

Molecular complexity around evolved stars

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The Cosmic Cycle of Dust and Gas in the Galaxy: From Old to Young stars
9-13 July 2018, Guy Nhon (Vietnam)

Interstellar and circumstellar molecules

2 atoms		3 atoms		4 atoms		5 atoms		6 atoms		7 atoms		8 atoms	
H ₂	CP	H ₃ ⁺	MgCN	CH ₃	NH ₃ D ⁺	C ₂ H ₄	CH ₃ NH ₂	CH ₃ CHNH					
LiH ?	AlO	CH ₂	NaCN	NH ₃	CH ₄	CH ₃ OH	CH ₃ C ₂ H	CH ₂ CHCHO					
CH													
CH ⁺													
NH													
OH													
OH ⁺													
HF													
C ₂													
CN	SO ⁺	HCO ⁺	AlNC	C ₃ H	HNCNH	H ₂ C ₄	CH ₃ NCO	H ₂ C ₆					

Large prevalence of organic molecules
 ≈3/4 (all with 6 or more atoms) contain at least one C atom

Large organic molecules around evolved stars:

- Presence of unsaturated carbon chains
- No saturated O-, N-bearing stable molecules

9 atoms		10 atoms	
HC ₄ N	CH ₂ CHCH ₃	CH ₃ COCH ₃	C ₃ H ₆ O
HC ₃ NH ⁺	CH ₃ OCH ₃	OHCH ₂ CH ₂ OH	CH ₃ OCH ₂ OH
HC ₂ CHO	CH ₃ CH ₂ OH	CH ₃ CH ₂ CHO	
c-H ₂ C ₃ O	CH ₃ CH ₂ CN	CH ₃ C ₅ N	
C ₅ H	CH ₃ CONH ₂		
C ₅ N	CH ₃ C ₄ H		
C ₅ N ⁻	C ₈ H		
C ₅ S	HC ₇ N		
SiH ₃ CN ?			

Metal-bearing molecules (Mg, Al, Ti, Fe, Na, K)
 They are only found around evolved stars

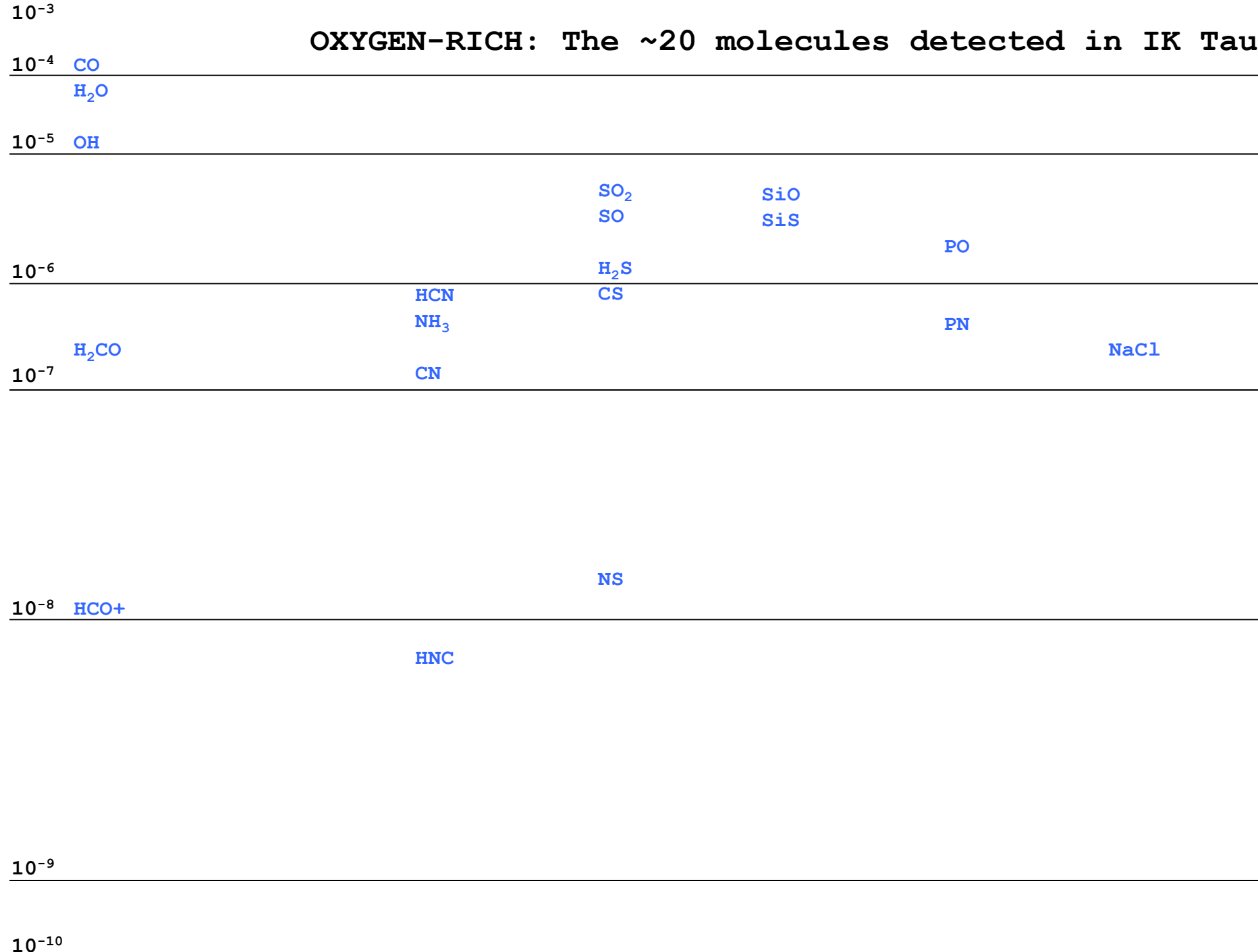
SH	AlOH	C ₃ N	CNCNH
SH ⁺	CO ₂	C ₃ N ⁻	C ₅
HCl	HCS ⁺	C ₃ O	H ₂ NCO
HCl ⁺	C ₂ O	HNCS	NCCNH
SiC	C ₃	HSCN	CH ₃ Cl
SiN	MgNC	c-SiC ₃	
ArH ⁺	CCN	C ₃ S	
NO ⁺ ?	Si ₂ C	HMgNC	
NS ⁺	S ₂ H	MgCCH ?	
	HCS, HSC	NCCP ?	
	NCO	HCCO CNCN	

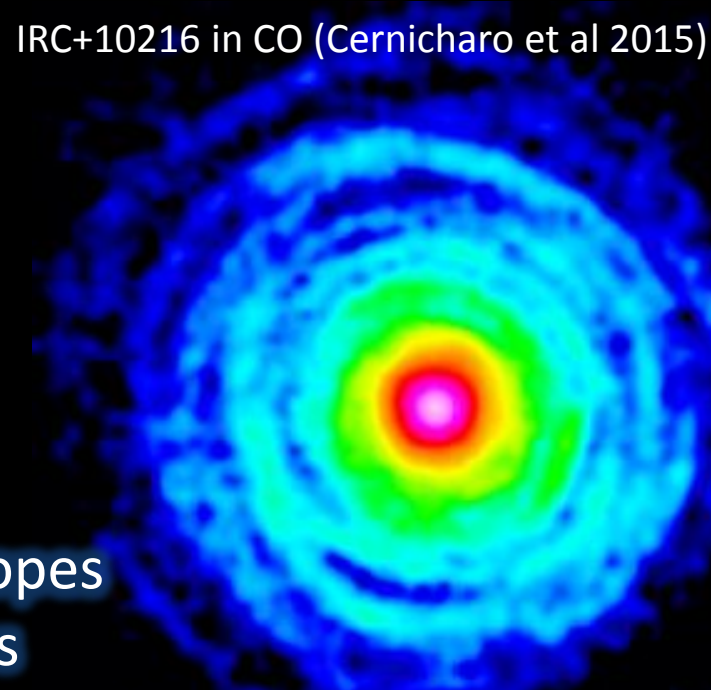
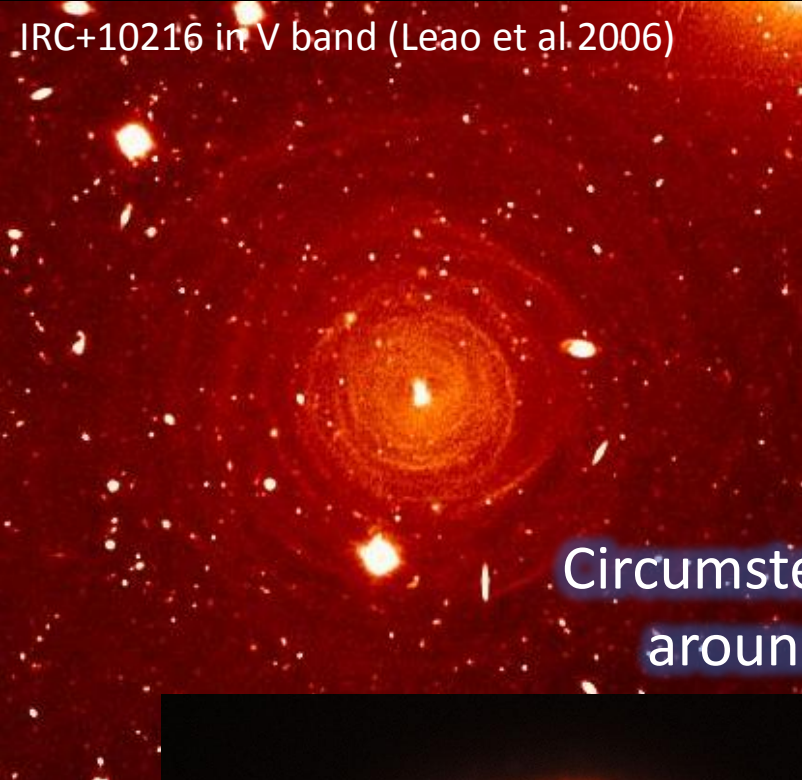
c-C₆H₅CN

CARBON-RICH: The ~80 molecules detected in IRC+10216

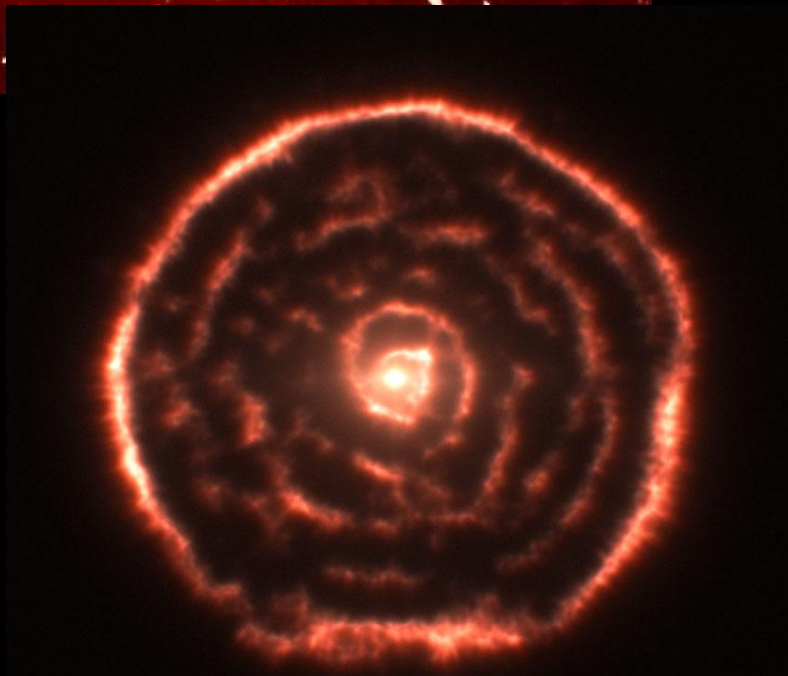
10^{-3}	CO						
10^{-4}		C ₂ H ₂					
10^{-5}			HCN				
		CH ₄					
		C ₂ H	NH ₃				
		C ₄ H	CN				
		C ₂	HC ₃ N		SiC ₂		
10^{-6}		C ₃			SiS		
			C ₃ N	CS	Si ₂ C		
					SiH ₄		
			HC ₅ N		SiO		HCl
10^{-7}	H ₂ O	C ₅	HNC				
		l-C ₃ H	CN-				
	OH	C ₆ H			SiC		
		C ₅ H	CH ₃ CN	C ₂ S			AlCl
		c-C ₃ H ₂					
		CH ₃ C ₂ H					
		c-C ₃ H	HC ₇ N			HCP	
		C ₂ H ₄					NaCN
10^{-8}	H ₂ CO	H ₂ C ₄		C ₃ S	CH ₃ SiH ₃		
						CP	HF
		C ₈ H	HC ₉ N	H ₂ CS	SiN	PH ₃	MgNC
			CH ₂ CN				AlF
			HC ₂ N				
			C ₅ N				
		C ₇ H	HCCNC				
		H ₂ C ₆	C ₂ H ₃ CN	H ₂ S	c-SiC ₃		
		C ₆ H-	C ₅ N-		SiC ₄		
	C ₃ O	C ₈ H-	HC ₄ N		SiCN		
		H ₂ C ₃	C ₃ N-	C ₅ S	SiNC	PN	NaCl
10^{-9}						C ₂ P	AlNC
	HCO+		HNCCC				MgCN HMgNC
		C ₄ H-					KCl FeCN KCN
10^{-10}							

