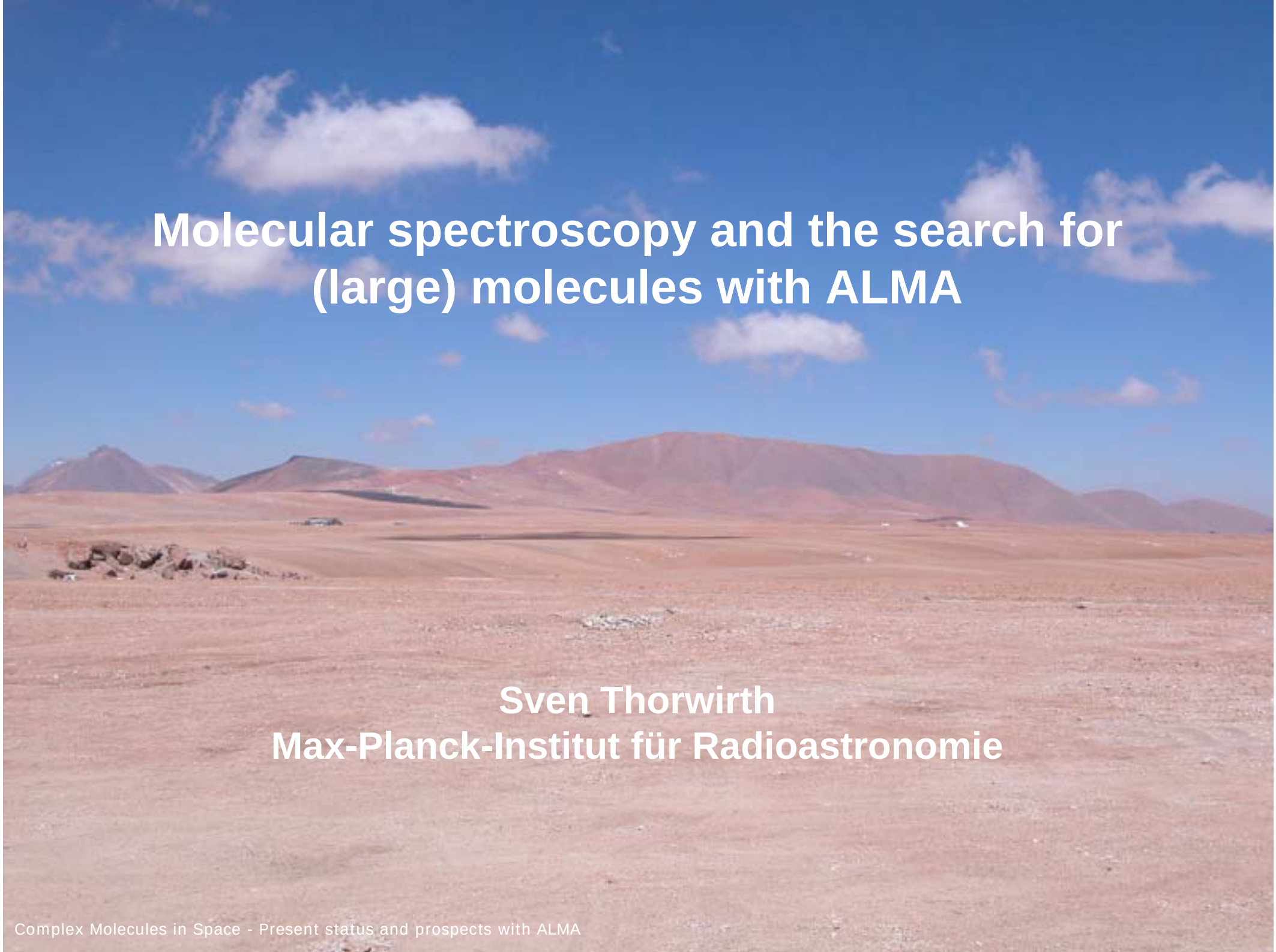
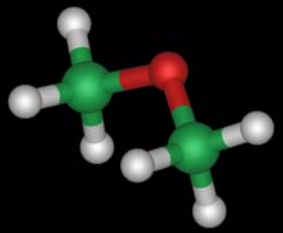


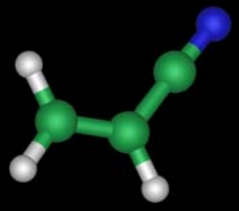
Molecular spectroscopy and the search for (large) molecules with ALMA

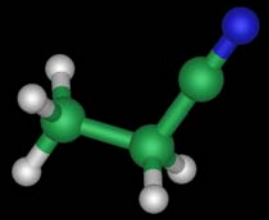
Sven Thorwirth
Max-Planck-Institut für Radioastronomie

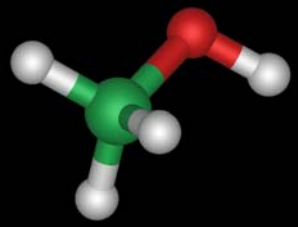
Molecules in Space

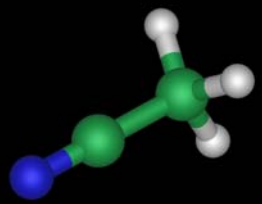
2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	13 atoms
H_2	C_3	c-C_3H	C_5	C_5H	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N	HC_9N	C_6H_6	$HC_{11}N$
AlF	C_2H	l-C_3H	C_4H	l-H_2C_4	CH_2CHCN	$HCOOCH_3$	CH_3CH_2CN	$(CH_3)_2CO$	CH_3C_6H	$CH_3OC_2H_5$	
AlCl	C_2O	C_3N	C_4Si	C_2H_4	CH_3C_2H	CH_3COOH	$(CH_3)_2O$	$(CH_2OH)_2$ (?)		$(CH_2OH)_2CO$ (?)	
C_2	C_2S	C_3O	l-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH	H_2NCH_2COOH (?)			
CH	CH_2	C_3S	c-C_3H_2	CH_3NC	CH_3CHO	H_2C_6	HC_7N	CH_3CH_2CHO			
CH^+	HCN	C_2H_2	CH_2CN	CH_3OH	CH_3NH_2	CH_2OHCHO	C_8H				
CN	HCO	NH_3	CH_4	CH_3SH	c-C_2H_4O	l-HC_6H (?)	CH_3CONH_2				
CO	HCO^+	HCCN	HC_3N	HC_3NH^+	H_2CCHOH	CH_2CHCHO (?)					
CO^+	HCS^+	$HNCH^+$	HC_2NC	HC_2CHO		$H_2CCCHCN$					
CP	HOC^+	HNCO	HCOOH	NH_2CHO							
SiC	H_2O	HNCS	H_2CNH	C_5N							
HCl	H_2S	$HOCO^+$	H_2C_2O	l-HC_4H							
KCl	HNC	H_2CO	H_2NCN	l-HC_4N							
NH	HNO	H_2CN	HNC_3	c-H_2C_3O							
NO	MgCN	H_2CS	SiH_4								
NS	MgNC	H_3O^+	H_2COH^+								
NaCl	N_2H^+	c-SiC_3									
OH	N_2O	C_3H									
PN	NaCN										
SO	OCS										
SO^+	SO_2										
SiN	c-SiC_2										
SiO	CO_2										
SiS	NH_2										
CS	H_3^+										
HF	H_2D^+, D_2H^+										
SH	SiCN										
HD	AlNC										
FeO (?)	SiNC										
O_2 (?)											

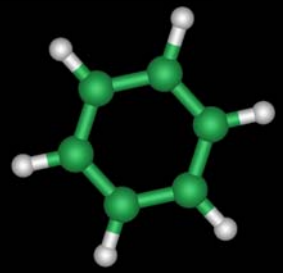












Max-Planck-Institut für Radioastronomie

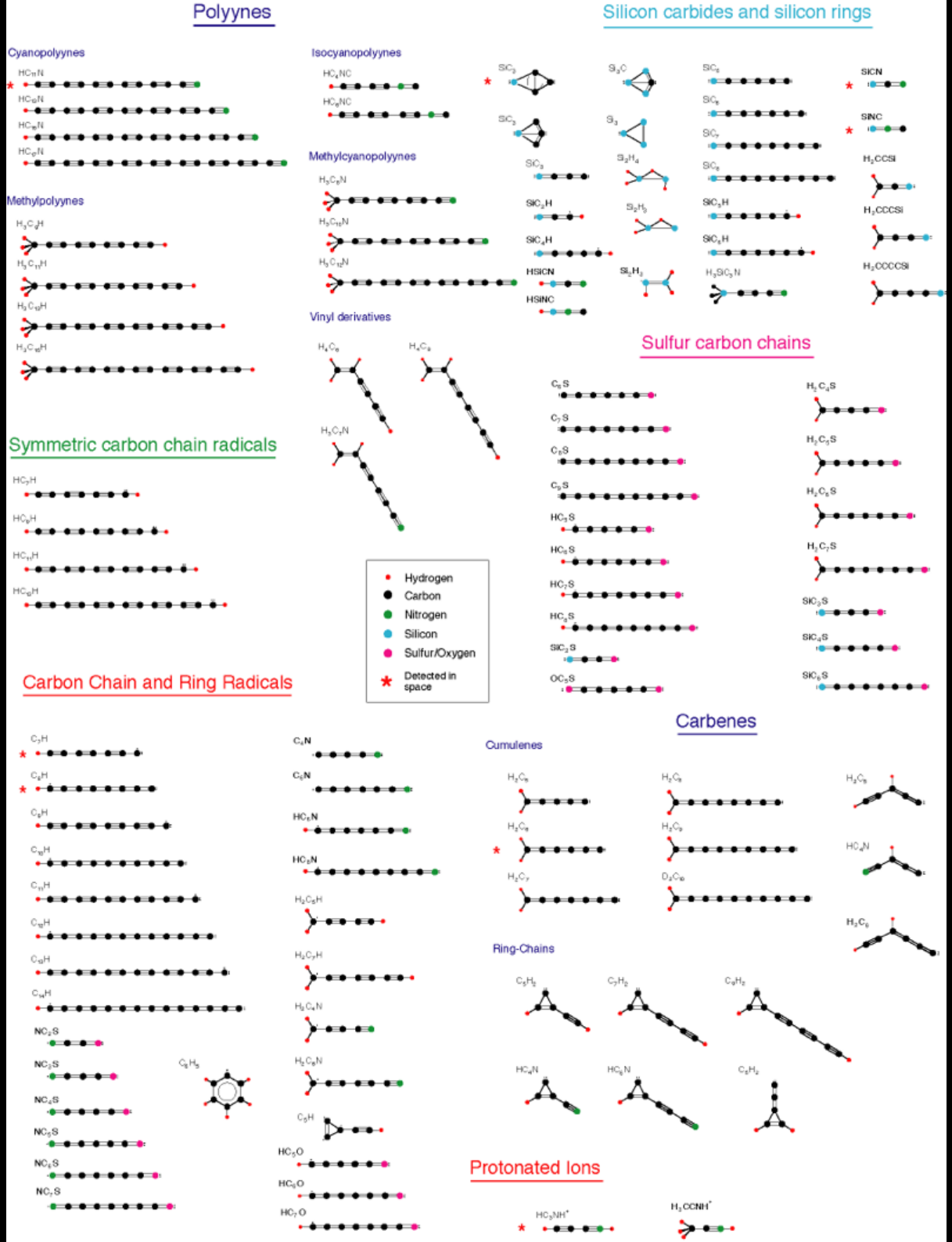
Gas phase spectroscopic characterization in the laboratory

Centimeter wave spectroscopy: Waveguide spectrometers
Fourier transform microwave spectroscopy (FTMW)
(Heated sources, Laser ablation)
2.5 to 45 GHz
(⇨ S. Brünken)

Mm-/submm wave spectroscopy: Klystrons/Multipliers
Backward Wave Oscillators (BWOs)
BWOs/Multipliers
Laser sideband spectrometers (Laser/BWO)
< 3 THz
ALMA, HERSCHEL/HIFI (up to 1.9 THz)
(F. DeLucia, S. Schlemmer, T. F. Giesen, H. Müller, J. Pearson)

