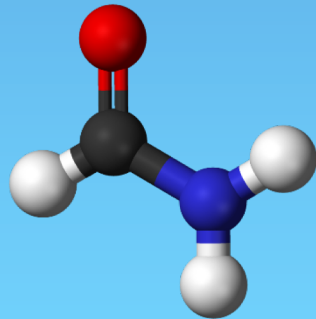
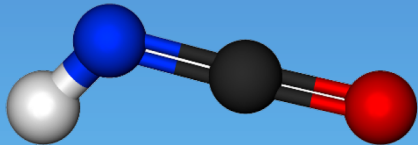
6-atom	7-atom	8-atom	9-atom
CH ₂ DOH	CH ₃ CDO	CH ₂ DOCHO	CH ₂ DOCH ₃
CH ₃ OD		CH ₃ OCDO	CH ₂ DCH ₂ CN ?
CHD ₂ OH		CH ₂ OH CDO	CH ₃ CHDCN ?
CD ₃ OH		CHDOHCHO	CH ₂ DCH ₂ OH
CH ₂ DCN		CH ₂ ODCHO	CH ₃ CHDOH
NHDCHO			
NH ₂ CDO			

Recent detection of doubly-deuterated methyl formate
CHD₂OCHO

HDO/H₂O < 0.1%

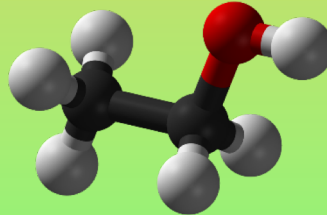
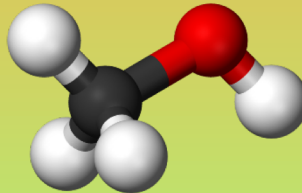
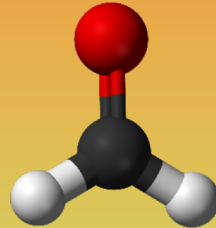
Very high deuteration: groups of COMs?

Isocyanic acid,
formamide



D/H ~ 1%

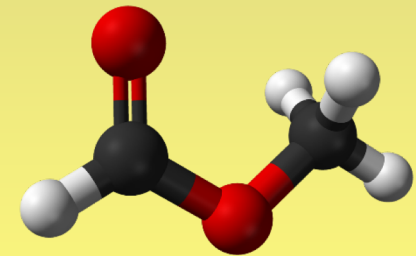
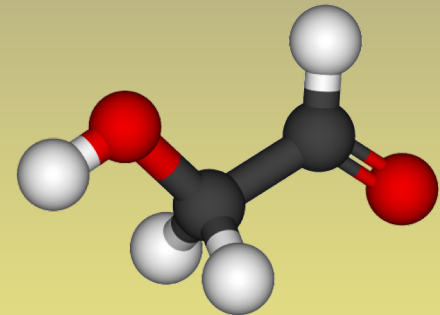
Formaldehyde,
methanol, ethanol



D/H ~ 2%

¹²C:¹³C ~ ISM

Glycolaldehyde,
methyl formate



D/H ~ 5%

¹²C:¹³C ~ 0.5 × ISM

COMs – Unexpected Consequences

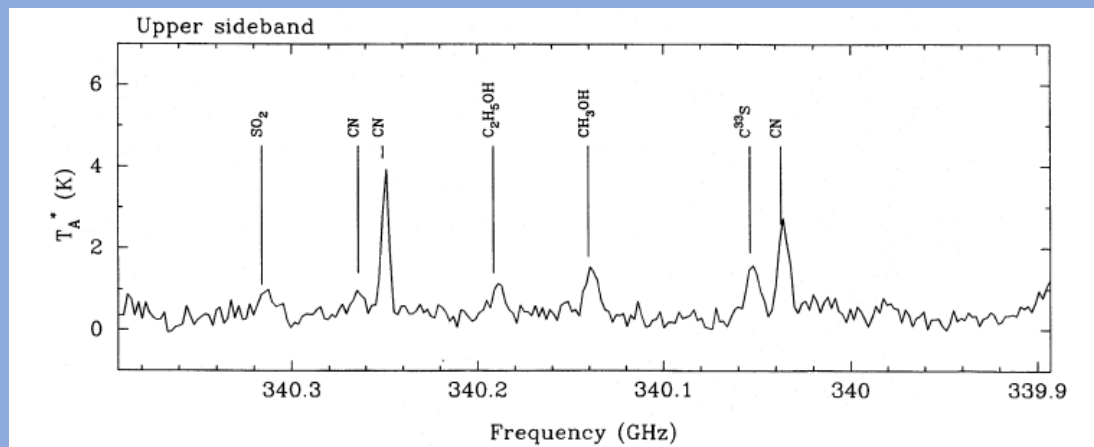
Mon. Not. R. Astron. Soc. **273**, 25–29 (1995)

The detection of hot ethanol in G34.3+0.15

T. J. Millar,¹ G. H. Macdonald² and R. J. Habing²

¹Department of Mathematics, UMIST, PO Box 88, Manchester M60 1QD

²Electronic Engineering Laboratories, The University of Kent at Canterbury, Canterbury, Kent CT2 7NT



300,000 pints of beer a day for every person on Earth for next Billion years

The Sun, March 18 1995

3 G

THE SUN, Saturday, March 18, 1995 7

Sun's the



Jamie... set up fondling

I planned TV grope

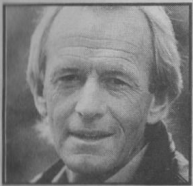
MOVIE star Jamie Lee Curtis has admitted she TOLD a comedian to grope her boob at a Hollywood awards bash.

Millions of TV viewers saw Jon Lovitz fondle her as she received a prize at the American Comedy Awards this month.