OXYGEN-RICH: The ~20 molecules detected in IK Tau

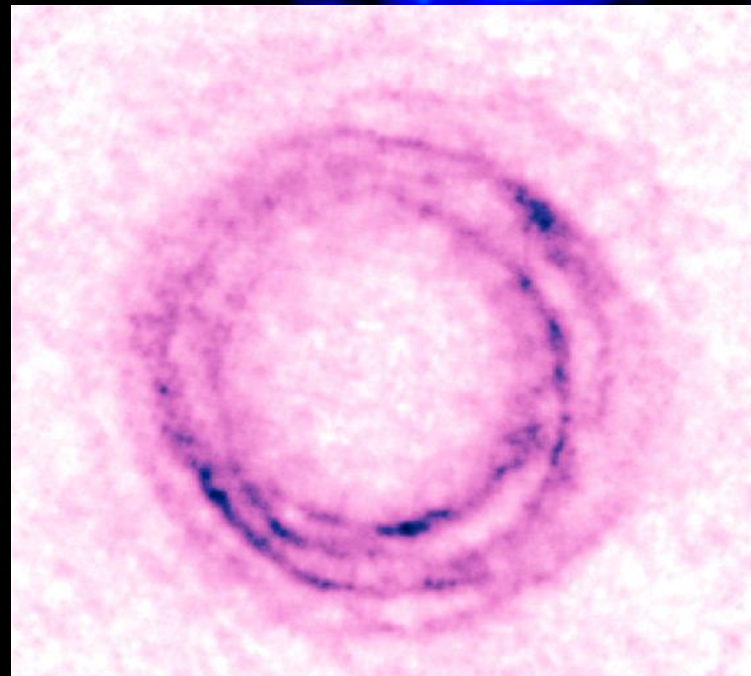




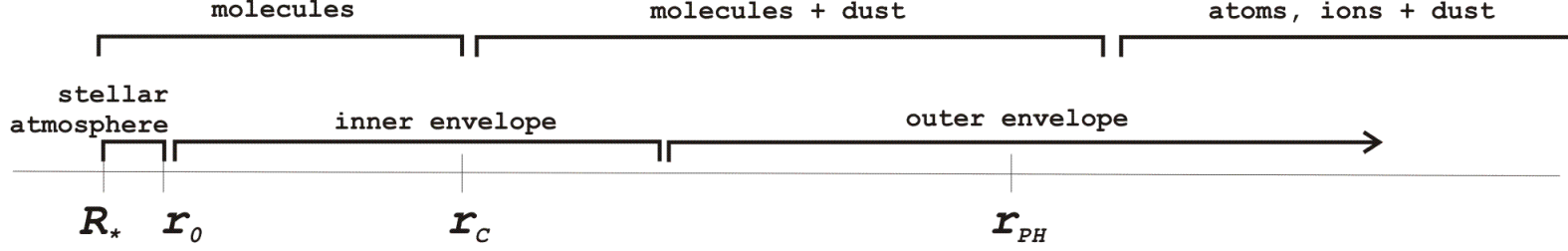
Circumstellar envelopes
around AGB stars



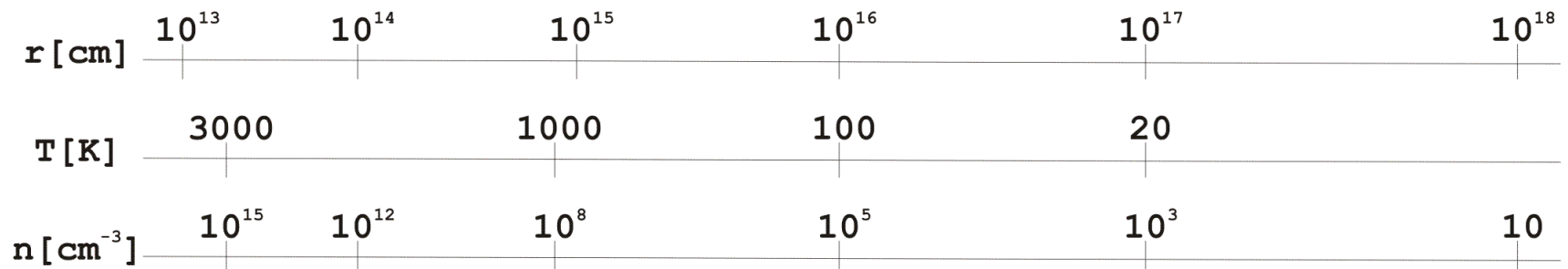
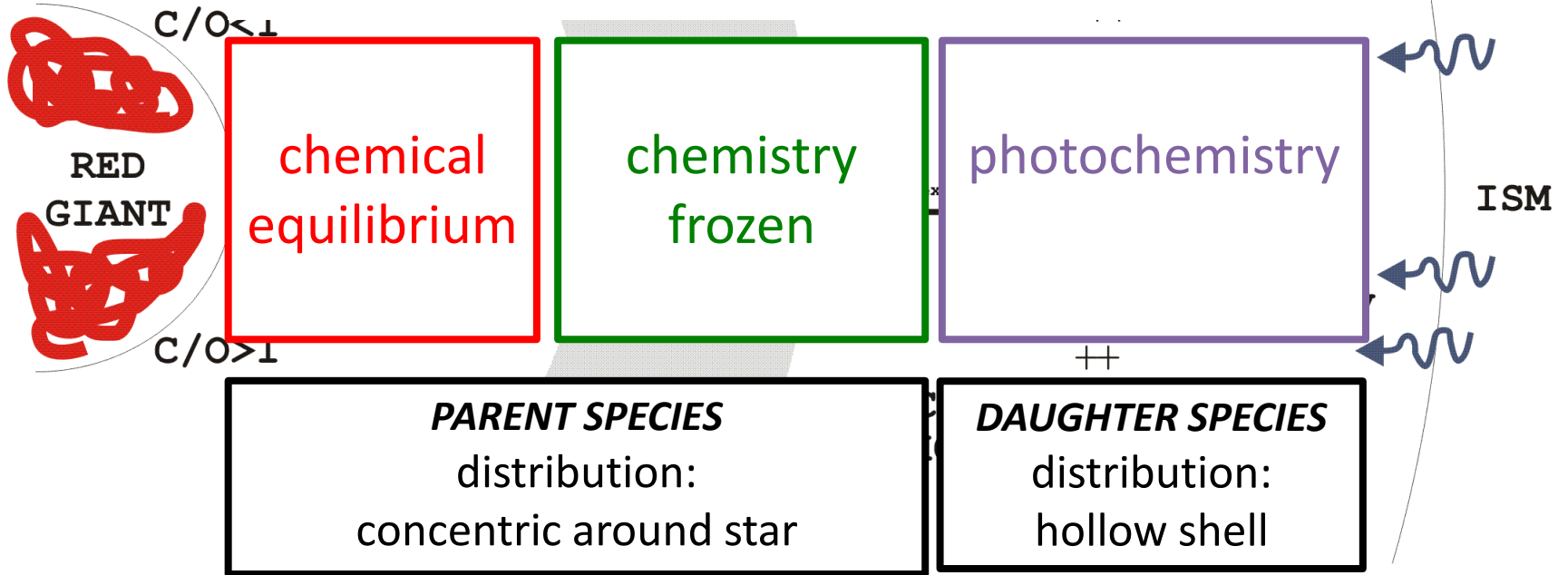
R Sculptoris in CO (Maercker et al 2012)

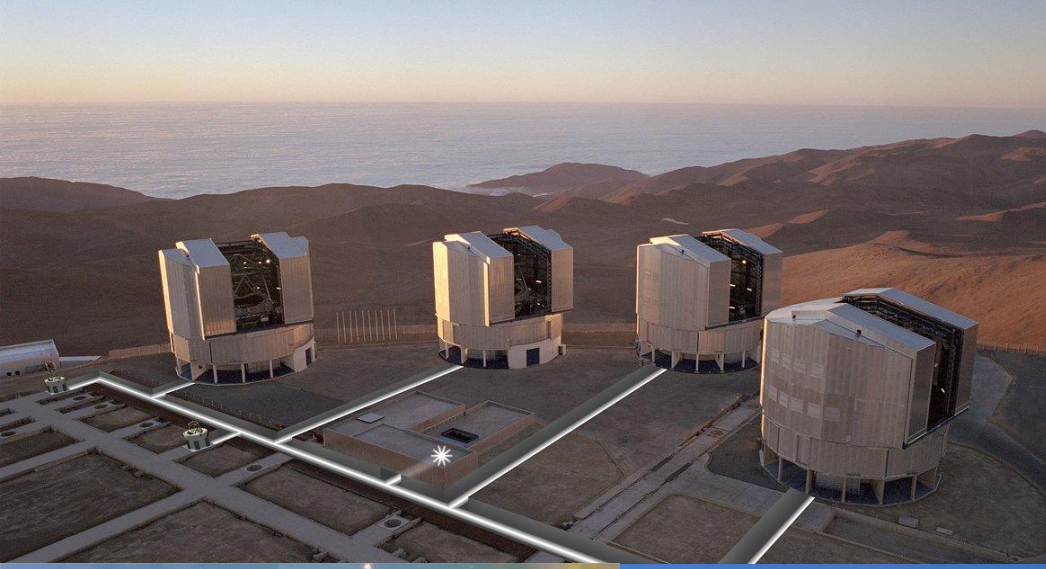


IRC+10216 in CN (Agúndez et al 2017)



standard scenario





Outline of the rest of the talk:

1) Some introduction (already done)

1) Chemistry in the inner layers

1) Chemistry in the outer envelope

1) Concluding remarks

The inner circumstellar layers

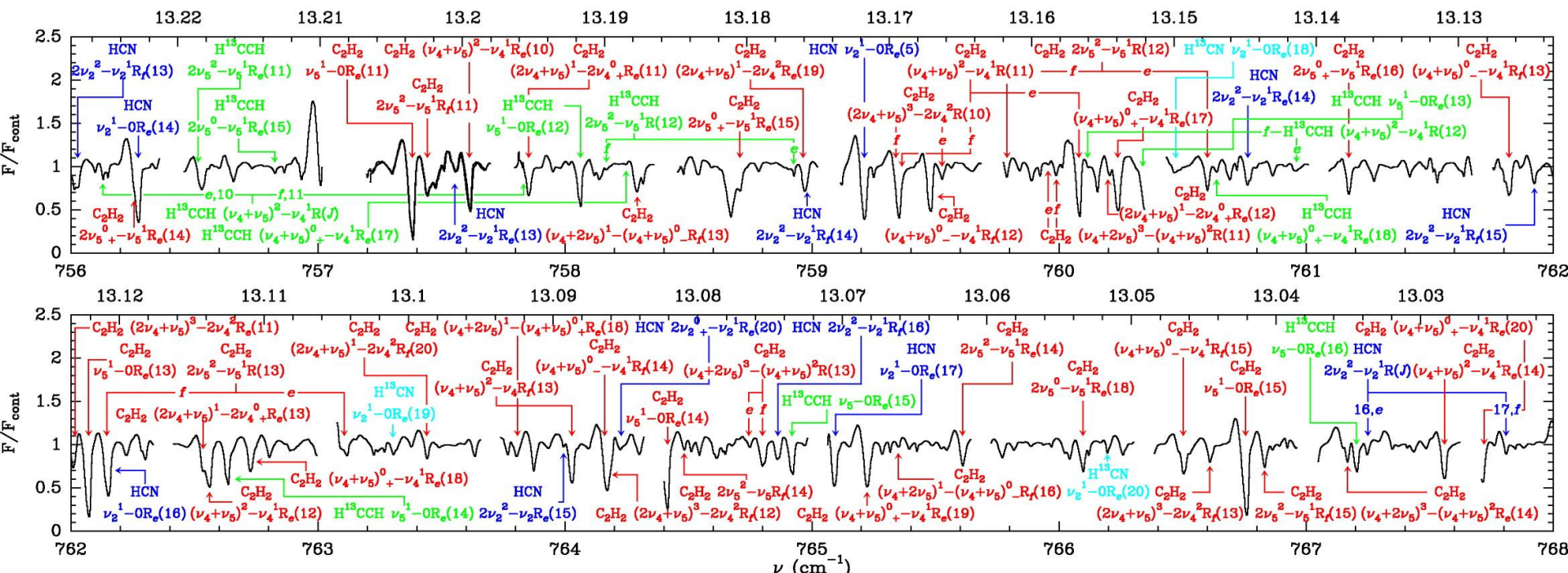


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CW Leo observed in the MIR (11-14 μm) with IRTF/TEXES (Fonfría et al 2008)

Spectra shows absorption lines from C_2H_2 and HCN present in the inner circumstellar envelope