Max-Planck-Institut für Radioastronomie

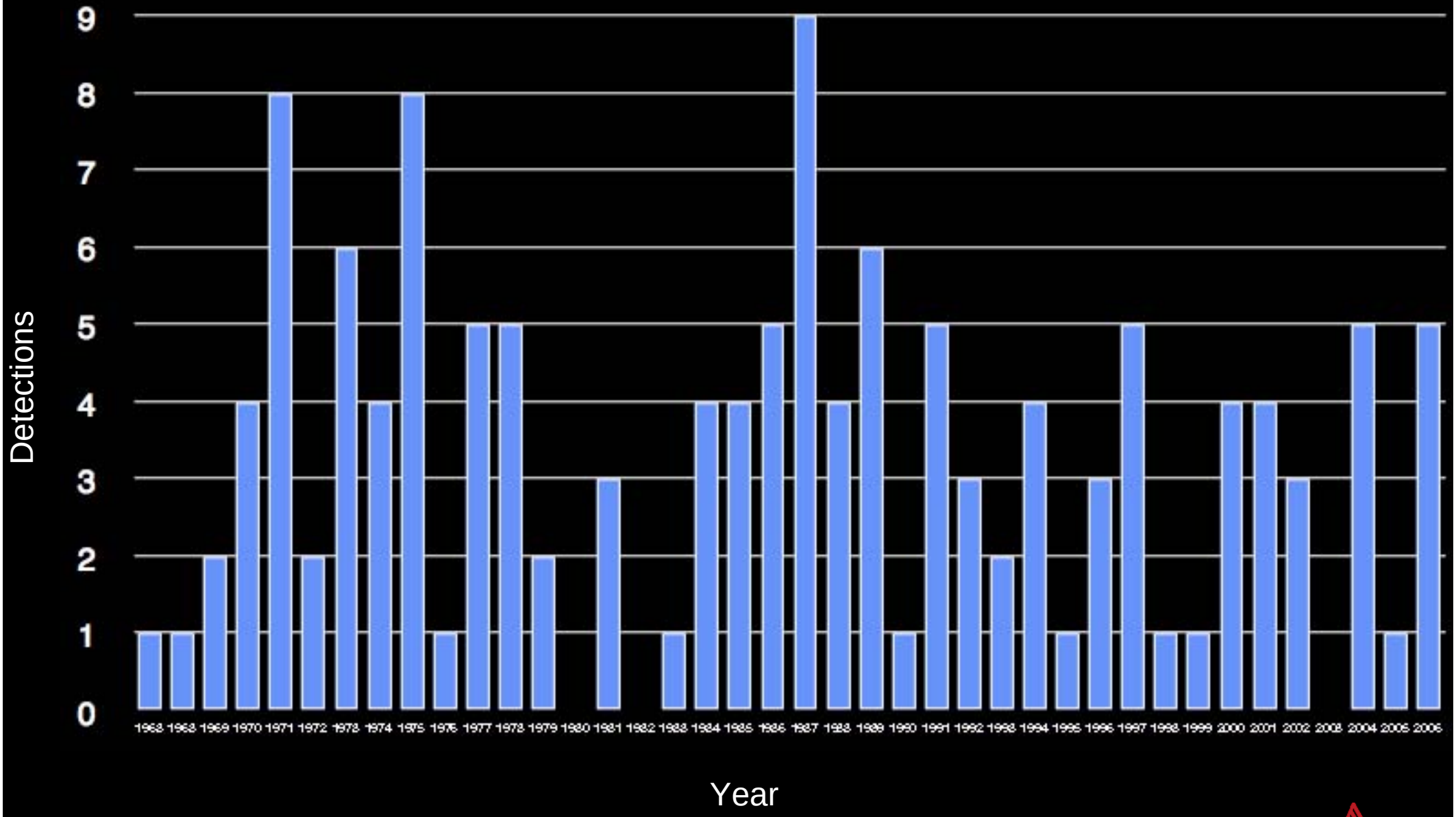
Carbon Chain and Ring molecules



Thaddeus, McCarthy and Thorwirth,
Proceeding 4th Cologne-Bonn-Zermatt Symposium
Springer, p.43 (2004)