Jamie seemed shocked and retaliated by grabbing his groin.

Critics branded Lovitz "crude." But Jamie, 36, said: "I don't want Jon to take the heat. They asked us to do funny things. It was my idea."

biz for



Hogan... £2m movie role

Hogan's Flipped

CROCODILE Dundee star Paul Hogan is set to make a splash in a film version of Flipper.

CRATER BROWN ALE

Boffins
find huge
cloud of
alcohol
in space



ET foam home... how movie favourite would look enjoying a pint of outer-space ale

By DAVID WOODING, Spaced-Out Correspondent

STARGAZERS have found a boozers' paradise in outer space — a gigantic mass of pure alcohol.

They stumbled across a mystery cloud while peering through their telescopes at a distant constellation.

Now after months of research they have learned the mystery object is the final front-beer... enough alcohol to make **400 TRILLION, TRILLION** pints of beer.

That's 300,000 pints a day for every person on Earth for the next **BILLION** years. It would fill the world's oceans tens of thousands of times over.

Frozen

But star-trekkers who want to beam up for a quick one had better think again — the bar at the end of the Universe is 10,000 light years away — or 58,656,960,000,000 miles.

Last night, the three British astronomers who made the discovery were raising their glasses in a more down-to-Earth toast.

Geoff Macdonald and Rolf Habing, of the University of Kent and Tom Miller, of the University of Manchester Institute of Science and Technology, were the boffins who spotted the cloud.

They were looking through the powerful James Clerk Maxwell Telescope on Hawaii at a newly formed star called G184 in the

10 STOUT OF THIS WORLD DRINKS

- 1 Interstellar Artois
- 2 Carling Black Hole Label
- 3 Tennants Extra Terrestrial
- 4 Adnams Alien
- 5 Mars-tons Pedigree
- 6 Watneys Red Planet
- 7 Miller Lite Years
- 8 Rolling Rocket
- 9 Castlemoon XXXX
- 10 Red Spock Cider

constellation of Aquila. Further studies revealed that heat from the new star is producing alcohol faster than all the world's breweries and distilleries put together.

At minus 140°C the cloud is warm by space standards — but the brew could be comfortably drunk without ice.

As Captain Kirk might say if he stumbled across the alcoholic haze: "Booze me up, Scotty."

Only one problem in outer space, though: the rules.

ILS ONT DÉCOUVERT DE

A des milliers d'années-lumière, c'est un nuage dans l'espace. Et c'est la plus grande "cave" de l'univers : des milliards de milliards de litres d'alcool pur. Deux chercheurs viennent de découvrir cette chose stupéfiante.

PAR PATRICE LANOY

Vous pouvez imaginer une pile de quatre cent mille milliards de pintes de bière ? Cela ferait un joli mur, non ? De quoi boire pendant des milliers d'années pour tous les Terriens.

A l'évidence, Geof MacDonald, sujet de Sa Majesté et astronome à l'université du Kent, est ravi de son petit calcul. Pour ponctuer sa phrase, il vient d'ailleurs d'écopier d'un trait sa « lady » ambrée. Au Loss O' Gowrie, un très honorable pub, haut lieu des adorateurs de la pure malt de Manchester, nous avons sacrifié au culte, en compa-

gnie de Tom Miller, chimiste et mathématicien à l'université locale. Le temps, pour les deux scientifiques, d'expliquer pourquoi leur trouvaille d'un gigantesque nuage d'alcool, flottant dans l'espace, à une distance d'environ 10 000 années-lumière de distance de notre planète (une année-lumière équivaut à 9 500 milliards de kilomètres) constitue une affaire de la plus intersidérale importance.

— *Cela ressemble à une plaisanterie, mais c'est très sérieux, renchérit MacDonald, c'est même une nouvelle étape de la cosmochimie.* Ne fouillez pas des yeux la nuit

du printemps. Si les chercheurs britanniques, en coopération avec une équipe de l'université de l'Ohio (Etats-Unis), ont déniché de l'alcool dans la constellation de l'Aigle (l'étoile principale en est Altaïr), le nuage, même gigantesque, restera invisible à vos yeux. C'est en analysant des ondes radio millimétriques, captées par une antenne située à 4 000 mètres d'altitude, sur les hauteurs volcaniques du Mauna Kea d'Hawaï (radiotélescope anglo-hollandais James Clerk Maxwell), que les chercheurs ont pu localiser cette étrange formation. Il se trouve que les

A LA SANTÉ DU COSMOS !

Le Pr Geof MacDonald (à gauche, photo de gauche) a calculé le nombre de pintes de bière représenté par le nuage d'alcool qu'il a découvert dans le cosmos, avec son ami le Pr Tom Miller (à droite). Un chiffre... astronomique. Ci-contre : ils nous montrent la constellation de l'Aigle (en blanc), où flotte ce gigantesque nuage.

PHOTOS: PASCAL CHEUREUX



Le Figaro, May 1995

Open Questions

- Physics of PPDs and Hot Cores/Corinos
- Results **sensitive** to physical model assumed
 - Grain size distribution, porosity
 - Gas and grain temperatures
- **Accurate** reaction rate coefficients
 - Routes to COM formation in gas-phase (hot and cold)
- **Accurate** surface parameters (binding energies, diffusion energies, activation barriers, ice composition and morphology)
- **Accurate** description of surface (and bulk?) chemistry
 - H atom addition/abstraction
 - How complex is this chemistry?
 - Deterministic vs. stochastic
 - Thermal and non-thermal **desorption mechanisms**
- Conversion of laboratory rates to interstellar rates
- ALMA is a wonderful tool to probe PPDs, Hot Cores/Corinos but large COMs will be difficult to detect in PPDs