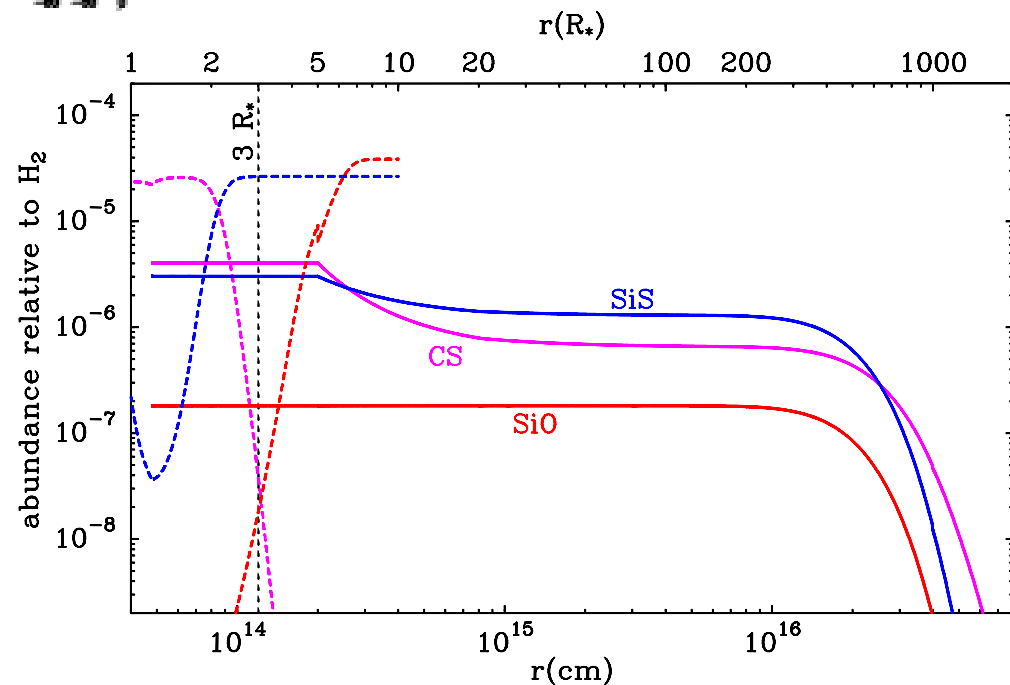
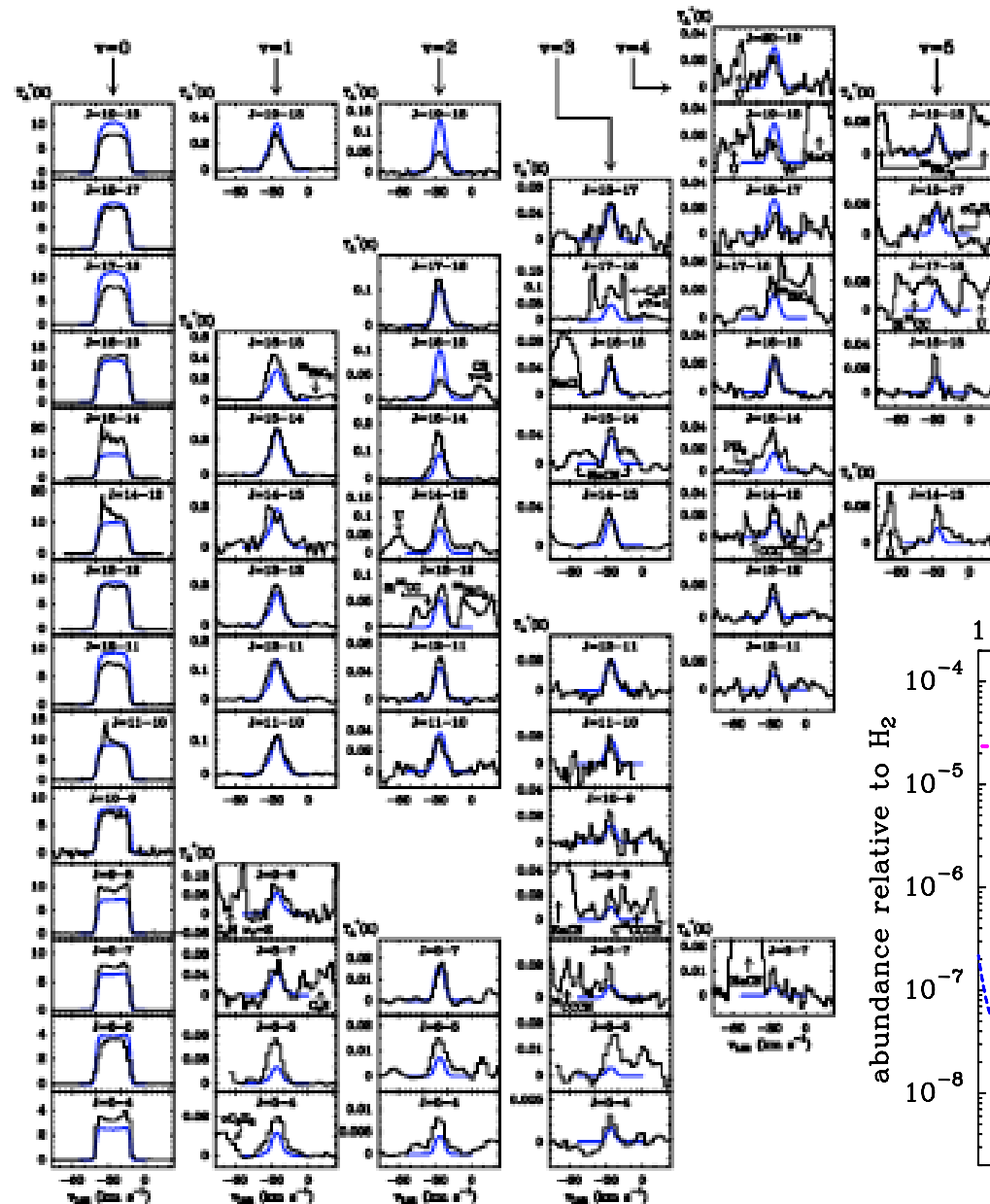


Single-dish millimeter observations

SiS ($v=0-6$) lines in IRC+10216 (Agúndez et al 2012)

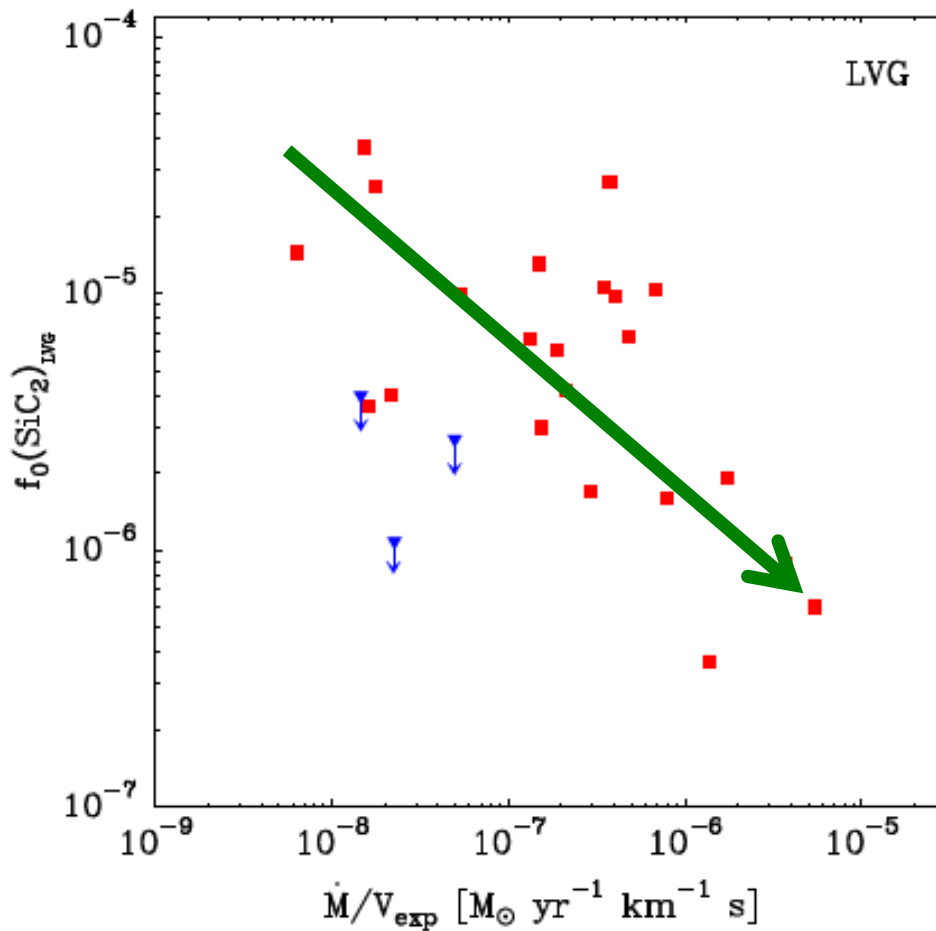


A detailed model allows to derive the radial abundance profile



Single-dish millimeter observations

SiC₂ in a sample of carbon stars
(Massalkhi et al 2018)



Gas-phase abundance of SiC₂
decreases with increasing density

Can be interpreted in terms of a
more efficient formation of dust
(and incorporation of SiC₂ on grains)
at high densities

Legacy of Herschel on circumstellar chemistry

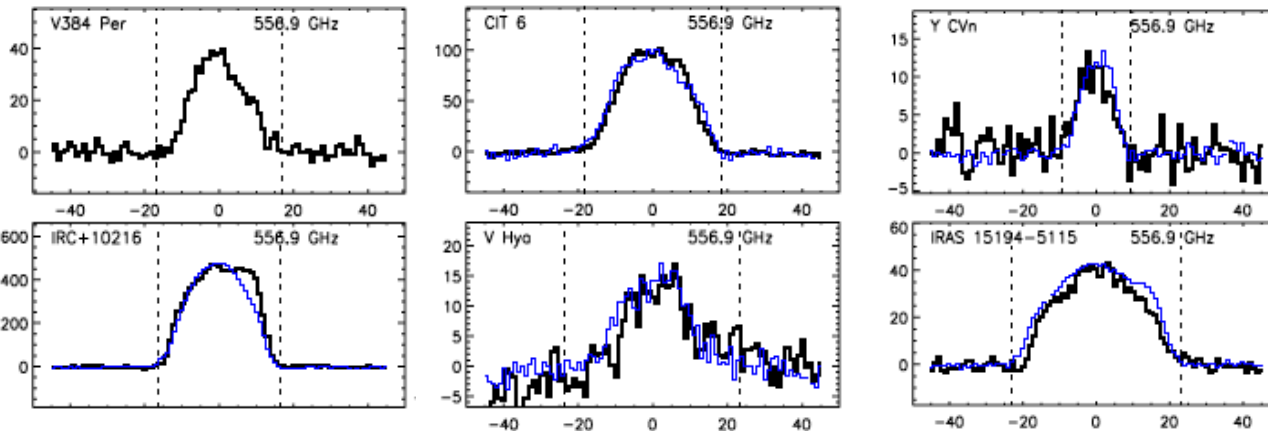
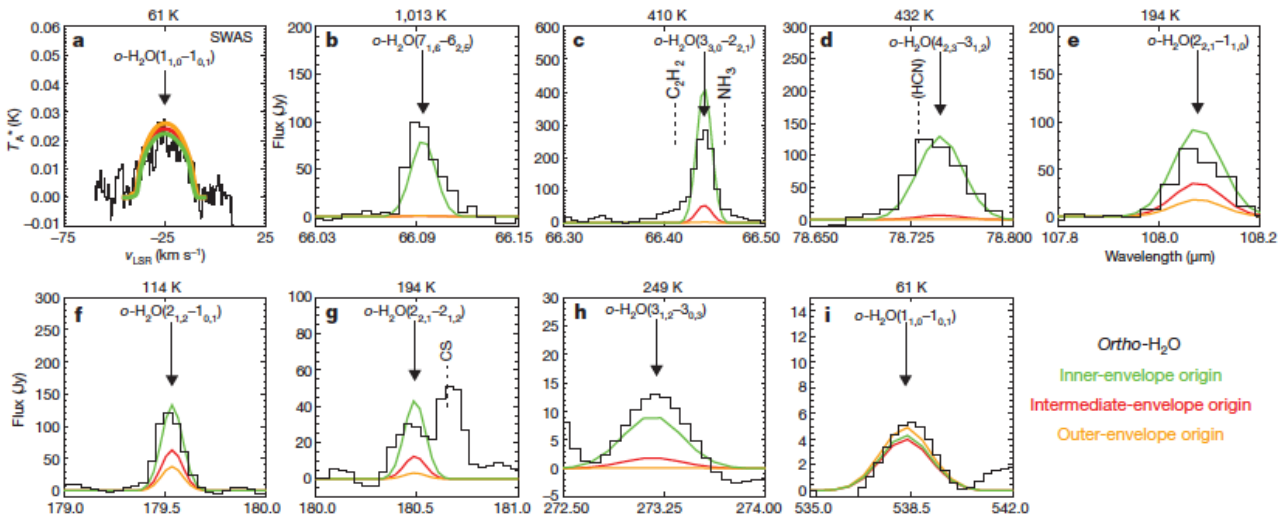
H₂O around carbon stars

Inner-envelope origin

Widespread occurrence in carbon stars



Decin et al (2010)



Neufeld et al (2011)