Max-Planck-Institut für Radioastronomie

Molecules in Space - Statistics



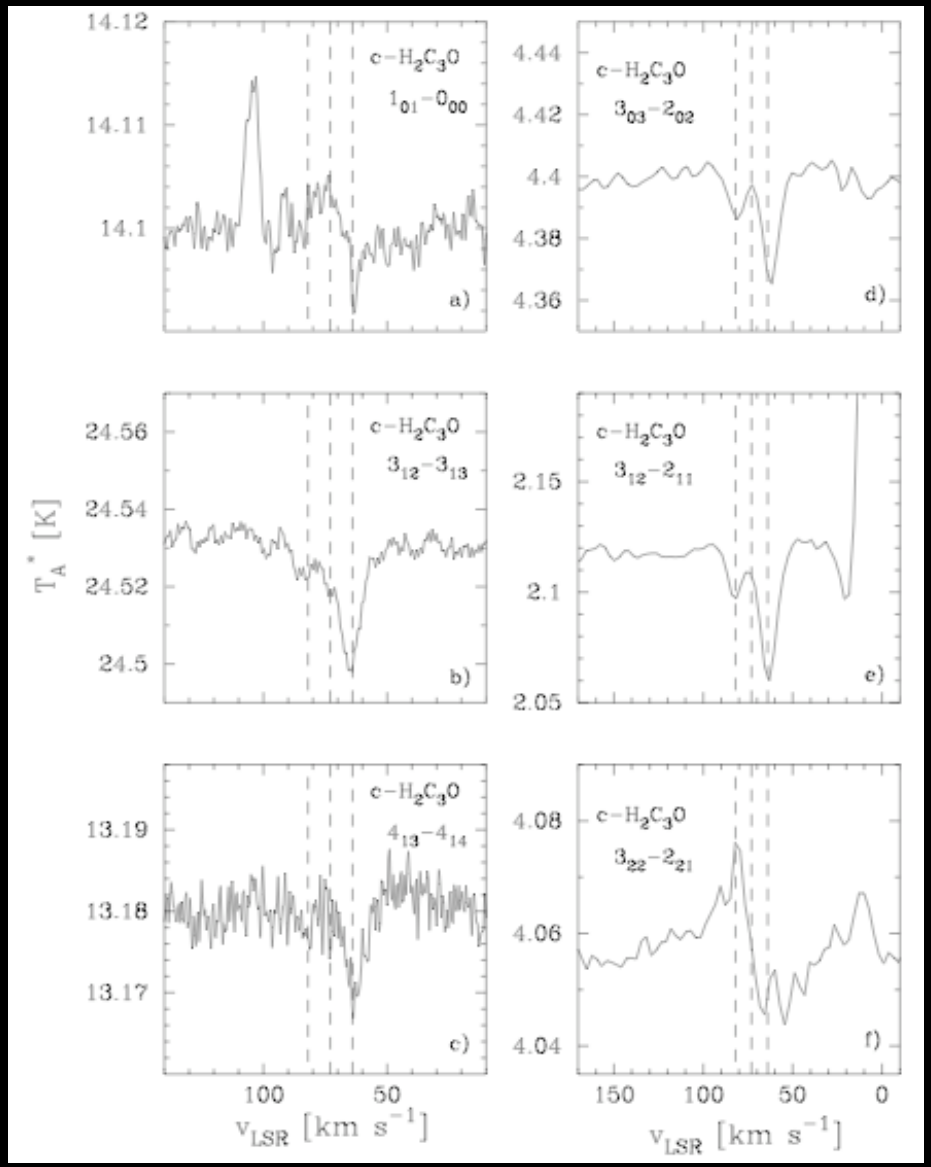
Max-Planck-Institut für Radioastronomie

How to chose candidate molecules

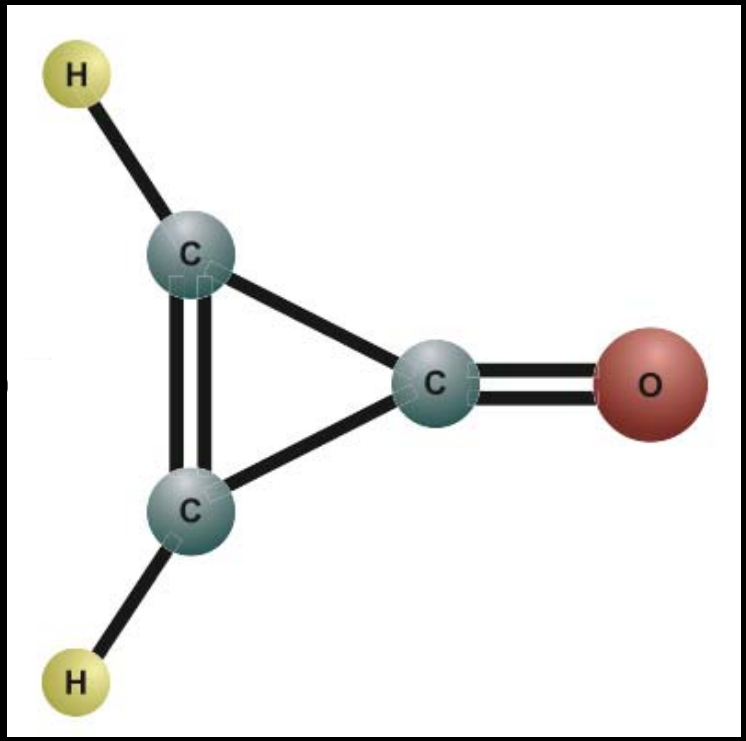
Variation of known structural themes

Astrochemical modeling

First Detections in 2006

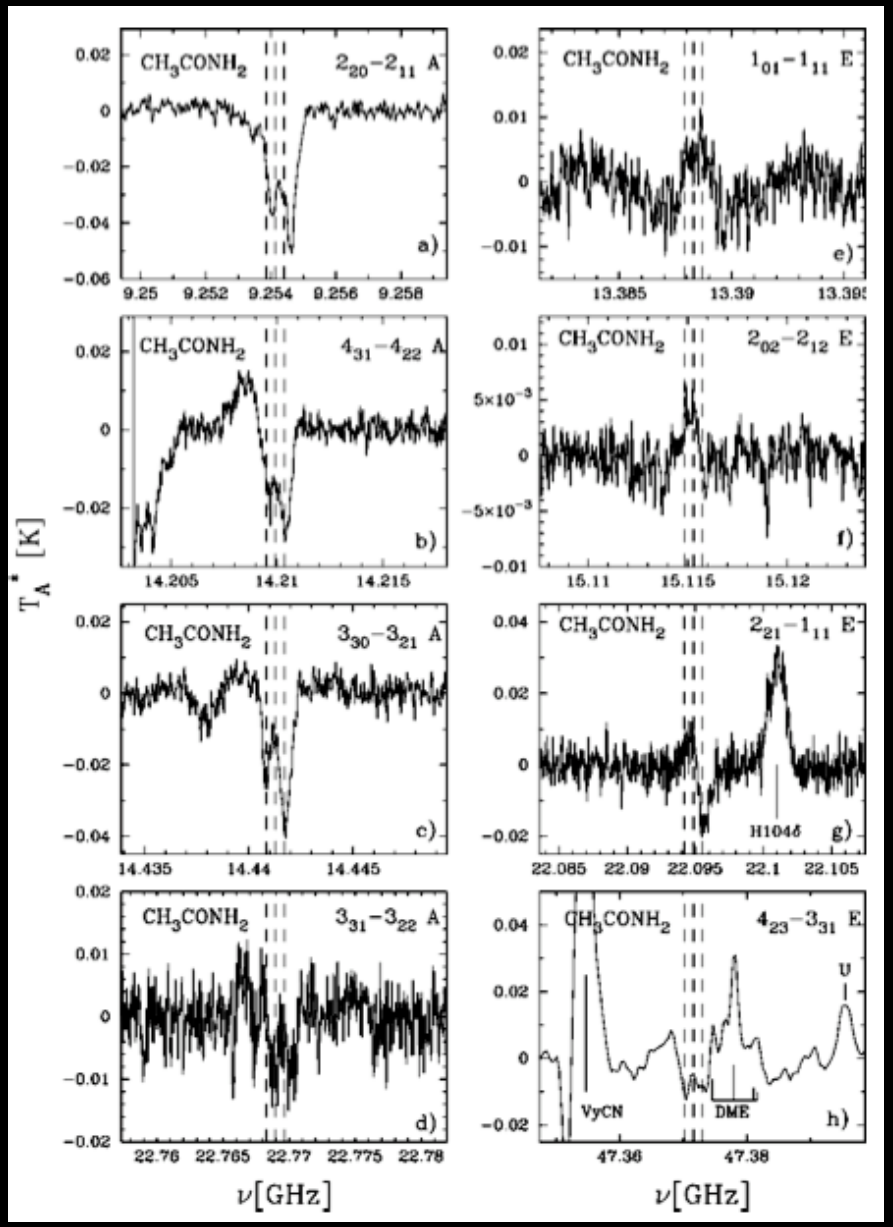


Cyclopropenone, c-H_2C_3O
Hollis et al., ApJ 642, 933 (2006)
SgrB2(N)
GBT

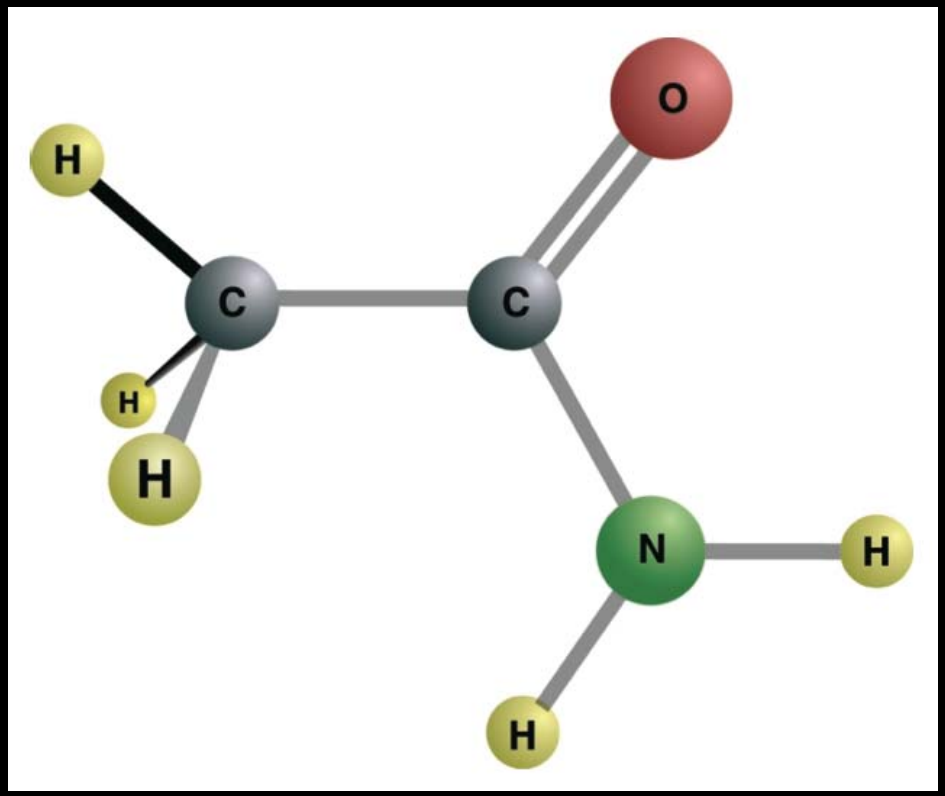


Max-Planck-Institut für Radioastronomie

First Detections in 2006

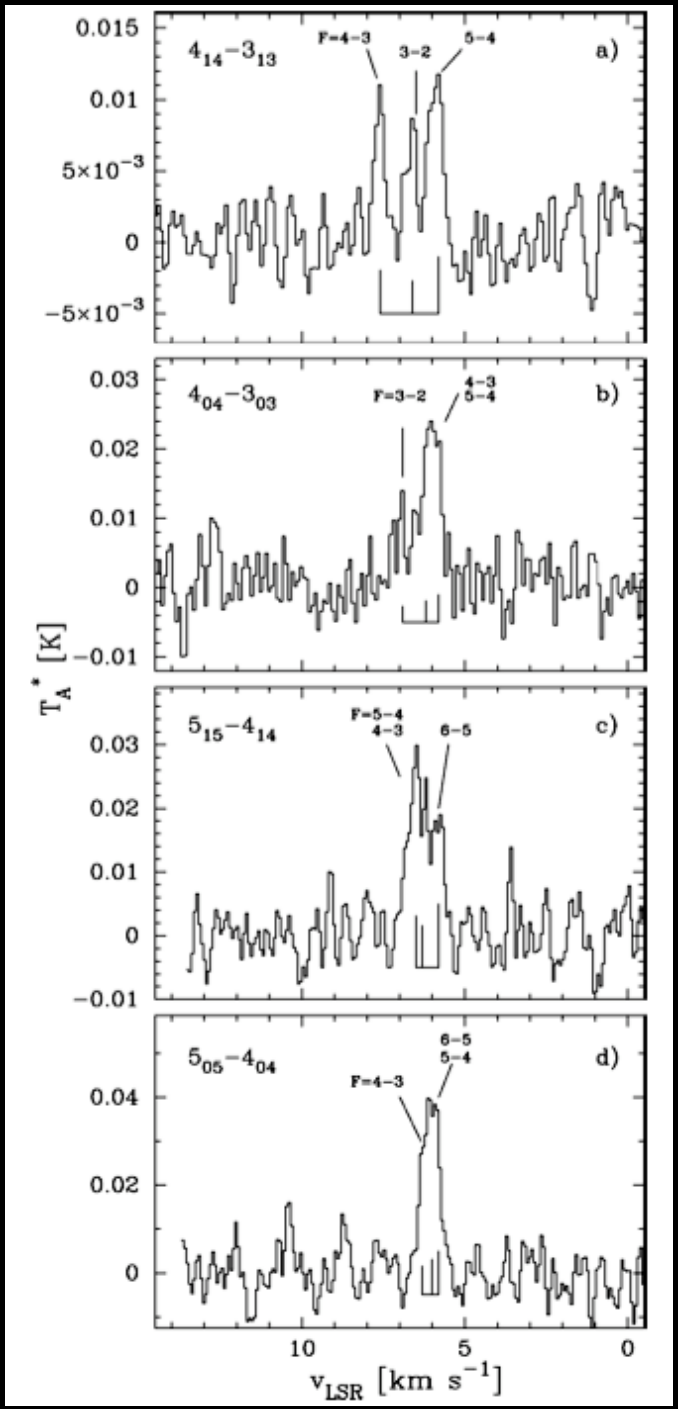


Acetamide
Hollis et al., ApJL 643, May 20 (2006)
SgrB2(N)
GBT



Max-Planck-Institut für Radioastronomie

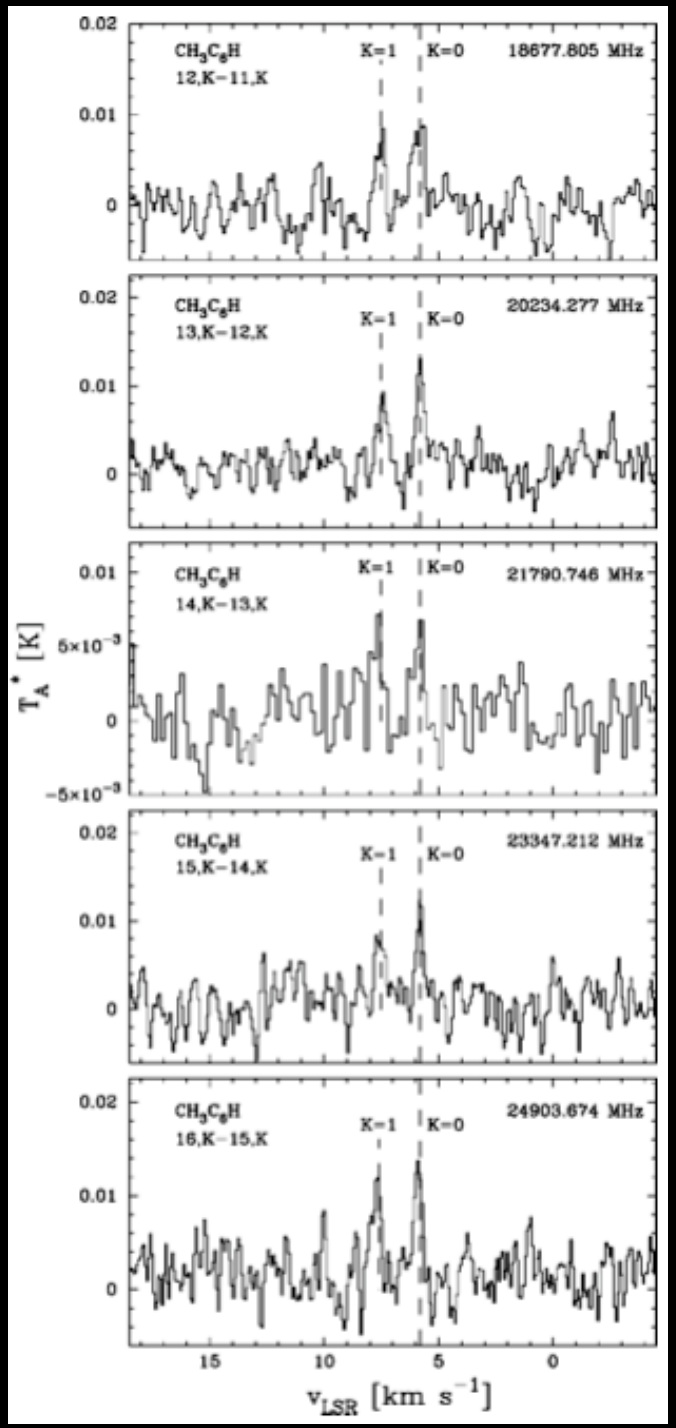
First Detections in 2006



Cyanoallene, $H_2C=C=CHCN$
Lovas et al., ApJ 637, L37 (2006)
TMC-1
GBT

Max-Planck-Institut für Radioastronomie

First Detections in 2006



Methyltriacetylene
Remijan et al., ApJL 643, May 20 (2006)
TMC-1
GBT

CH_3-C≡C-C≡C-C≡C-H

Max-Planck-Institut für Radioastronomie

Interstellar Fluorine Chemistry

Formation of HF

$F + H_2 \Rightarrow HF + H$

$F + H_2O \Rightarrow HF + OH$

Destruction of HF

$C^+ + HF \Rightarrow CF^+ + H$

$Si^+ + HF \Rightarrow SiF^+ + H$

$H_3^+ + HF \Rightarrow H_2 + H_2F^+$

HF

B = 616.4 GHz

J = 1 - 0 at 1.23 THz

J = 2 - 1 at 2.46 THz (*ISO*)