Legacy of Herschel on circumstellar chemistry

H₂O around carbon stars

Inner-envelope origin

Widespread occurrence in carbon stars

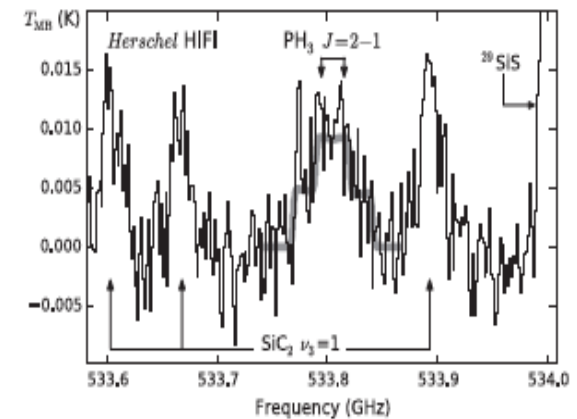
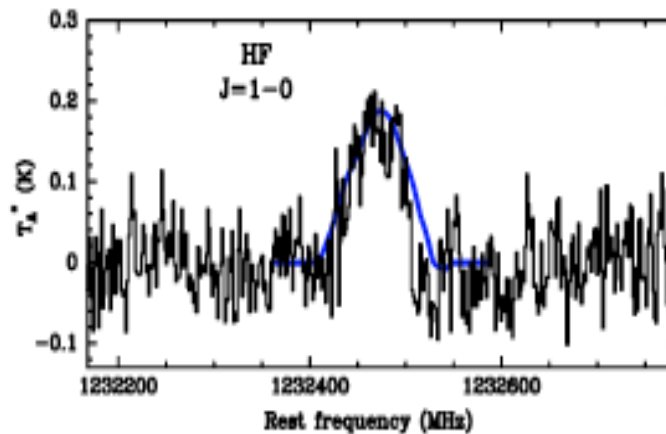
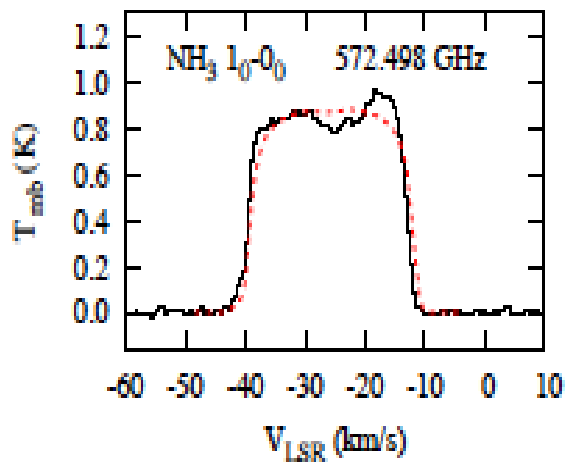
Other hydrides around AGB stars

NH₃ (Menten et al 2010; Schmidt et al 2016; Wong et al. 2018)

HCl (Cernicharo et al 2010; Agúndez et al 2011)

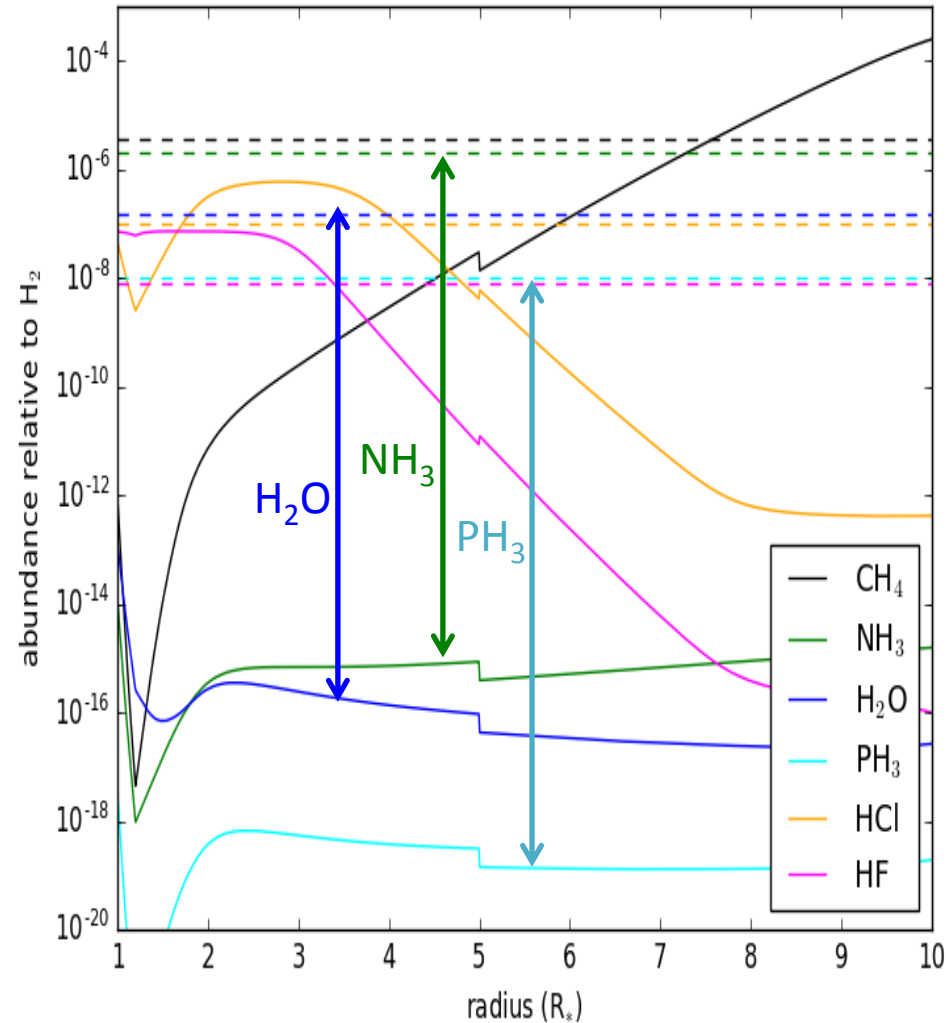
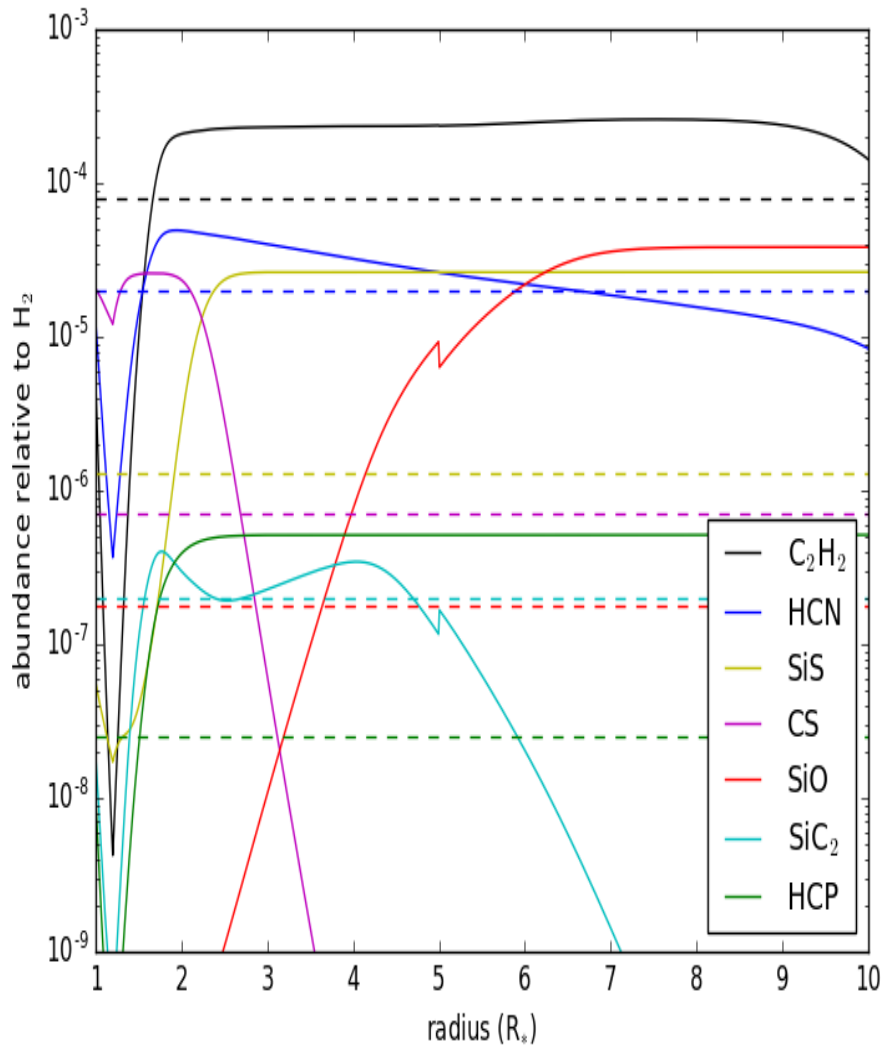
HF (Agúndez et al 2011)

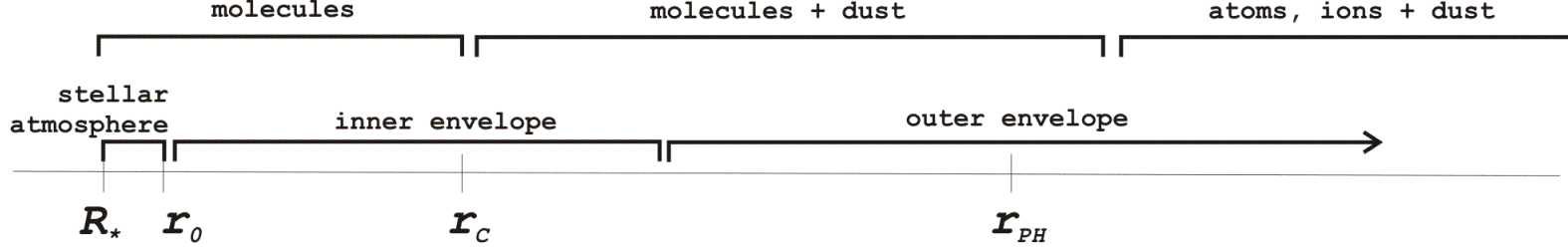
PH₃ (Agúndez et al 2014)



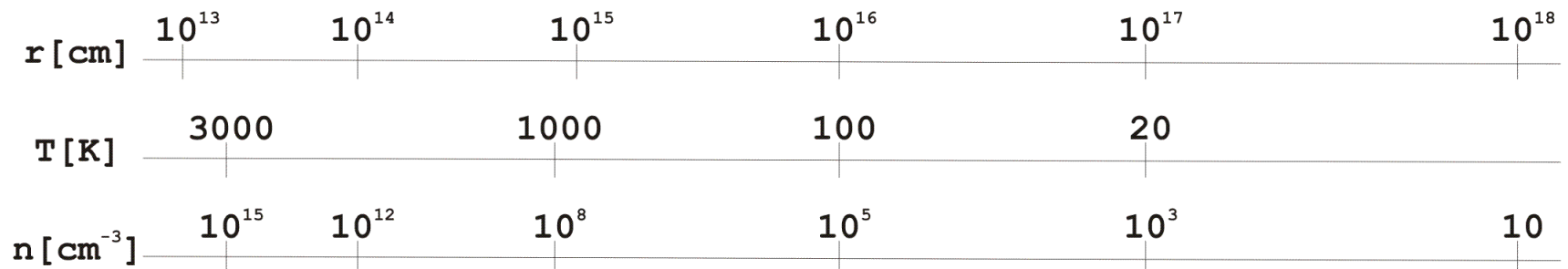
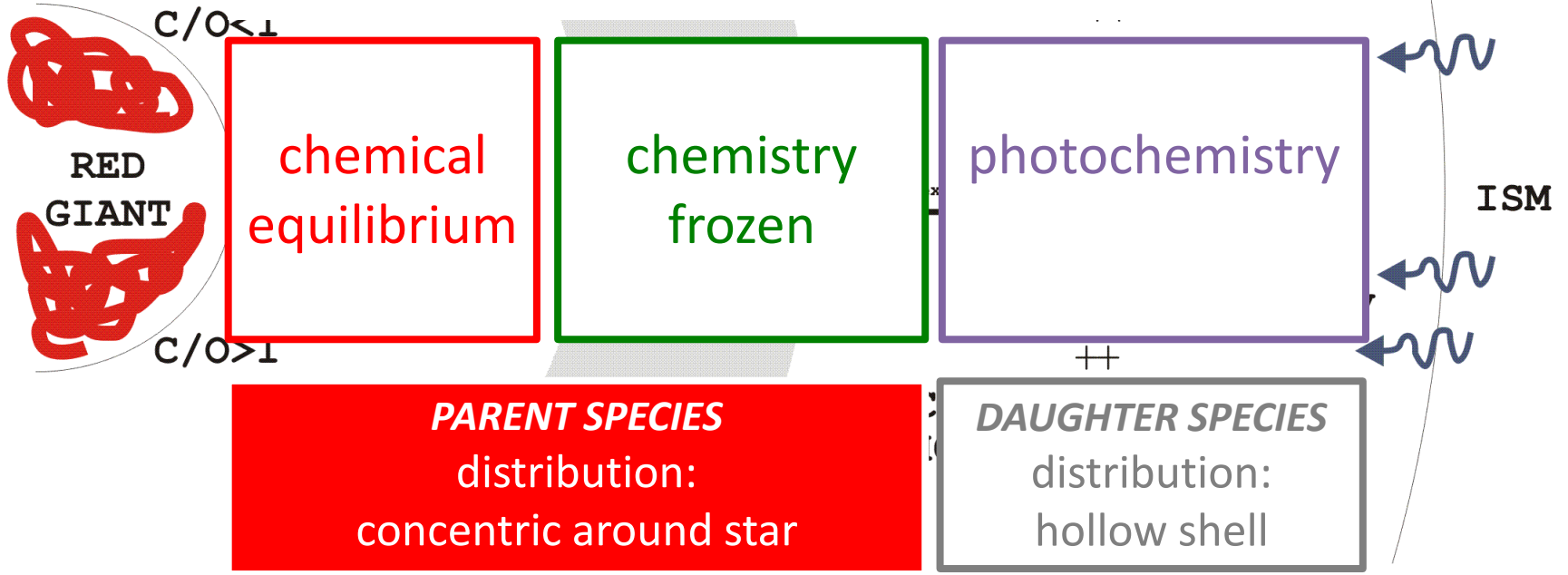
Comparison between observed abundances and calculated abundances at chemical equilibrium for the carbon star IRC+10216

— calculated at LTE
- - - observed

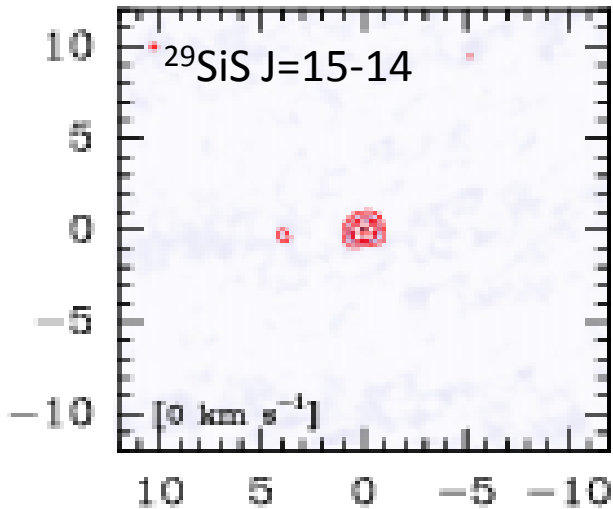
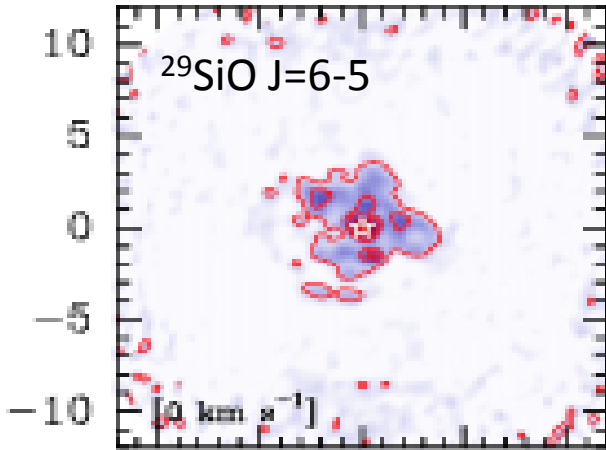




standard scenario



Small-scale distribution of parent species in IRC+10216

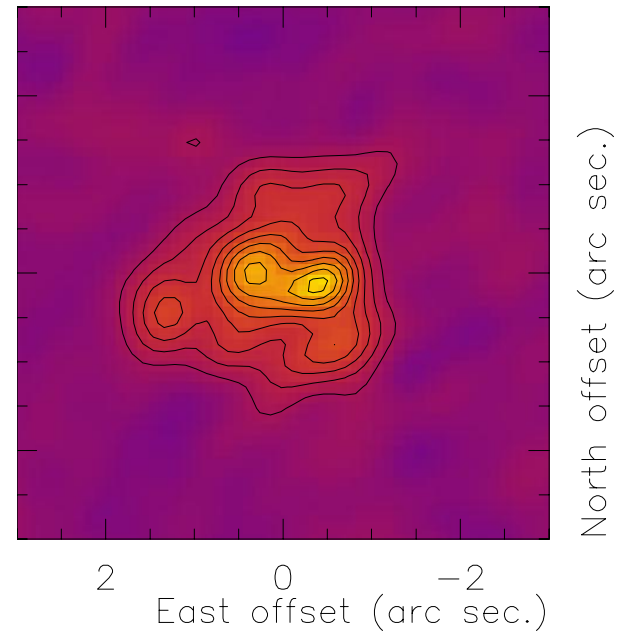


Velilla Prieto et al (2015)

The arrival of ALMA



$\text{NaCl } J=21-20$



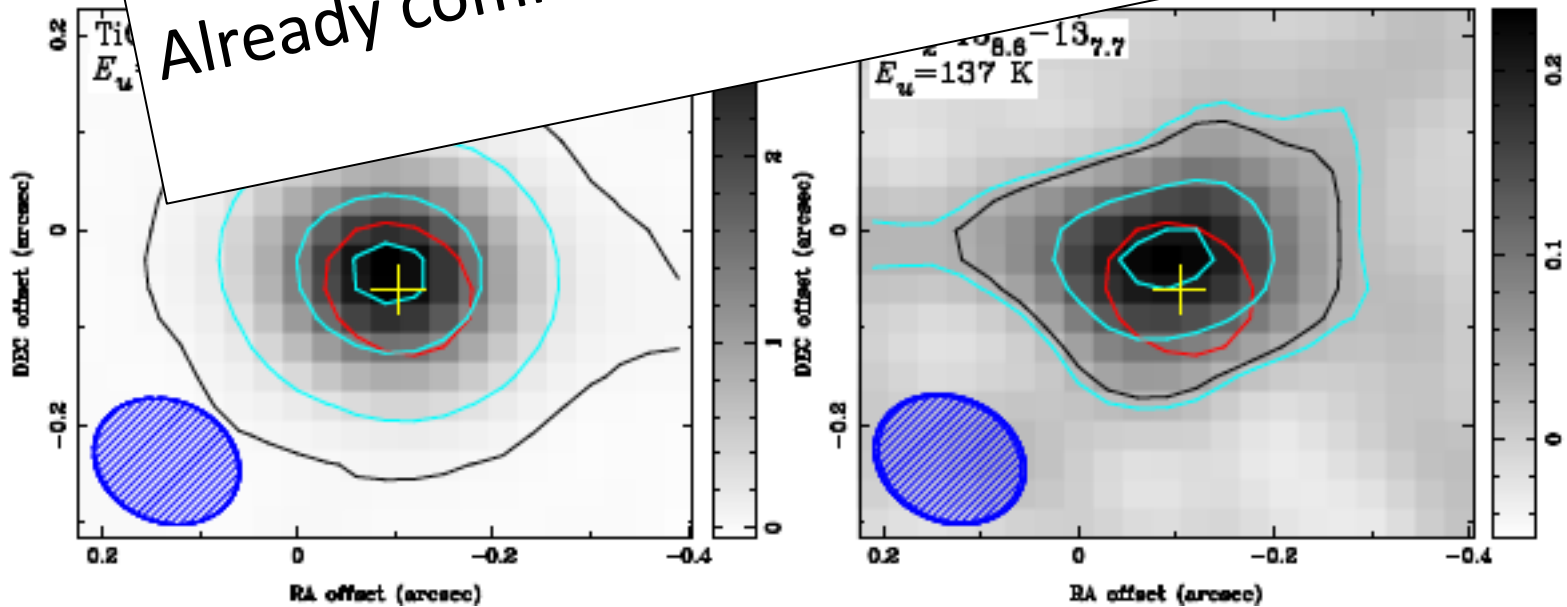
Quintana-Lacaci et al (2016)

Small-scale distribution of Ti and Al oxides in O-rich stars

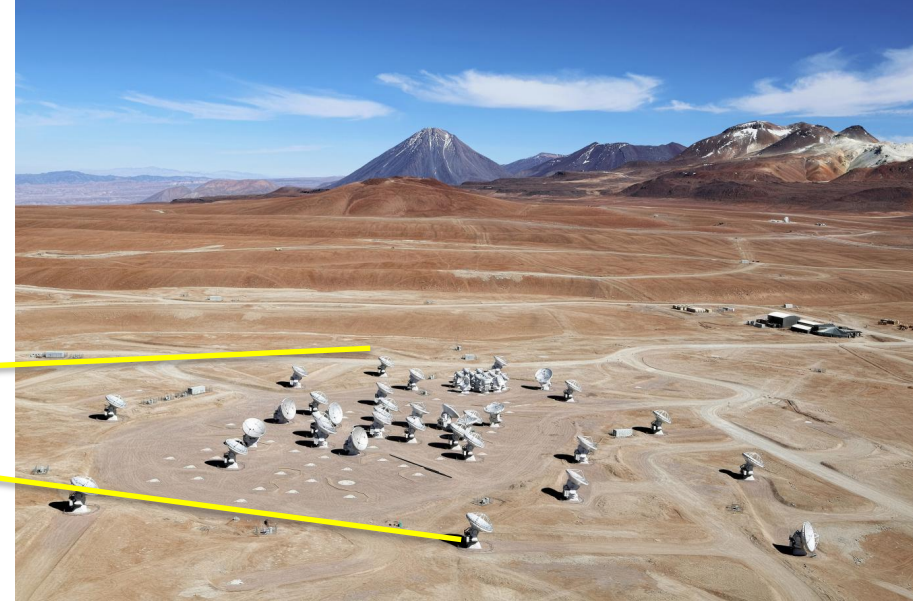
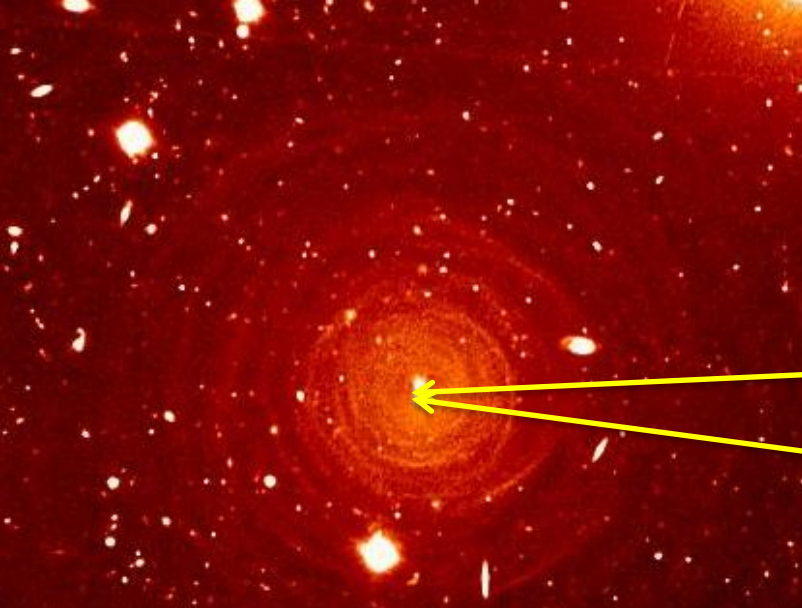


Evaluating the role of TiO , TiO_2 , AlO as gas-phase precursors

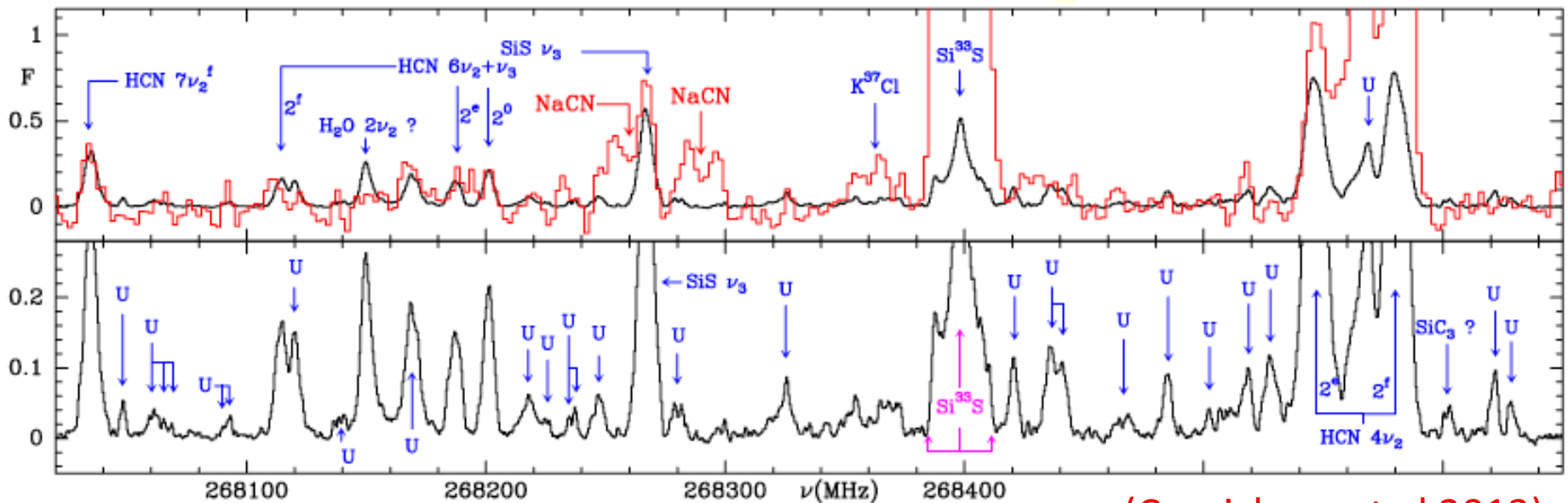
Already commented by Jean Martin Winters



Kaminski et al (2017). See also Kaminski et al (2016), Decin et al (2017).