CF^+

B = 51.3 GHz

J = 1 - 0 at 102.6 GHz

J = 2 - 1 at 205.2 GHz

J = 3 - 2 at 307.7 GHz

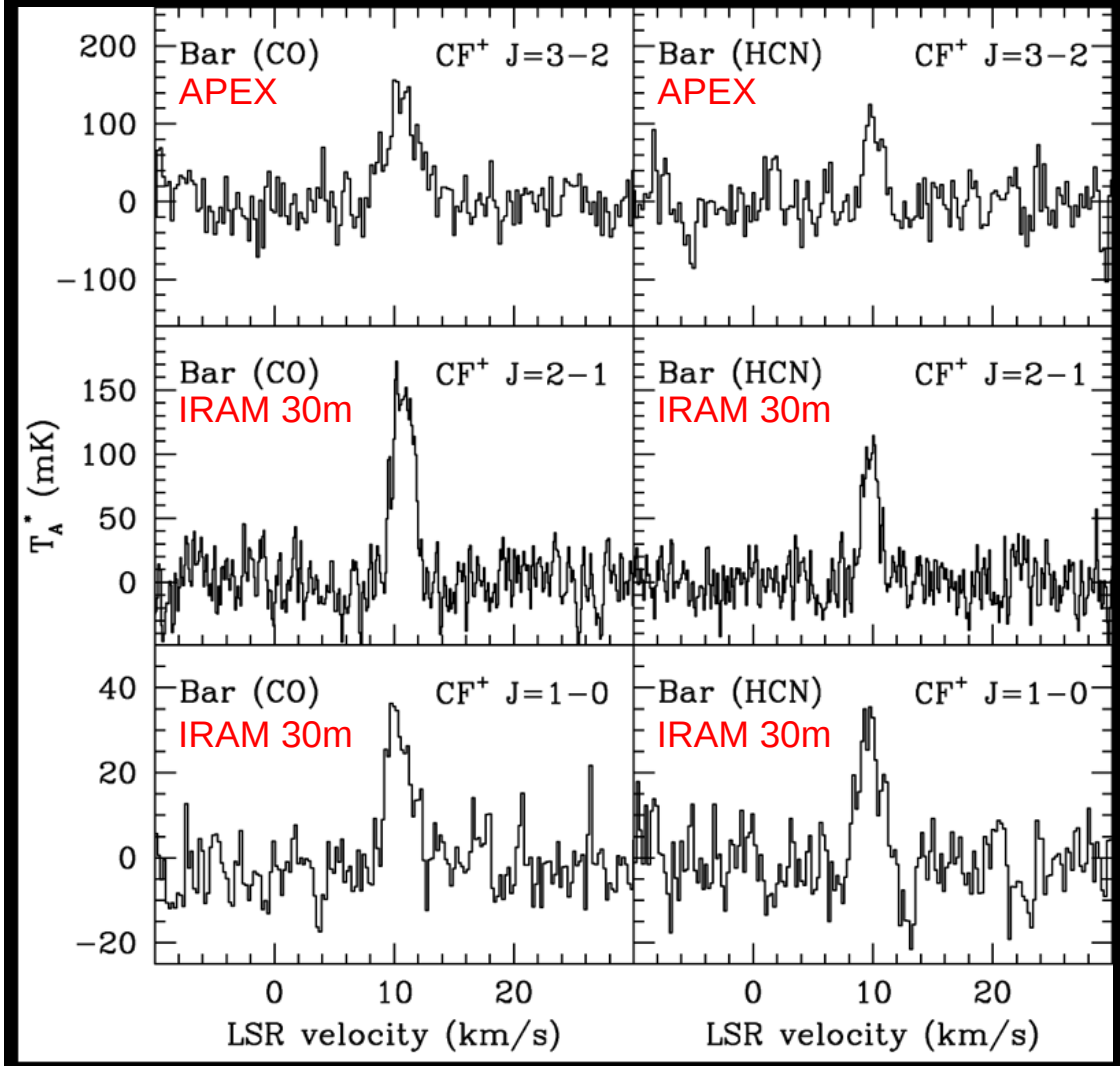
Destruction of CF^+

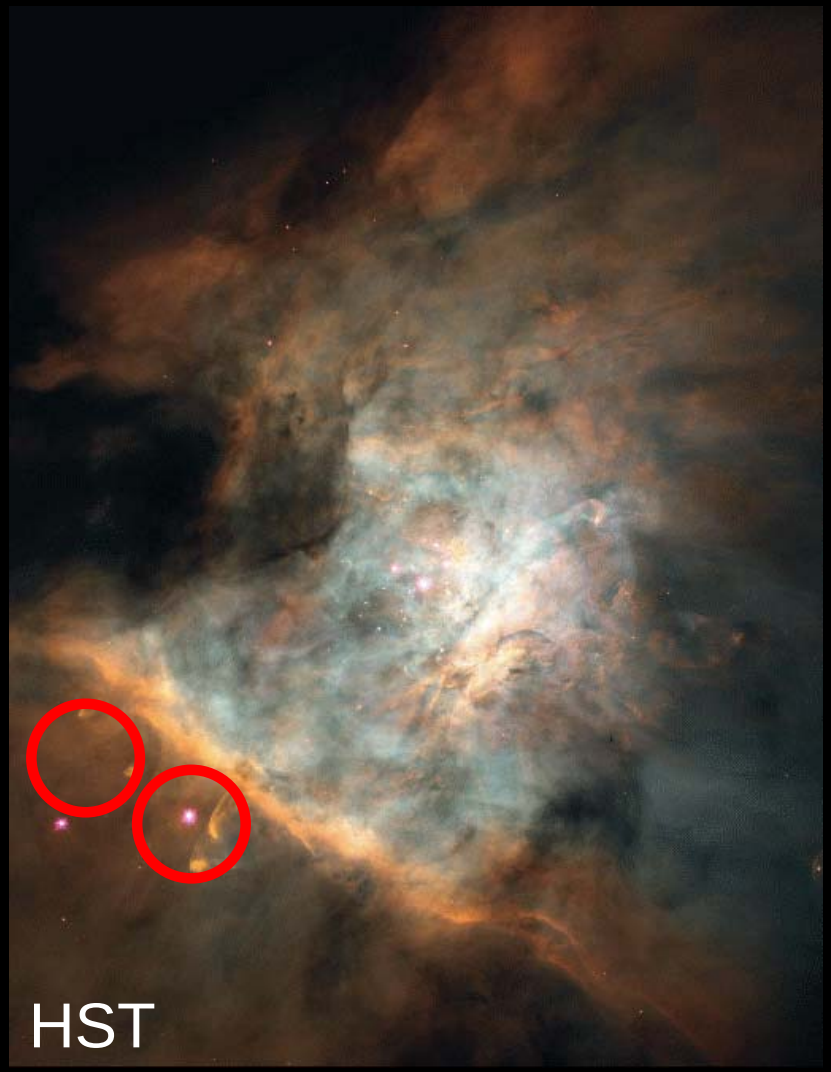
$CF^+ + e \Rightarrow C + F$

Neufeld, Wolfire, and Schilke,
ApJ 628, 260 (2005)

Max-Planck-Institut
für
Radioastronomie

Detection of CF^+ towards Orion Bar





Neufeld et al. 2006, A&A, accepted

Max-Planck-Institut für Radioastronomie

New detections benefit from

Detection at cm-wavelengths
Less confusion

Cold source (TMC-1), Q_{rot}

Absorption (GC)

Moderate line density (Orion Bar)

Max-Planck-Institut für Radioastronomie

Large molecules in space

8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	13 atoms
CH_3C_3N	CH_3C_4H	CH_3C_5N	HC_9N	C_6H_6	$HC_{11}N$
$HCOOCH_3$	CH_3CH_2CN	$(CH_3)_2CO$	CH_3C_6H	$CH_3OC_2H_5$ (?)	
CH_3COOH	$(CH_3)_2O$	$(CH_2OH)_2$		$(CH_2OH)_2CO$ (?)	
C_7H	CH_3CH_2OH	H_2NCH_2COOH (?)			
H_2C_6	HC_7N	CH_3CH_2CHO			
CH_2OHCHO	C_8H				
/-HC_6H	CH_3CONH_2				
CH_2CHCHO					
$H_2CCCHCN$					

Max-Planck-Institut für Radioastronomie

Recent searches for complex organics

Interstellar Glycine
Kuan et al., ApJ 593, 848 (2003)

A rigorous attempt to verify interstellar glycine
Snyder et al., ApJ 619, 914 (2005)

Interstellar glycolealdehyde: the first sugar
Hollis et al., ApJ 540, L107 (2000)

Green Bank Telescope Observations of Interstellar Glycolaldehyde: Low-Temperature Sugar
Hollis et al., ApJ 613, L45 (2004)

A Systematic Study of Glycolaldehyde in Sagittarius B2(N) at 2 and 3 mm:
Criteria for Detecting Large Interstellar Molecules
Halfen et al., ApJ 639, 237 (2006)

1,3-Dihydroxyacetone in Sagittarius B2(N-LMH): The First Interstellar Ketose
Widicus Weaver and Blake, ApJ 624, L33 (2005).

Investigating the Limits of Chemical Complexity in Sgr B2(N):
A Rigorous Attempt to Confirm 1,3-Dihydroxyacetone
Apponi et al., ApJL, accepted.

Max-Planck-Institut
für
Radioastronomie

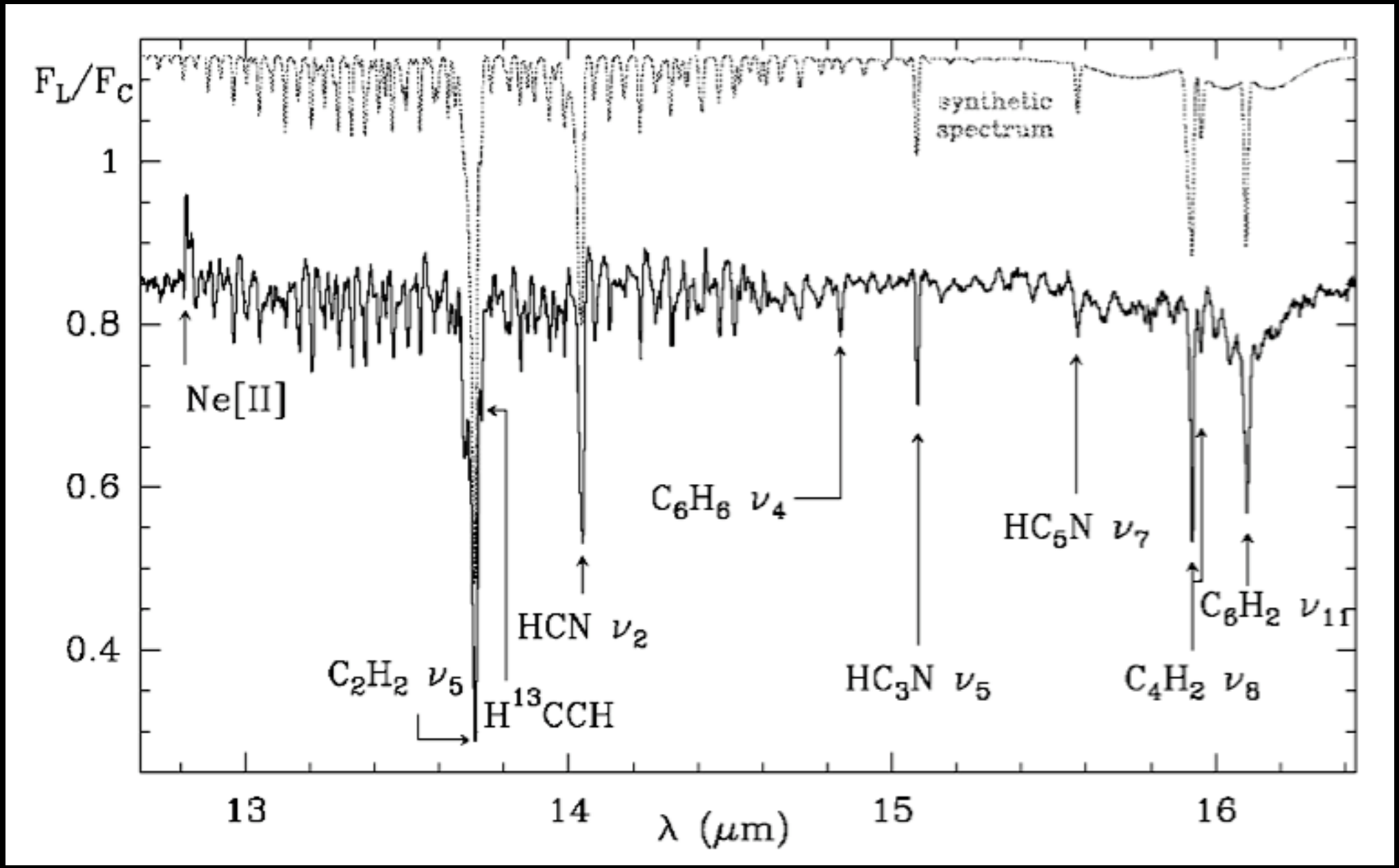
Astronomical searches for complex molecules

Complex organics: Aminomethanol, Aminoethanol, Diethylether, Glycine, etc.

Aromatic compounds: Benzene derivatives, PAHs, PANHs

Max-Planck-Institut für Radioastronomie

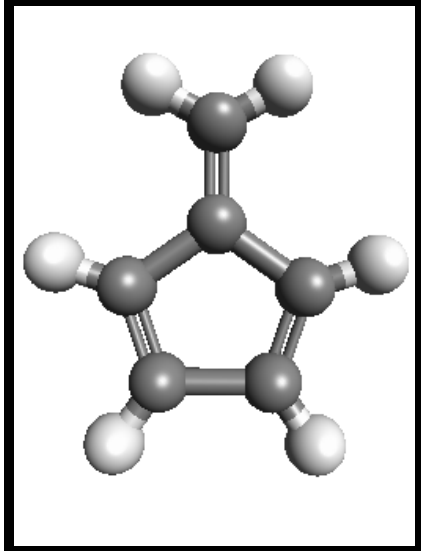
Benzene in CRL618



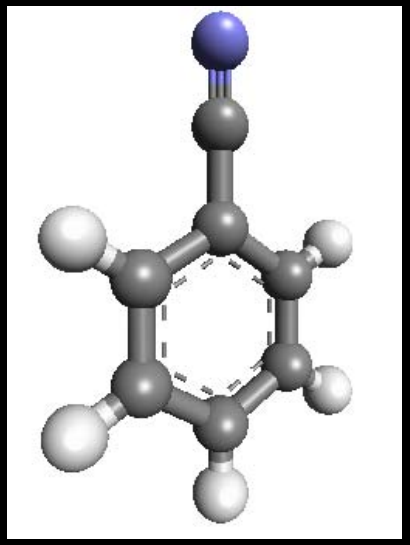
Cernicharo et al., ApJ 546, L123 (2001).