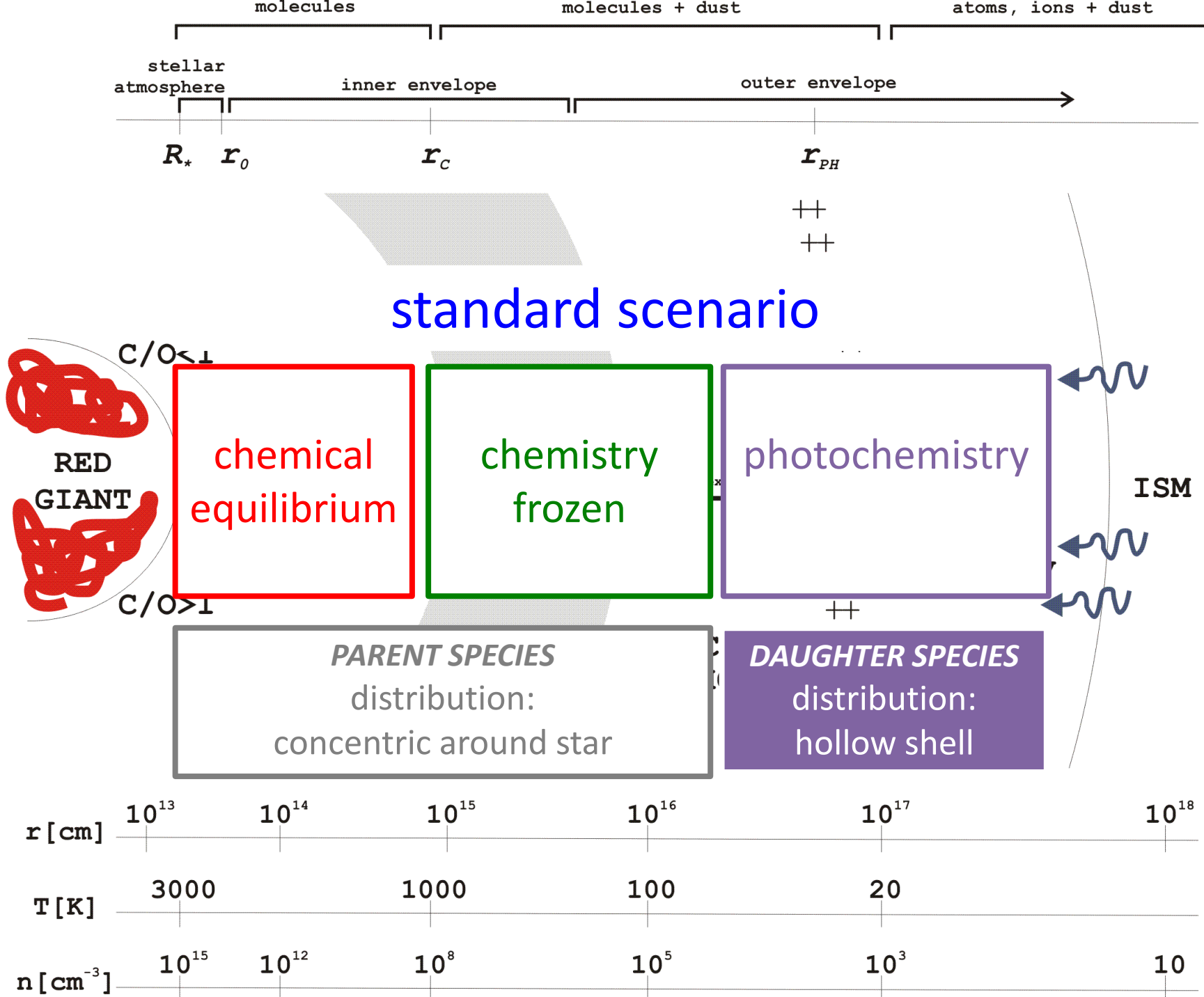


The ALMA view of IRC+10216:
 a forest of U lines arises from the surroundings of the star

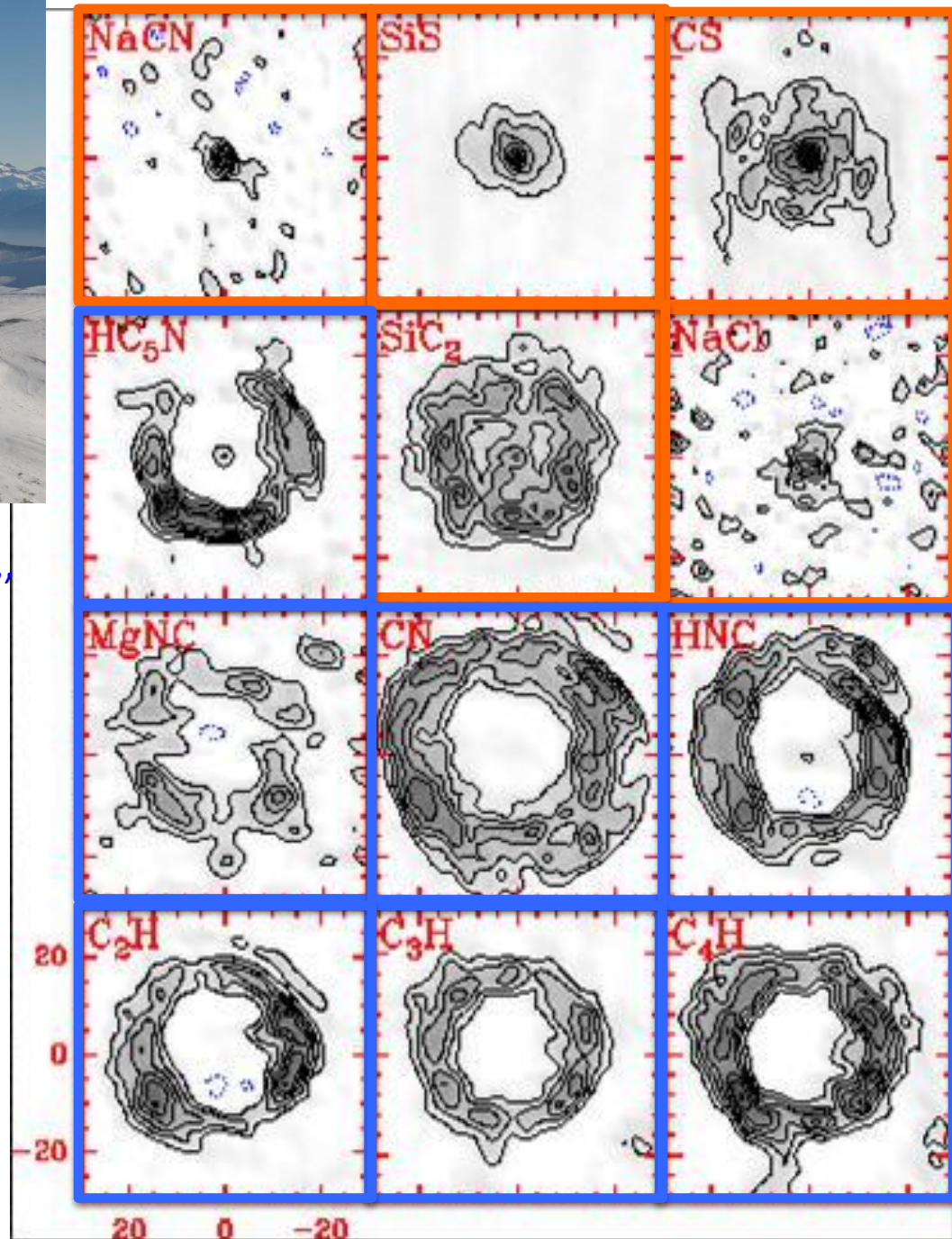


(Cernicharo et al 2013)

The outer circumstellar envelope

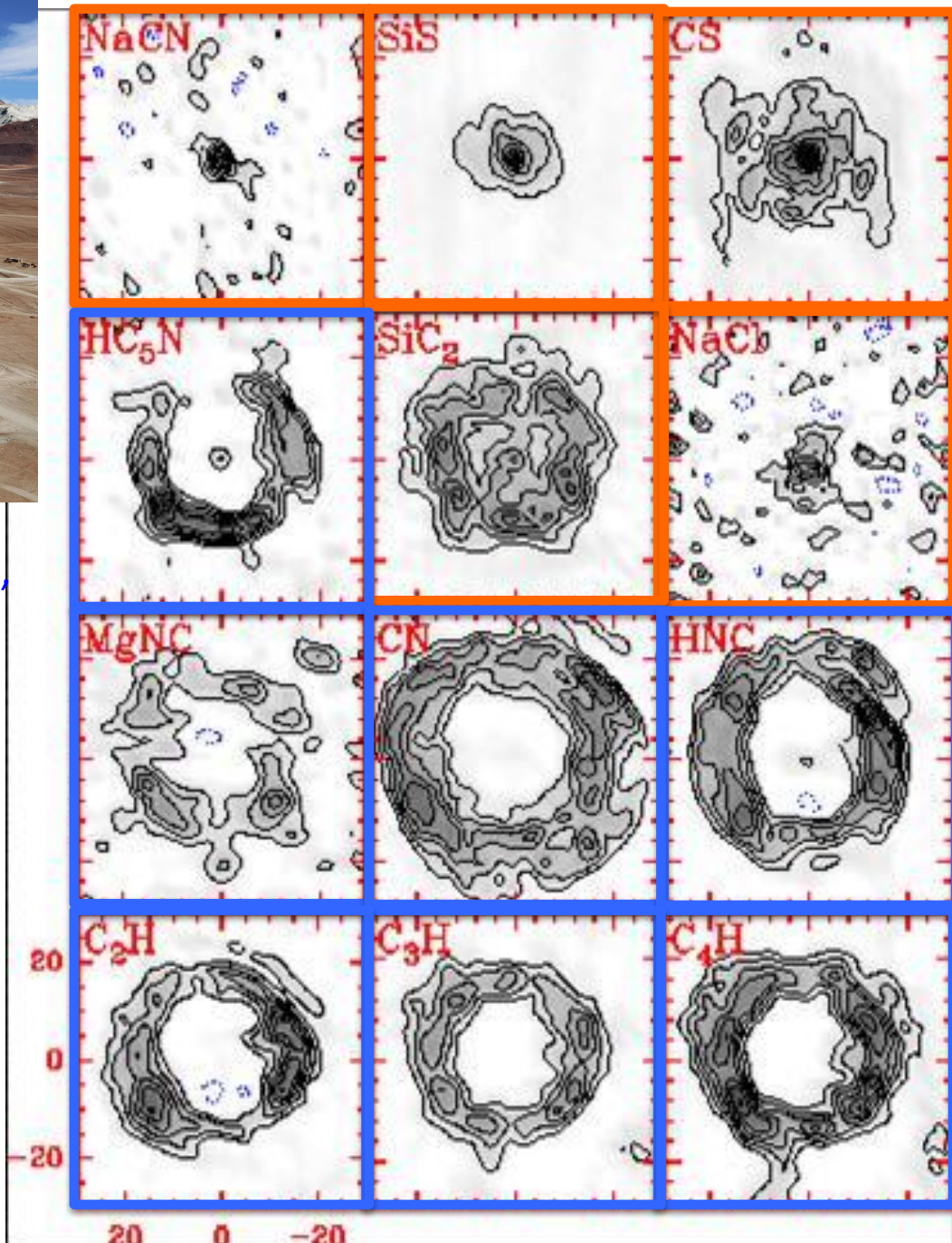


IRAM Plateau de Bure (1990s)



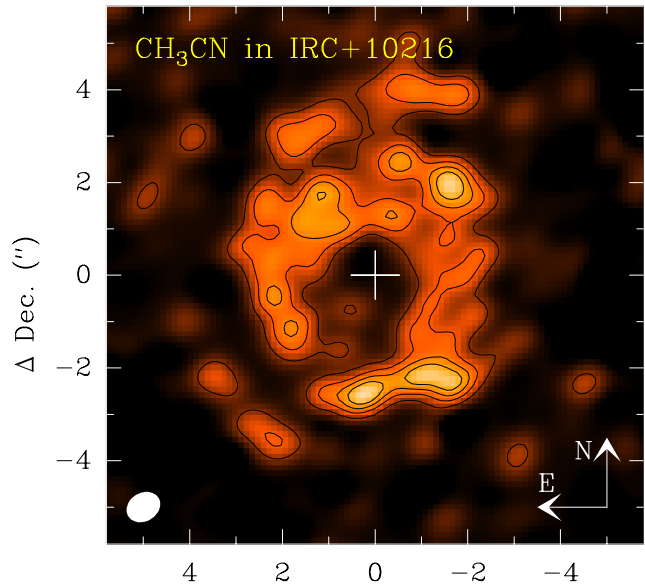
Parent species: concentric around star
Daughter species: hollow shell at $\approx 15-20''$

ALMA



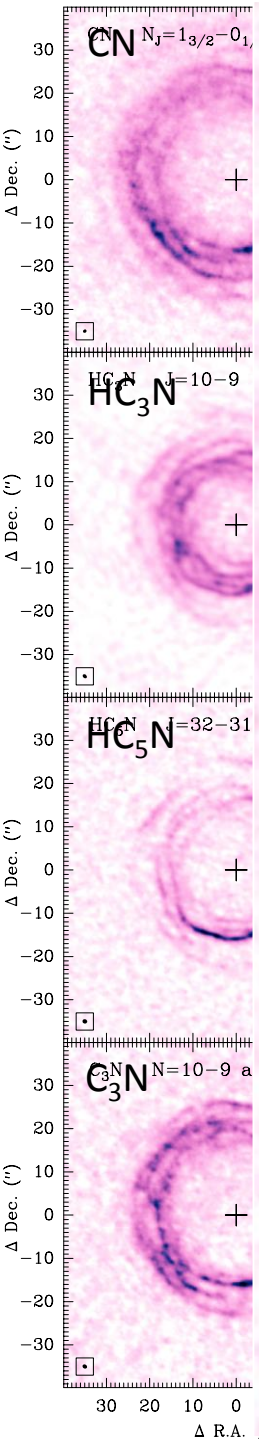
Parent species: concentric around star
Daughter species: hollow shell at $\approx 15-20''$

CH_3CN shows a peculiar distribution

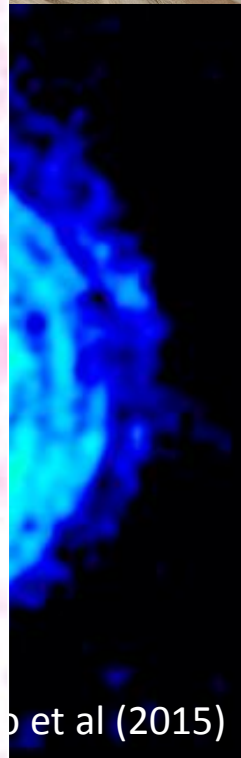
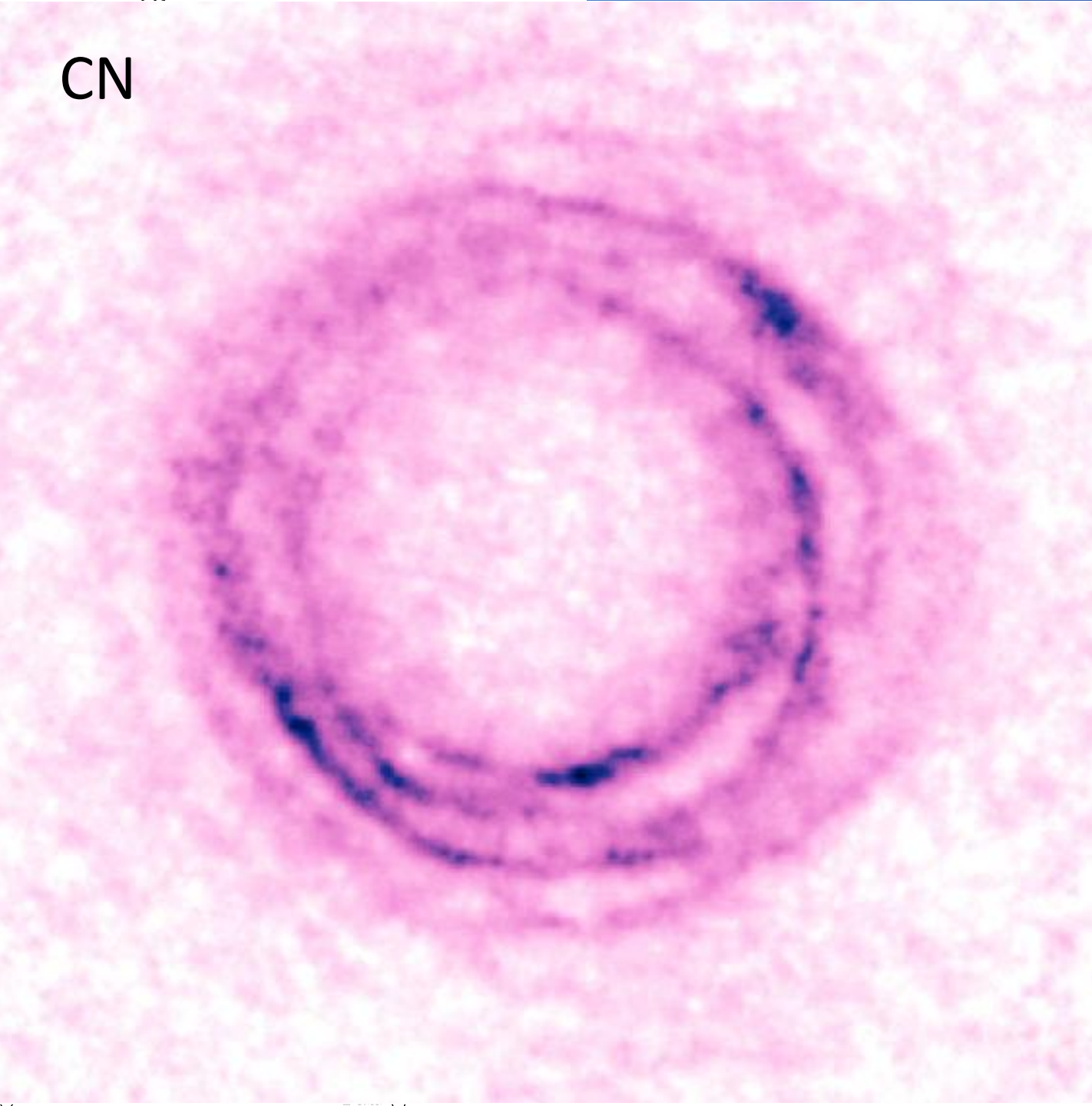


Agúndez et al. (2015)

Guélin et al. (IRAM PdBI data)



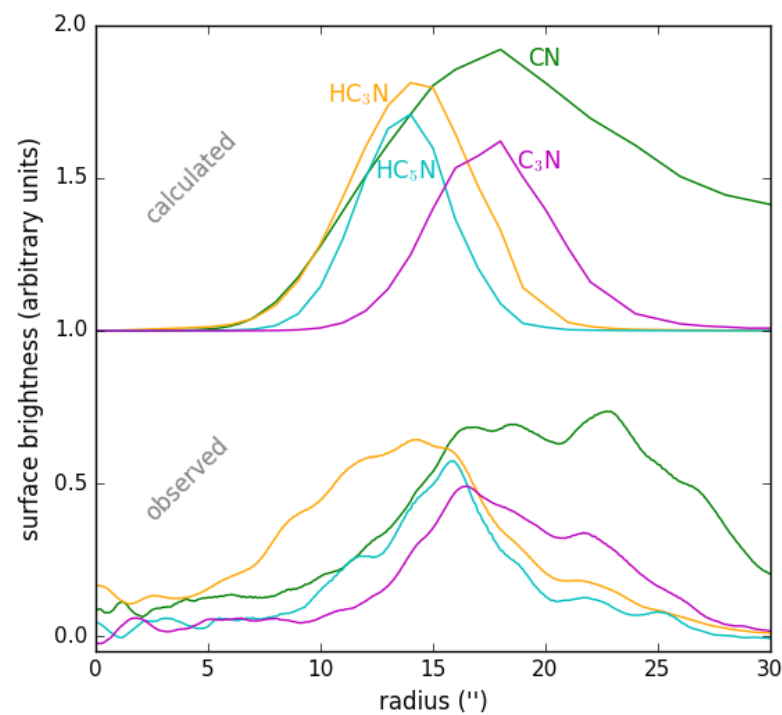
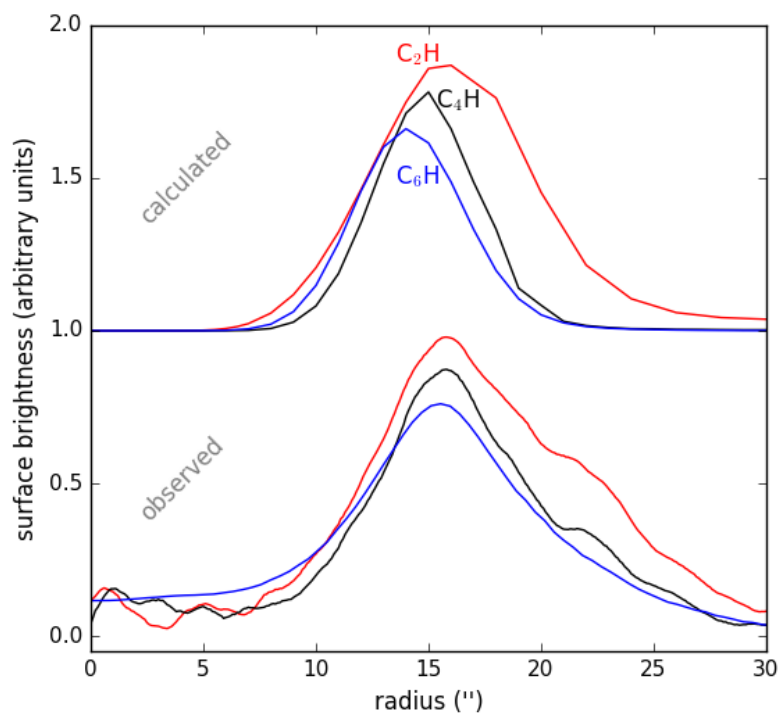
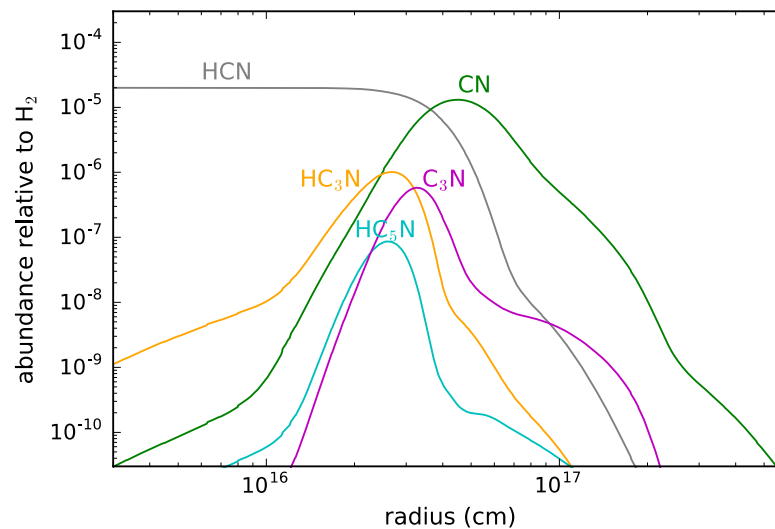
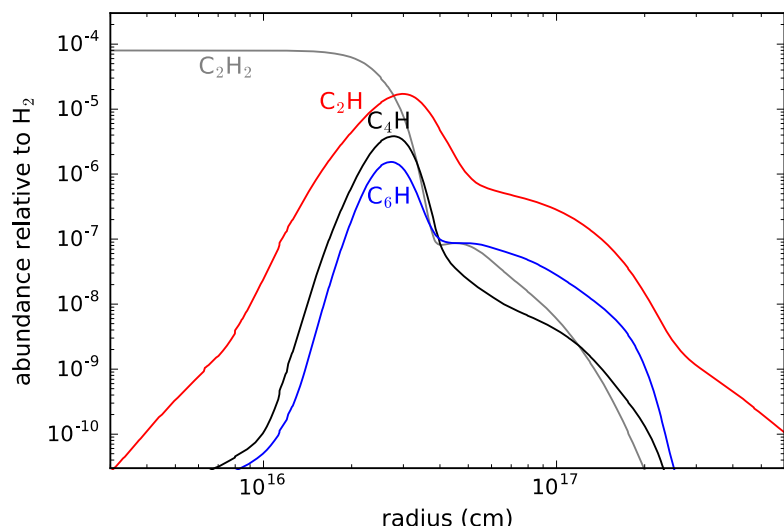
CN



et al (2015)

Carbon chain growth in IRC+10216

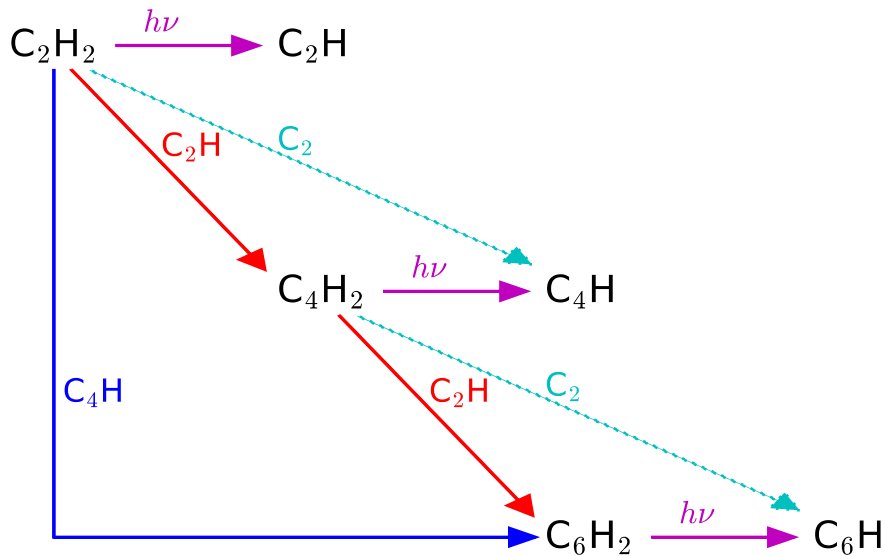
(Agúndez et al 2017)



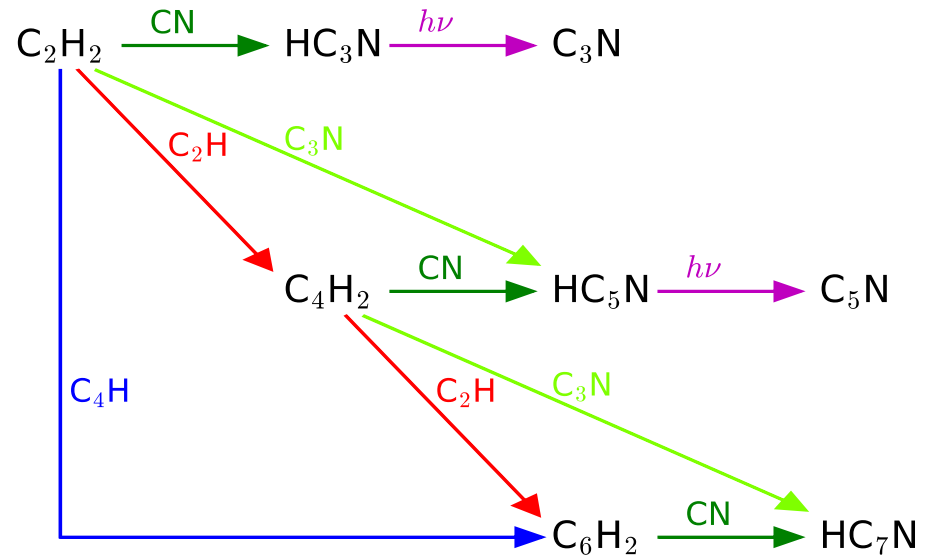
Carbon chain growth in IRC+10216 (schemes according to chemical model)