Max-Planck-Institut für Radioastronomie

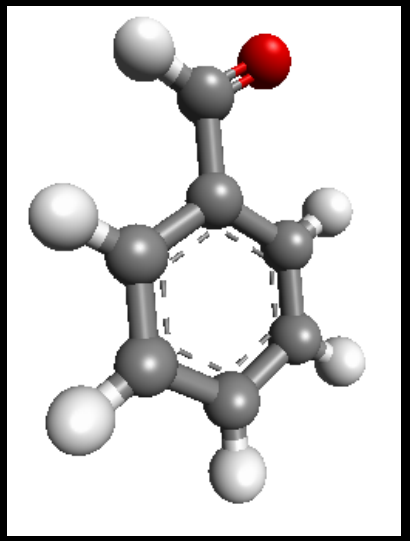
Benzene derivatives, dehydrobenzenes, azabenzenes



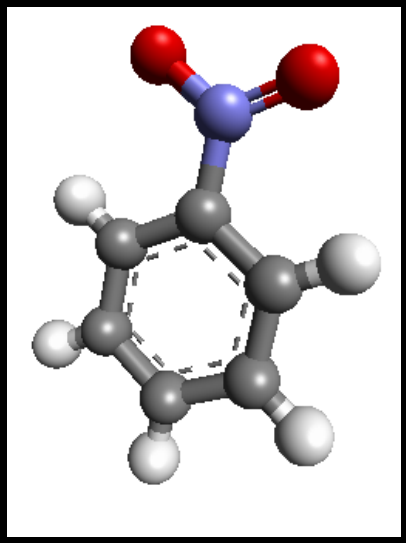
Fulvene



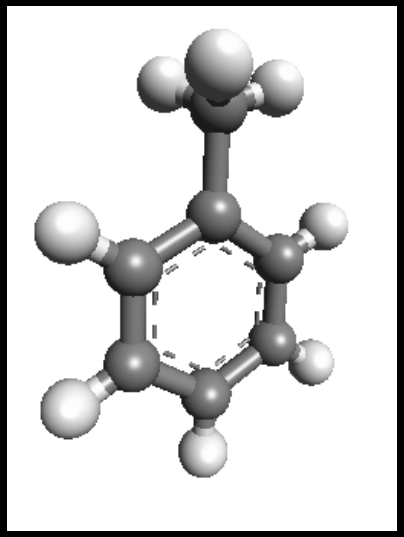
Benzonitrile



Benzaldhyde



Nitrobenzene



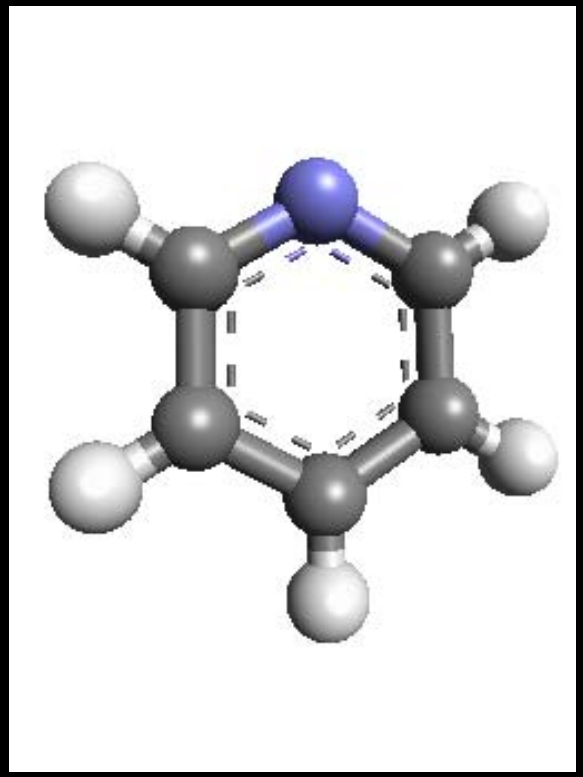
Toluene

Max-Planck-Institut für Radioastronomie

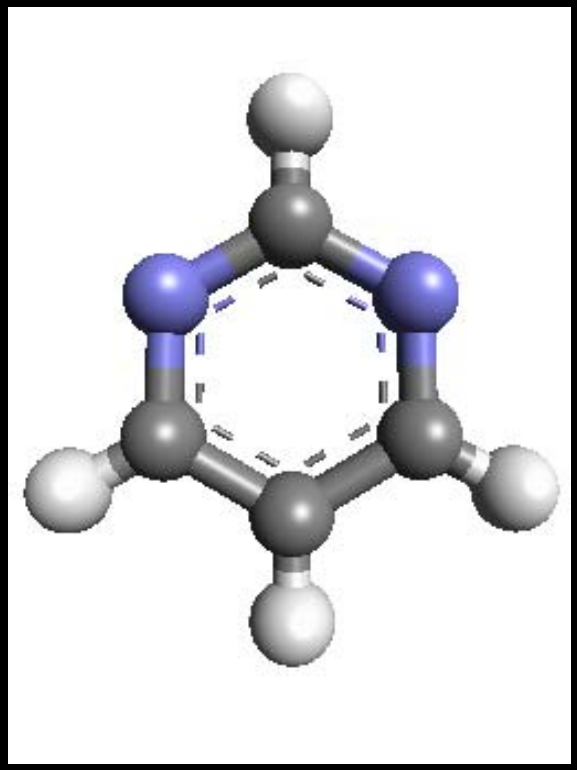
Benzene derivatives, dehydrobenzenes, azabenzenes

Phenyl radical, C_6H_5

o-Benzyne, C_6H_4



Pyridine



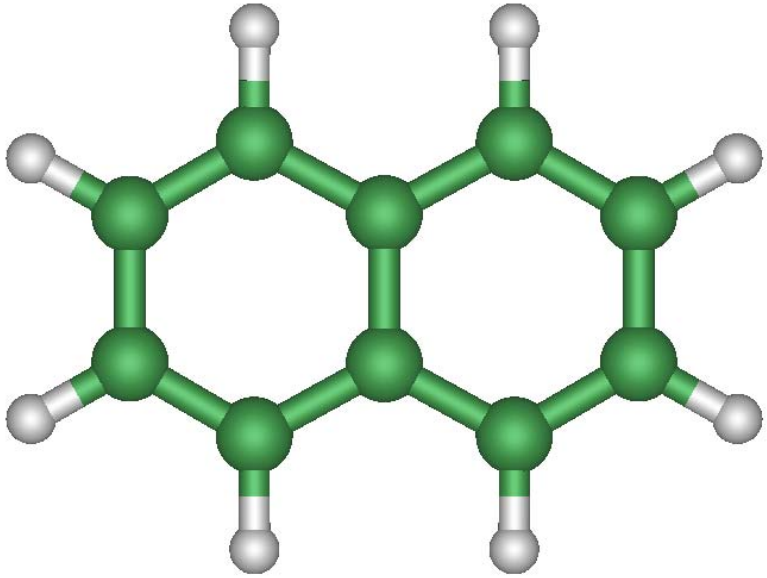
Pyrimidine

Max-Planck-Institut für Radioastronomie

PAHs

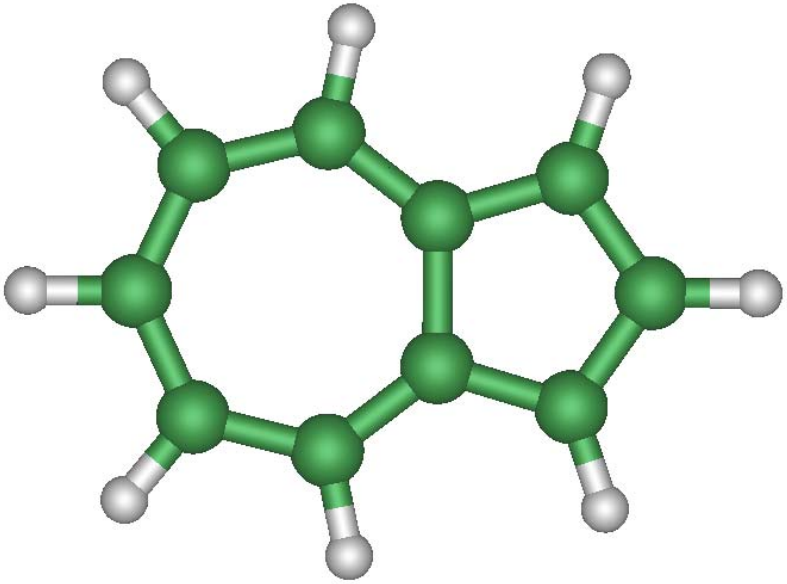
MW/FTMW Spectroscopy of Azulene

Naphthalene, $C_{10}H_8$



$\mu = 0$ D

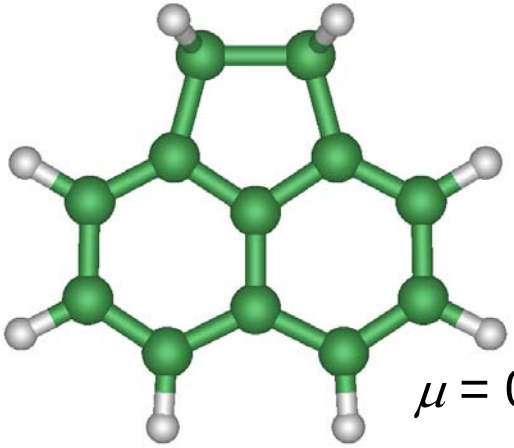
Azulene, $C_{10}H_8$



$\mu_{exp} = 0.9$ D

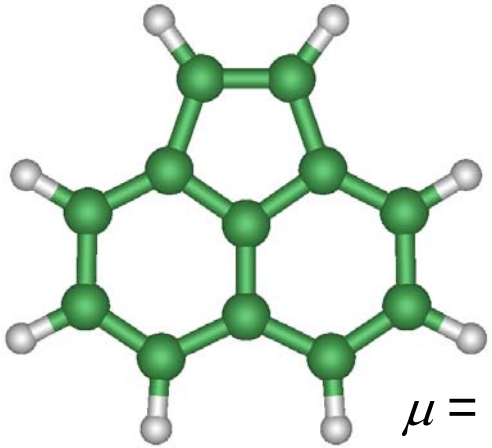
Tobler et al., J. Mol. Spectrosc. 18, 239 (1965)
Huber et al., Mol. Phys. 103, 1395 (2005)