(Agúndez et al 2017)

Polyynes



Cyanopolyynes



The growth of polyynes is driven by reactions involving C_2H and C_4H radicals

The growth of cyanopolyynes is driven by reactions involving CN and C_3N radicals

Low-temperature kinetics of these reactions studied with CRESU machines

Infrared detection of diacetylene (C_4H_2) in IRC+10216 (Fonfría et al 2018)

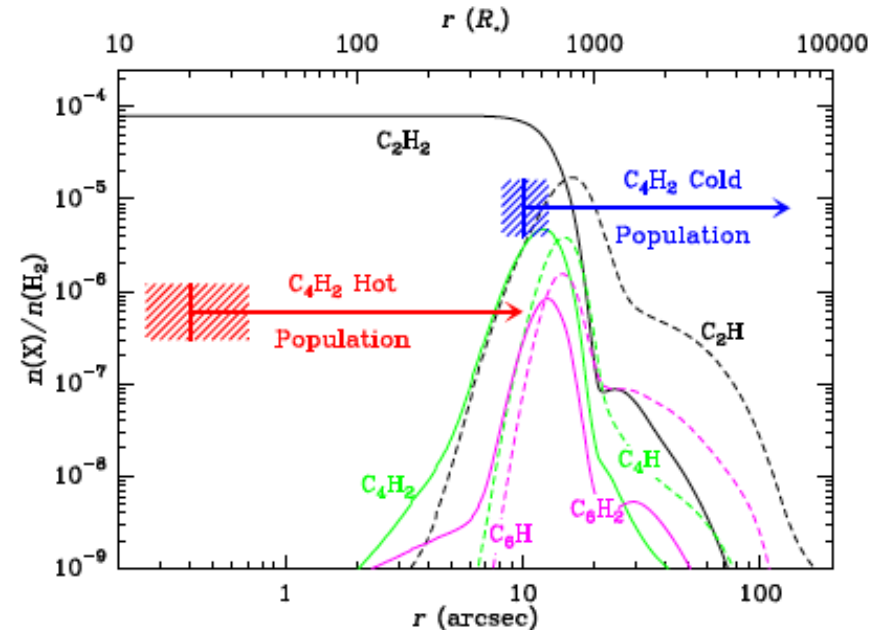
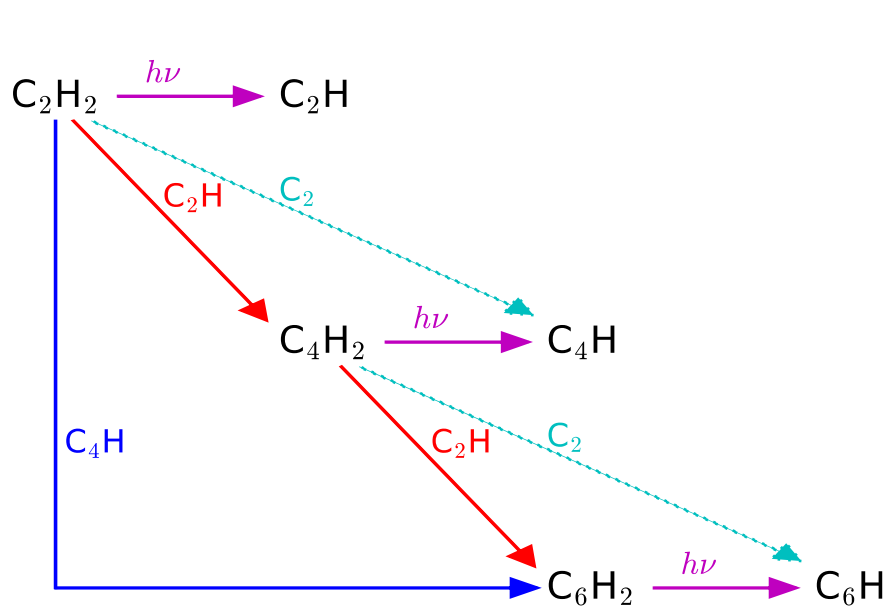
NASA

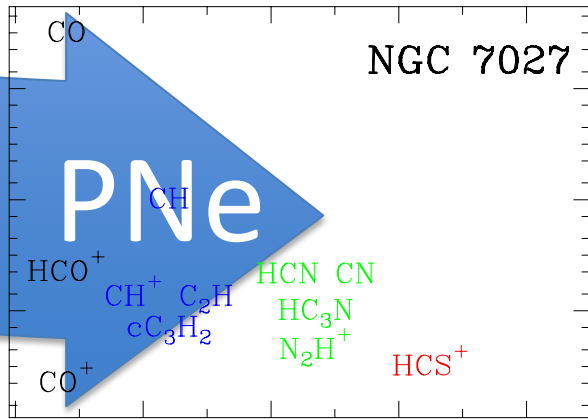
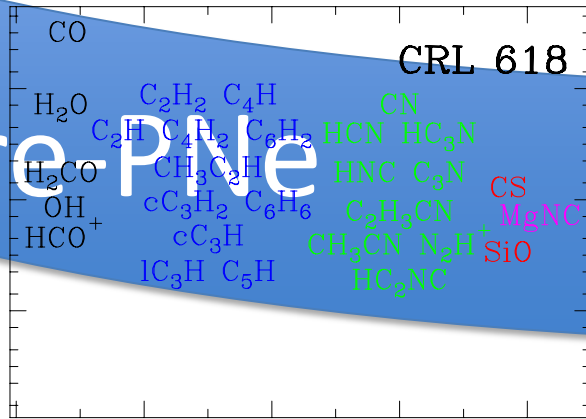
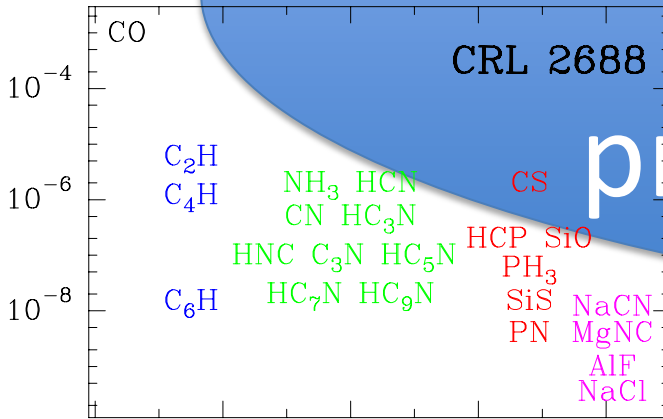
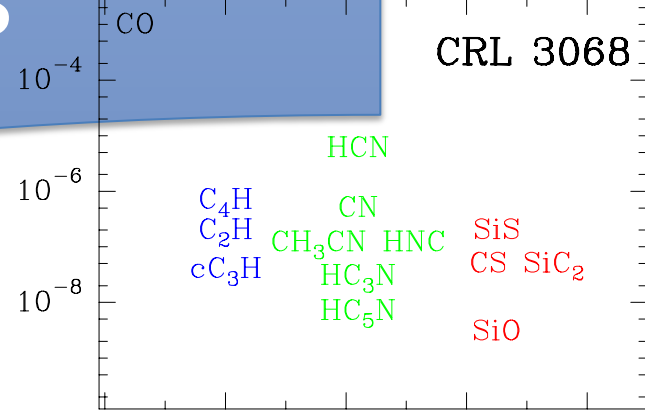
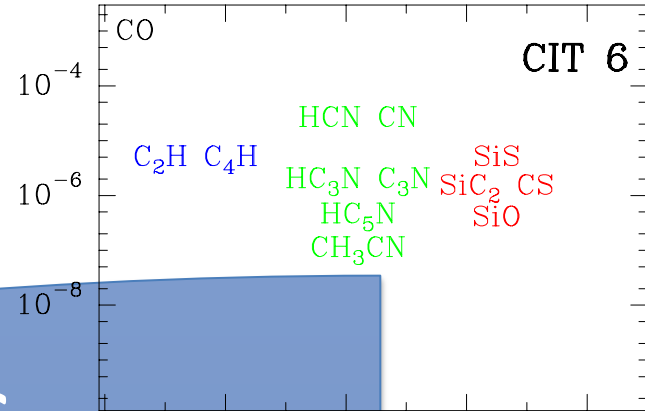
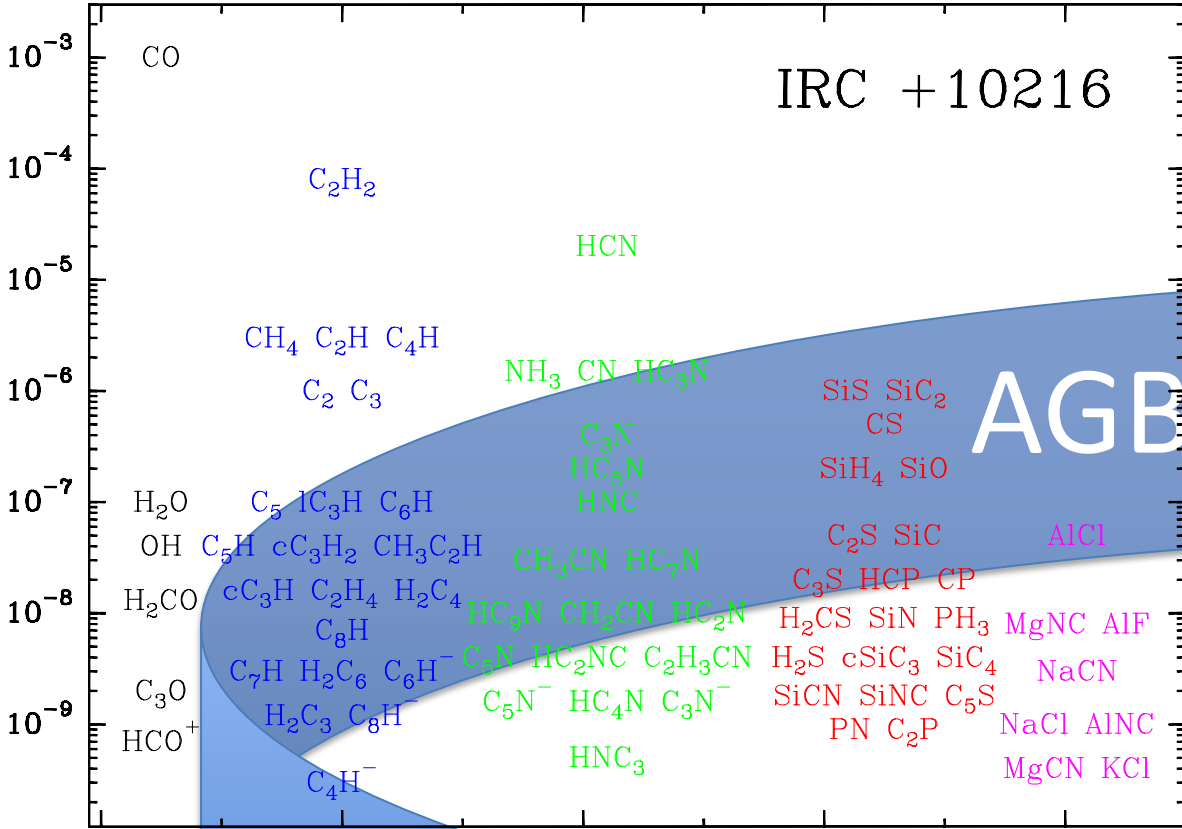
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C_4H_2 is a non polar molecule, predicted to form abundantly in the outer envelope. Important observation because it allows to put constraints on the chemical model.

Derived abundance of cold (outer) C_4H_2 in good agreement with chemical model. Presence of hot (inner) C_4H_2 is puzzling.





Concluding remarks:

- # Overall picture of the circumstellar chemistry around AGB stars well understood
 - > parent molecules formed under LTE close to the star
 - > daughter species formed by photochemistry in outer envelope

- # Observations are revealing a growing number of aspects not well understood yet
 - > Formation of H₂O in C-rich objects and other hydrides (NH₃, PH₃)
 - > Relevance of non-equilibrium chemistry in the inner envelope
 - different small-scale distribution of molecules: (NaCl, KCl) vs (SiS, SiO) in IRC+10216
 - role of refractory molecules as precursors of dust grains
 - distribution of CH₃CN in IRC+10216
 - existence of hot C₄H₂ in IRC+10216
 - carriers of unidentified lines arising just close to the star
 - > Discontinuous and non-isotropic mass loss

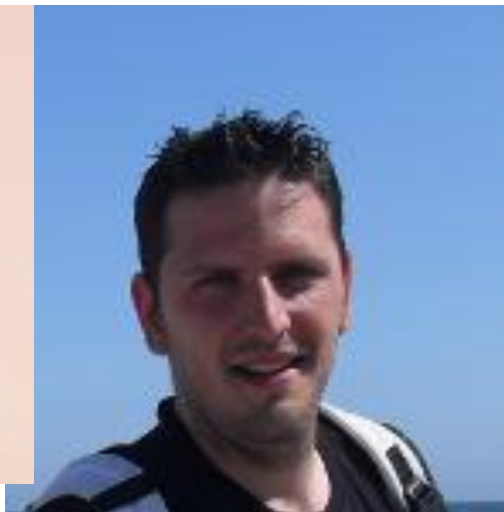
- # Need to revise the current paradigm of circumstellar chemistry
 - > Dust formation
 - > Shocks driven by the stellar pulsation
 - > Clumpiness
 - > Spiral-like structures caused by binarity

The evolved stars team at IFF, Madrid

José Cernicharo



Luis Velilla Prieto



José Pablo Fonfría



Guillermo Quintana-Lacaci



Sarah Massalkhi



Jason Champion