Acenaphthene, $C_{12}H_{10}$



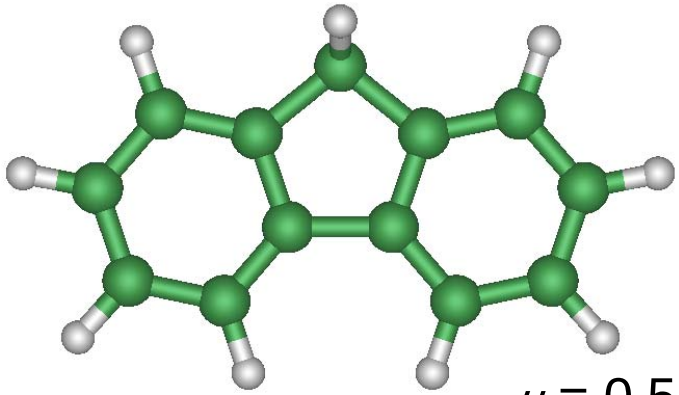
μ = 0.9 D

Acenaphthylene, $C_{12}H_8$



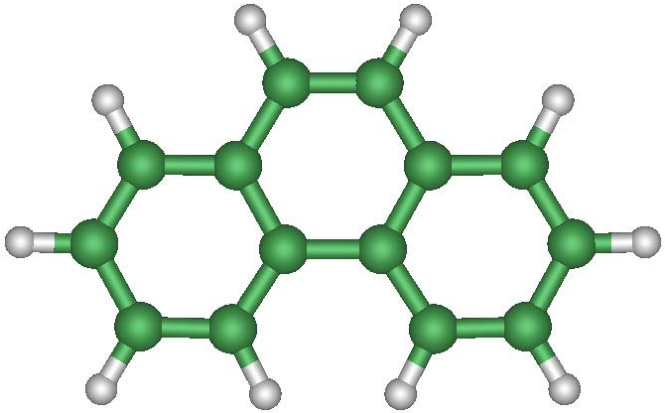
μ = 0.3 D

Fluorene, $C_{13}H_{10}$



μ = 0.5 D

Phenanthrene, $C_{14}H_{10}$



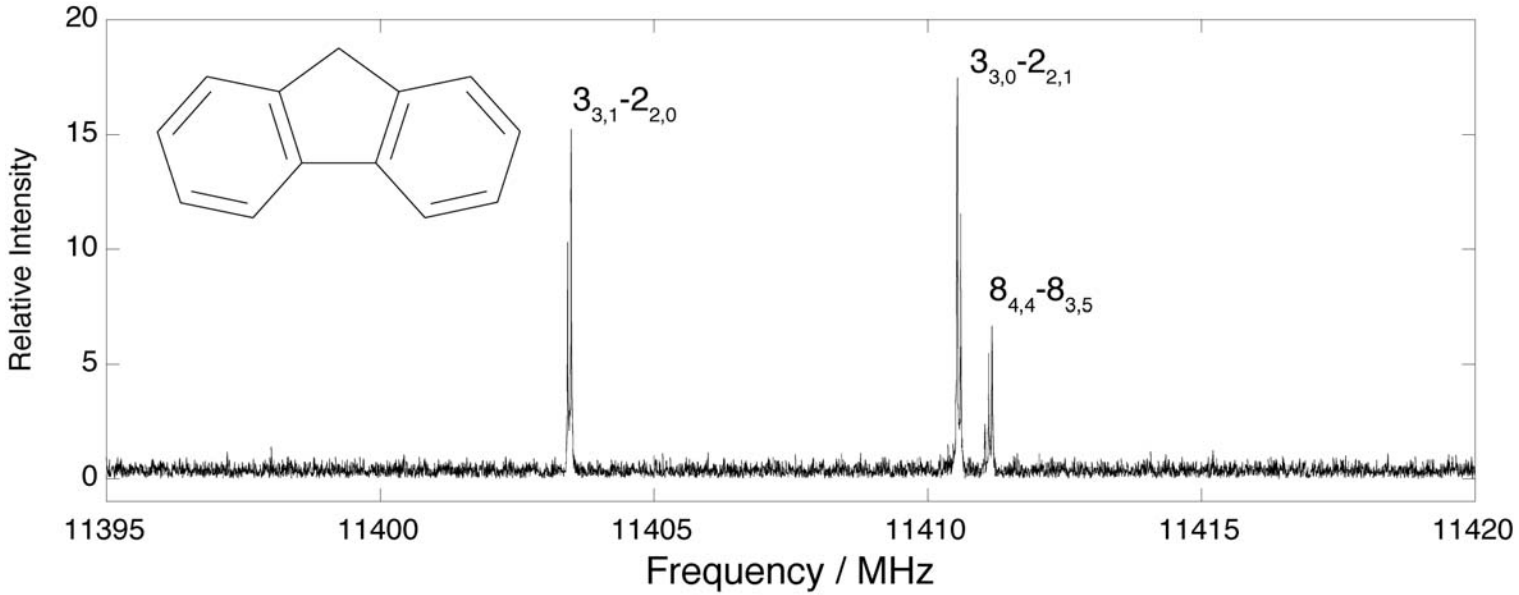
μ < 0.1 D

B3LYP/cc-pVTZ, Gaussian03

Thorwirth et al. 2006

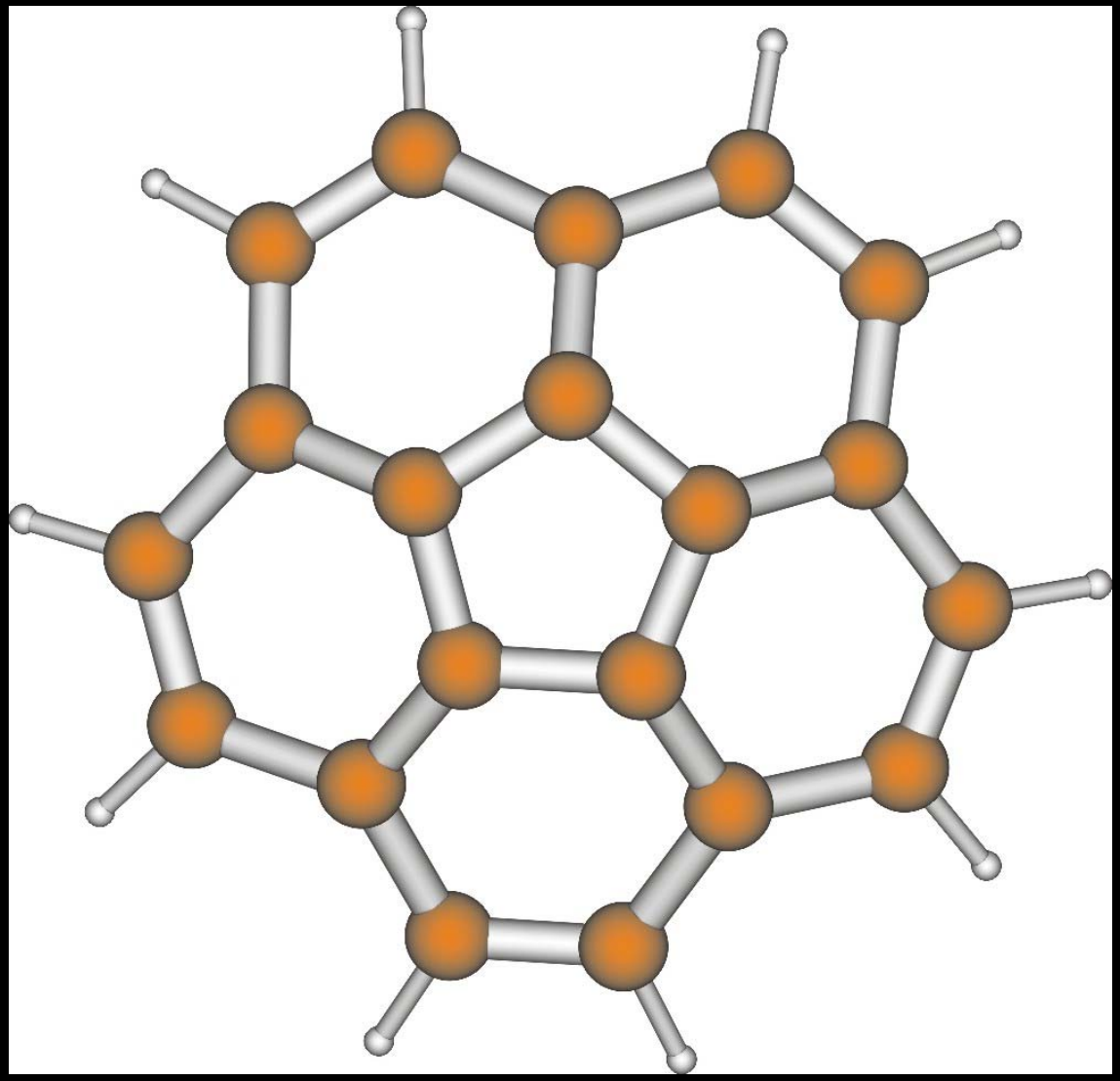
Molecular Constants of Fluorene

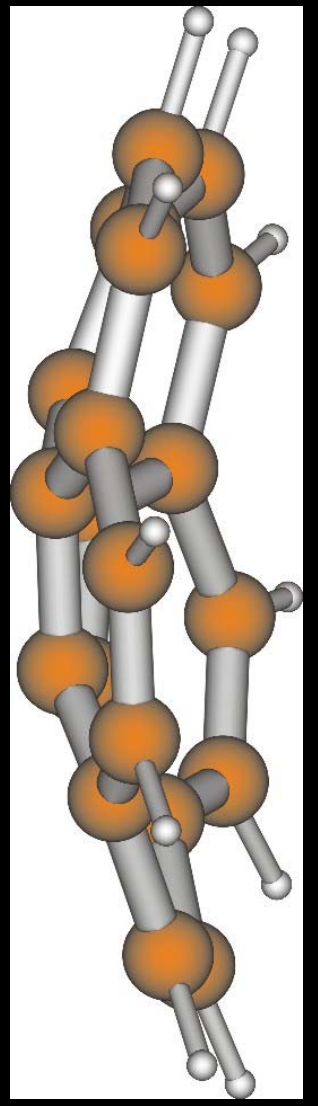
Constant / MHz	B3LYP/cc-pVTZ	Experimental
A	2195.1	2176.210
B	588.2	586.653
C	465.2	463.569



Thorwirth et al. 2006

Corannulene





μ_{exp} = 2.07(2)D

B = 509.8MHz

B_{HC7N} = 564.0MHz

Lovas et al., J. Am. Chem. Soc. 127, 4345 (2005)

Max-Planck-Institut für Radioastronomie

PANHs

Some evidence for N bearing PAHs from ISO spectra (6 micron feature)

However, dedicated searches to date unsuccessful

Pyridine, Pyrimidine, Quinoline, Isoquinoline
Charnley et al., Advances in Space Research 36, 137 (2005)

Laboratory gas-phase studies for larger PANHs missing so far (FTMW)

Nevertheless, quite a bit of data for selected PAHs molecules!

PAHs in late type stars? (cf. E. Herbst)
IRC+10216, CRL618

Where should we search for complex organics?

NGC6334

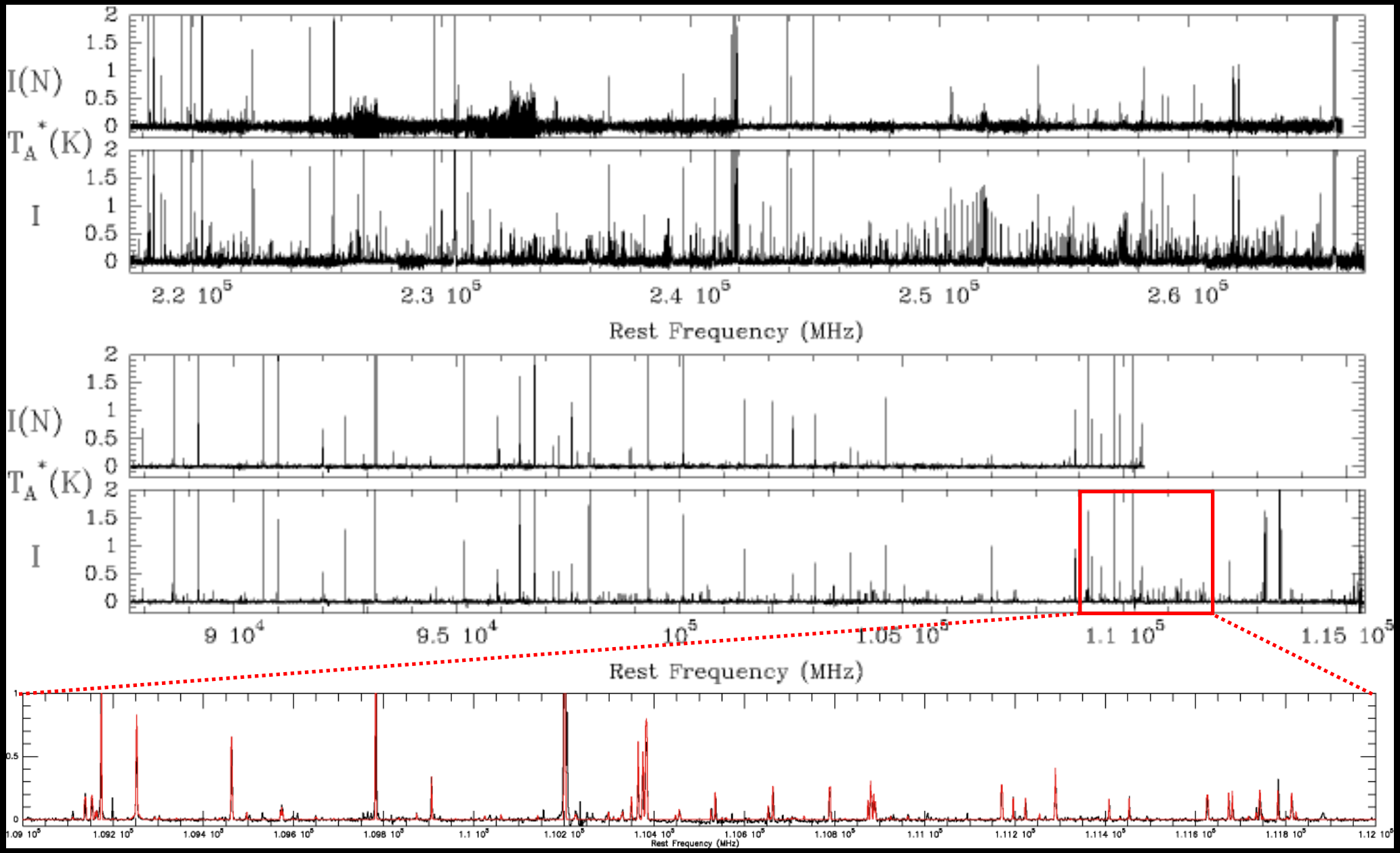
$\delta = -36^{\circ}$

G327.3-0.6

$\delta = -54^{\circ}$

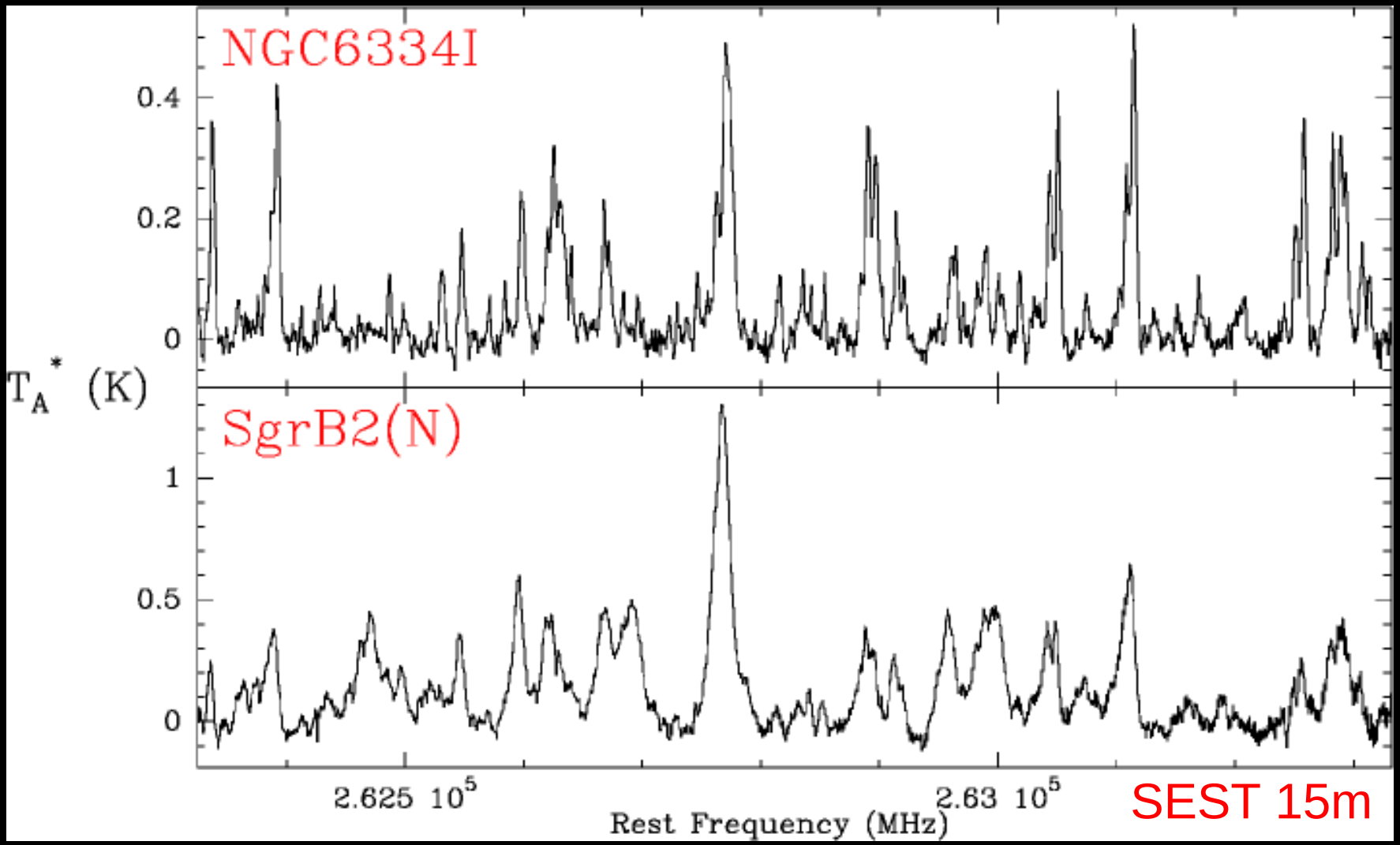
Max-Planck-Institut für Radioastronomie

NGC6334 I and I(N) with SEST



Max-Planck-Institut für Radioastronomie

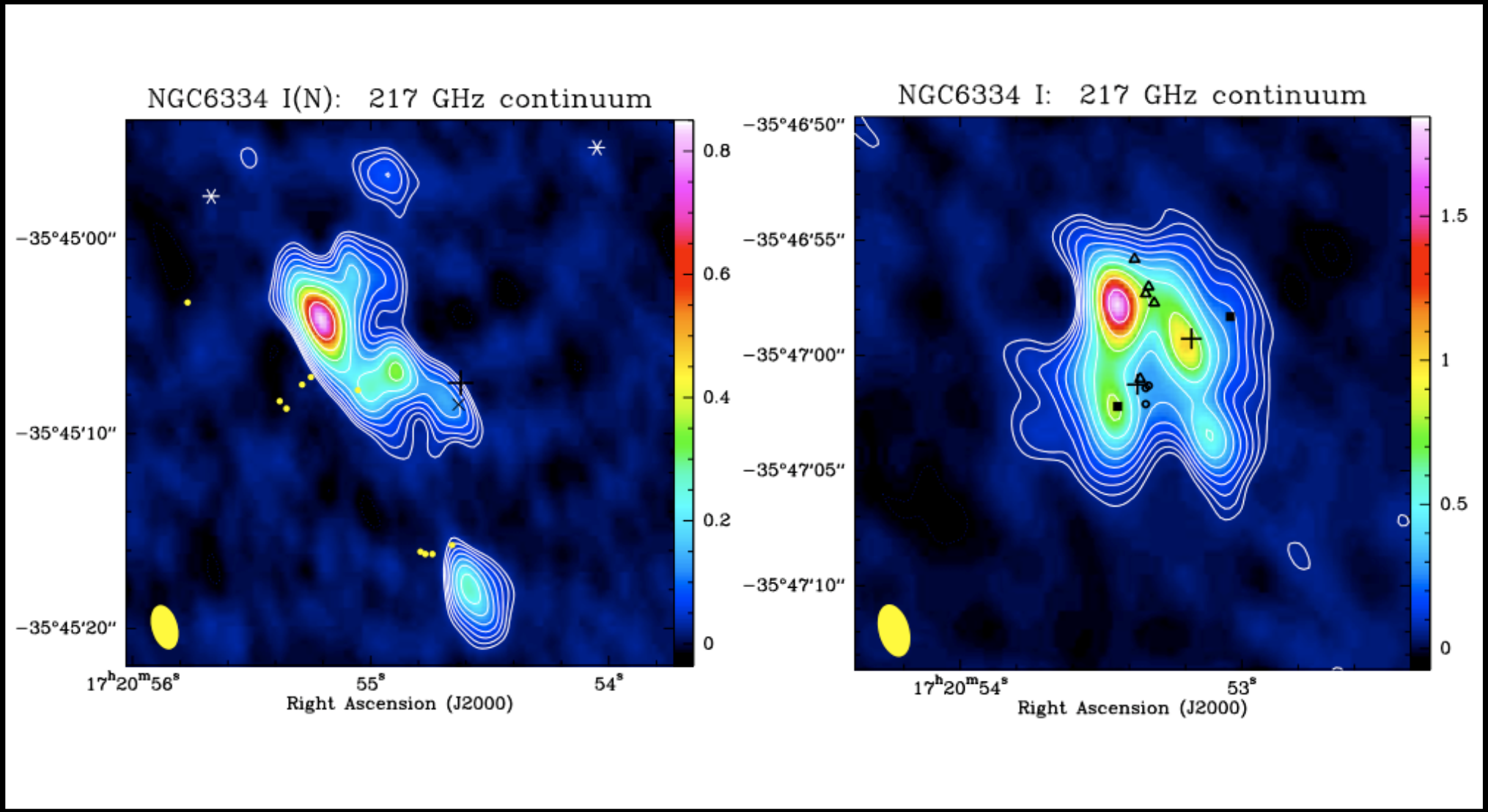
Chemistry and Linewidths NGC6334I vs. SgrB2(N)



High line density (comparable to SgrB2/Orion)
Rich chemistry, Narrow lines ~5km s^{-1}
Confusion limit is lower
More (weaker) lines can be detected

Max-Planck-Institut für Radioastronomie

NGC6334 I & I(N) with the SMA



Hunter et al., Protostars and Planets V, 8504 (2005).

Max-Planck-Institut für Radioastronomie

Observations at Submm Wavelengths

high-excitation transitions provide an insight into the hottest, densest regions of the ISM, high-*J*

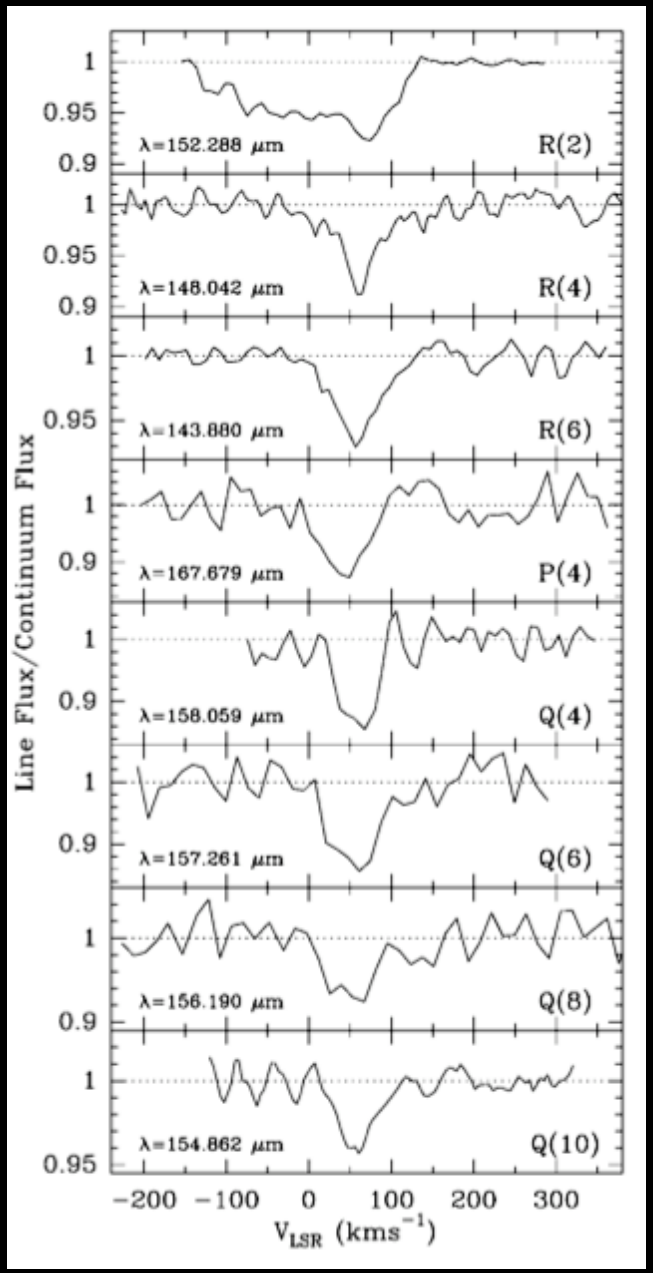
study of ground-state transitions of light species (such as the hydrides HCl, SiH, CH^+, NH_2, HDO, H_2D^+,...)

infrared pumping becomes important: selected molecular transitions provide a measure of the background dust radiation field

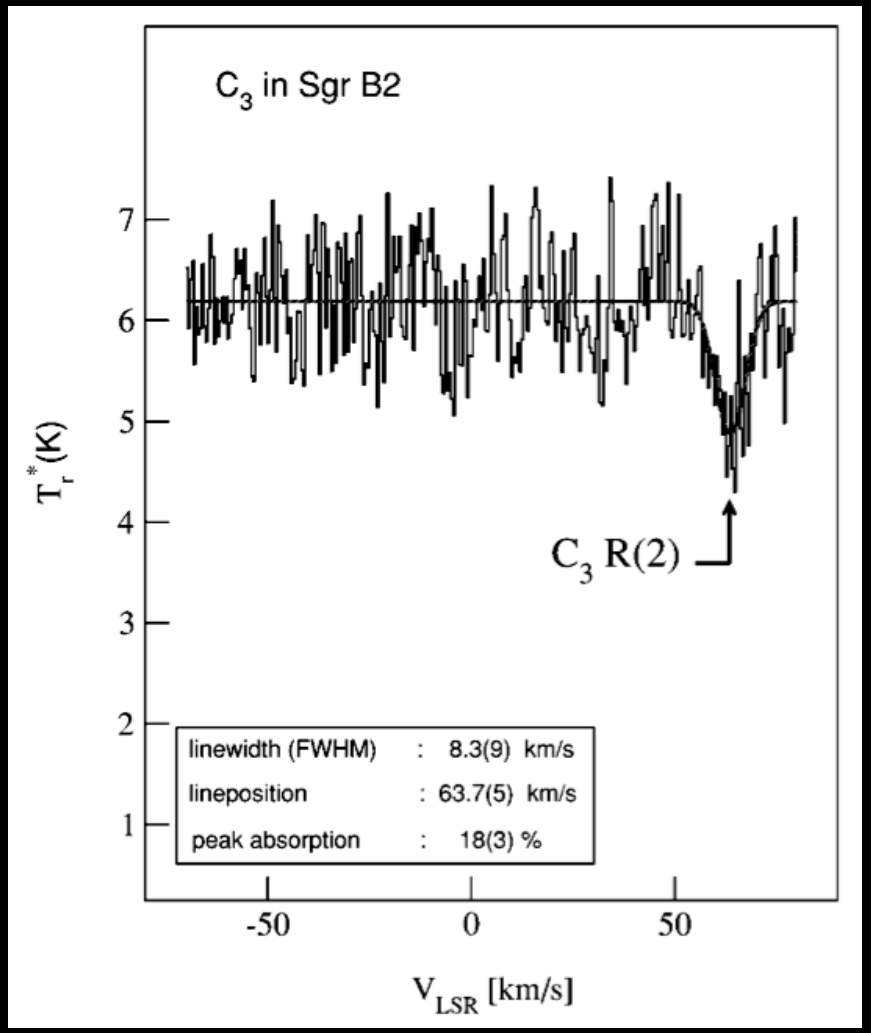
pure rotational transitions
rovibrational transitions (< 35 cm^{-1})

Max-Planck-Institut für Radioastronomie

Detection of C_3 at 2 THz



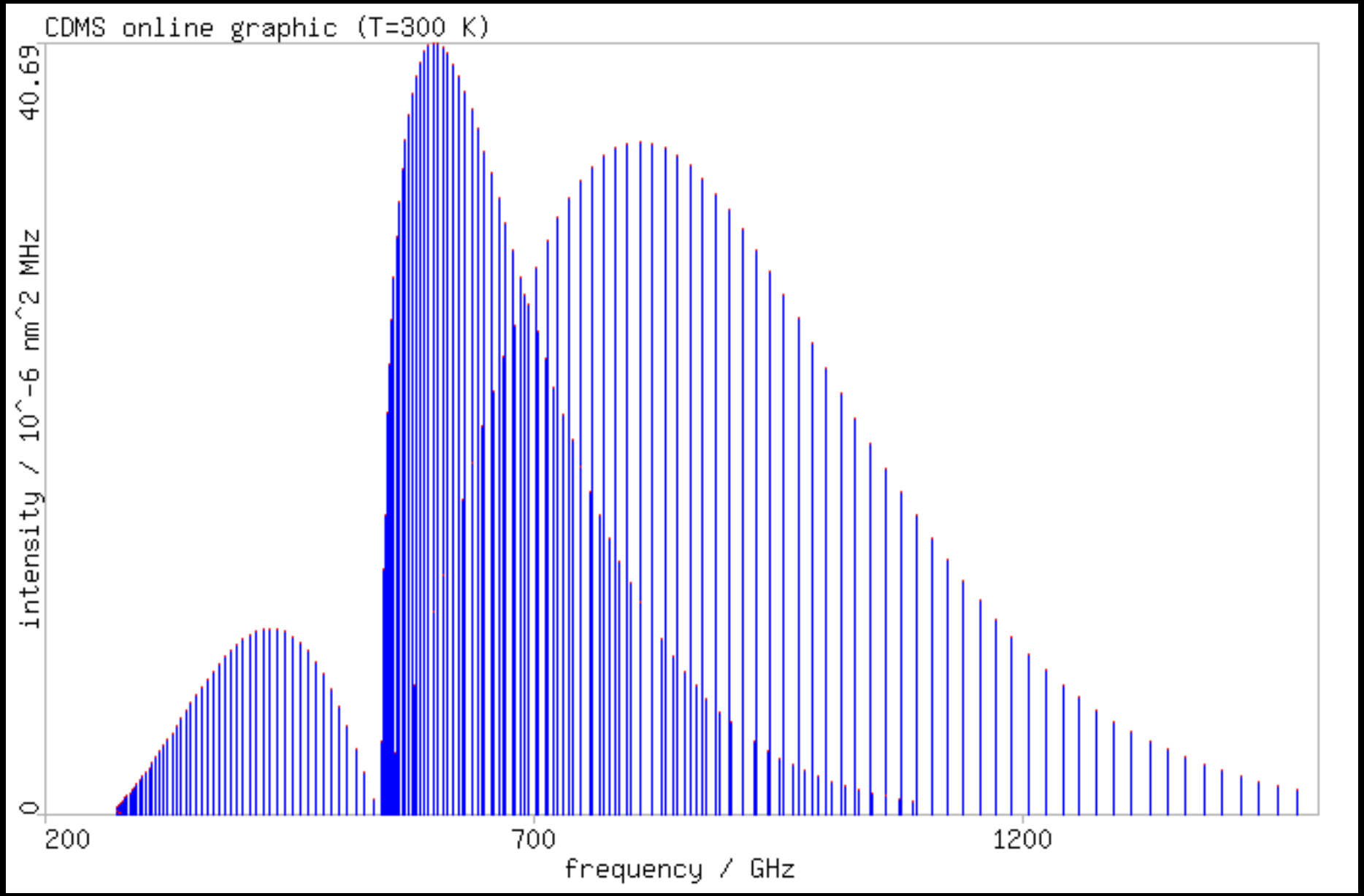
ISO, Cernicharo et al., ApJ 534, L199 (2000)



KAO, Giesen et al., ApJ 551, L181 (2001)

Max-Planck-Institut für Radioastronomie

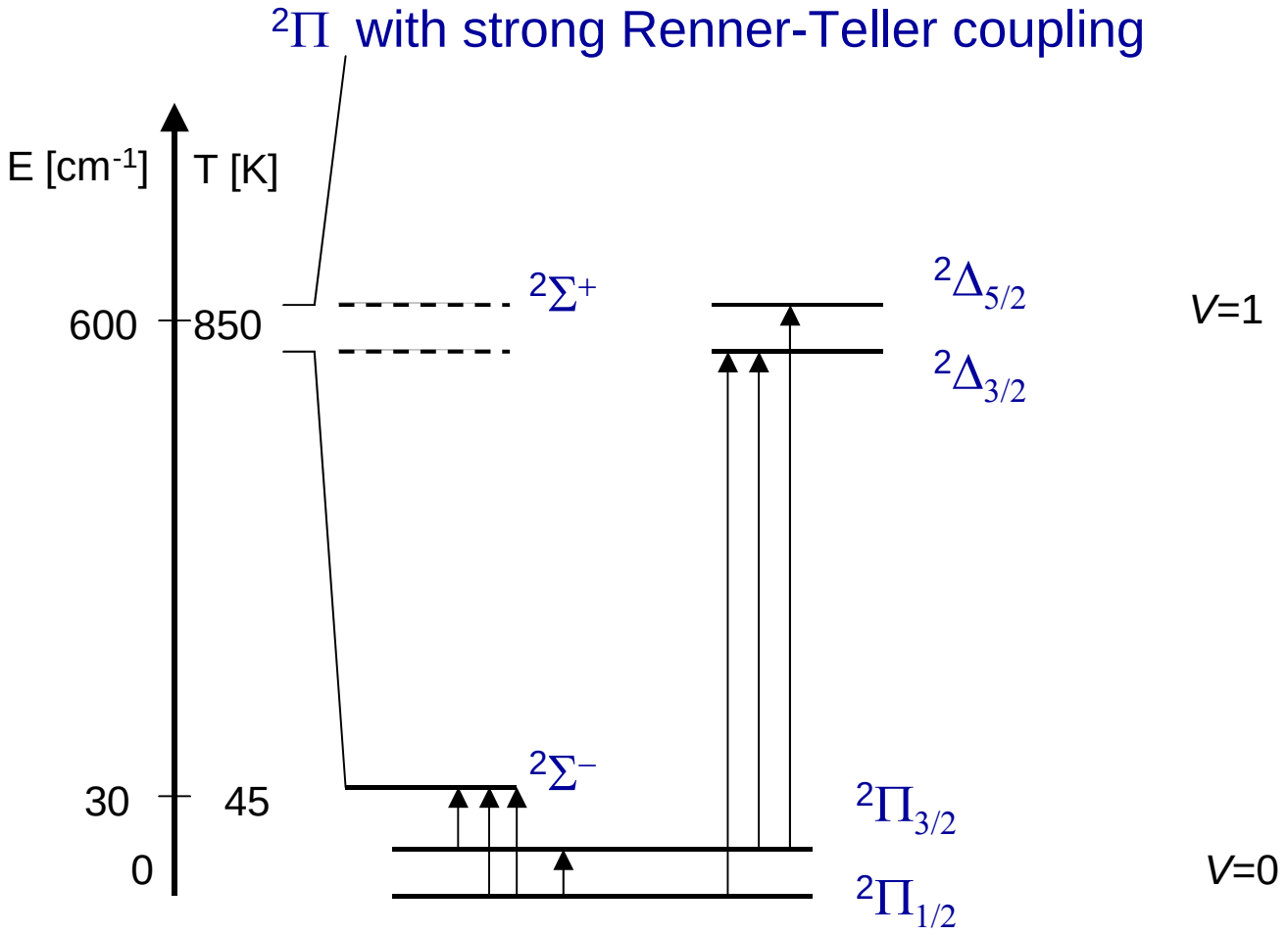
ν_7 of O=C=C=C=O at 18 cm^{-1}



μ = 0.08D

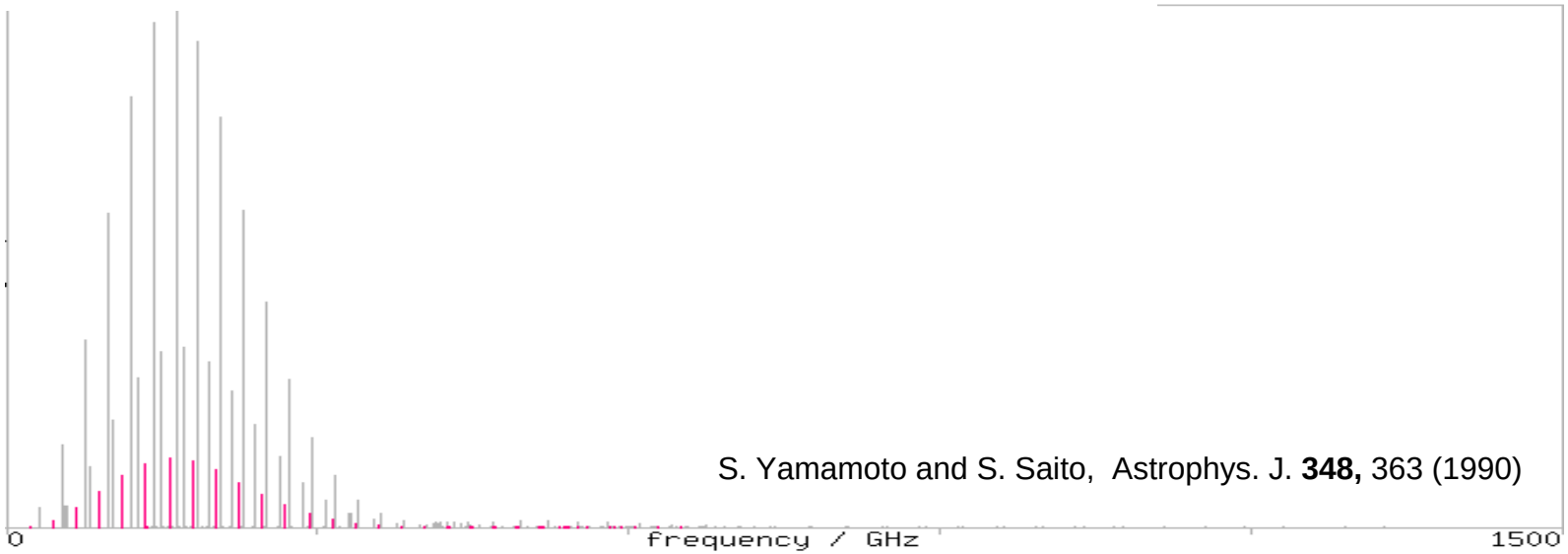
Max-Planck-Institut für Radioastronomie

C_3H



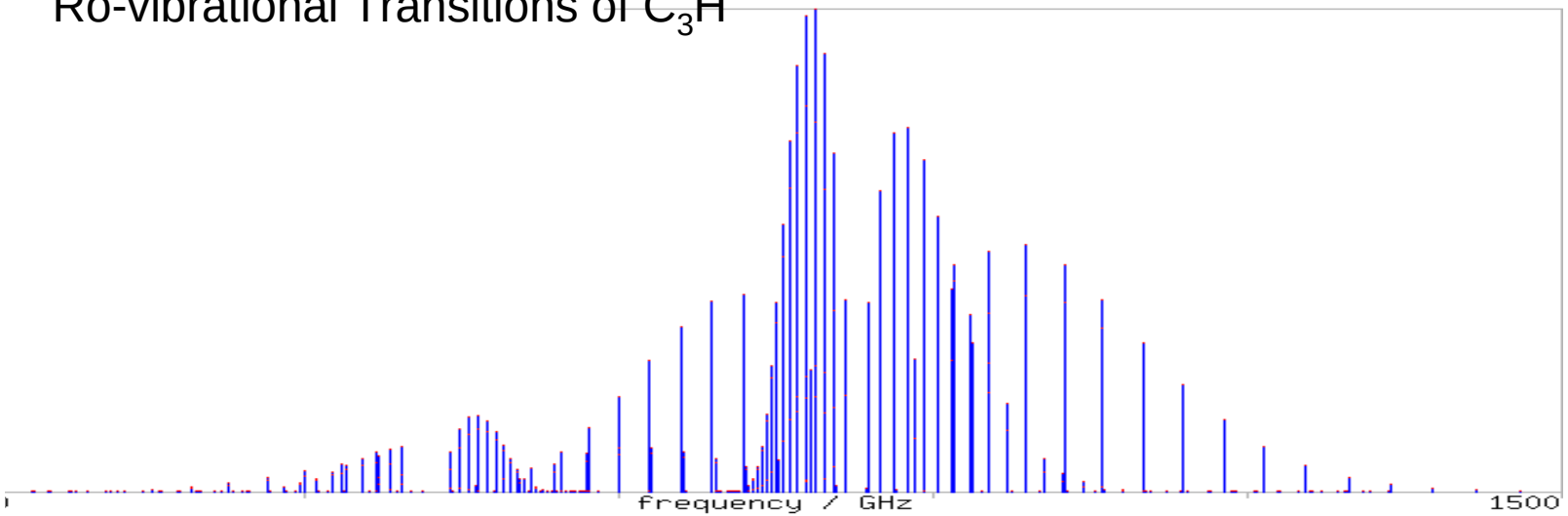
Max-Planck-Institut für Radioastronomie

Pure Rotational Transitions of C_3H



S. Yamamoto and S. Saito, Astrophys. J. **348,** 363 (1990)

Ro-vibrational Transitions of C_3H



0 GHz 500 GHz 1000 GHz 1500 GHz

Max-Planck-Institut für Radioastronomie

Conclusions

Homework!

Lab spectroscopy! Lab spectroscopy! Lab spectroscopy!
Can’t do the complex guys without knowing the simple ones
New species, isotopic species, vib. states

QCC

Astrochemical modeling

Databases (Funding!)

Analysis software

Pick the right sources

Max-Planck-Institut für Radioastronomie


Thanks!