Young and old, big and small: Chemical modelling at opposite ends of the stellar evolution spectrum

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Outline

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1. Whistle-stop tour of astrochemistry
2. Protoplanetary disks
   - Small molecules in AA Tau
   - Small molecules in GV Tau
   - Predictions of large molecules
   - Predictions of heavy molecules
3. Evolved stars
   - AGB stars
   - Protoplanetary nebulae

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What is astrochemistry?

Astrochemistry is the study of the chemical elements found in outer space, generally on larger scales than the Solar System, particularly in molecular gas clouds, and the study of their formation, interaction and destruction. – **Wikipedia**

What is astrochemistry?

Astrochemistry is the study of atoms, molecules, ions and radicals found outside of the Solar System and the processes which affect them. Generally this excludes the processes which occur inside stars (e.g., nucleosynthesis) – **PMW**

Why do we care?

H_2	C_3	c-C_3H	C_5	C_5H	C_6H	CH_3C_3N	CH_3C_4H
AlF	C_2H	l-C_3H	C_4H	l-H_2C_4	CH_2CHCN	$HCOOCH_3$	CH_3CH_2CN
AlCl	C_2O	C_3N	C_4Si	C_2H_4	CH_3C_2H	CH_3COOH?	$(CH_3)_2O$
C_2	C_2S	C_3O	l-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH
CH	CH_2	C_3S	c-C_3H_2	CH_3NC	$HCOCH_3$	H_2C_6	HC_7N
CH^+	HCN	C_2H_2	CH_2CN	CH_3OH	NH_2CH_3	CH_2OHCHO	C_8H
CN	HCO	CH_2D^+?	CH_4	CH_3SH	c-C_2H_4O	CH_2CHCHO	CH_3CONH_2
CO	HCO^+	HCCN	HC_3N	HC_3NH^+	CH_2CHOH	CH_2CCHCN	HC_6CN
CO^+	HCS^+	$HCNH^+$	HC_2NC	HC_2CHO		NH_2CH_2CN	CH_3CHCH_2
CP	HOC^+	HNCO	HCOOH	NH_2CHO			
CSi	H_2O	HNCS	H_2CHN	C_5N			
HCl	H_2S	$HOCO^+$	H_2C_2O	HC_4N			
KCl	HNC	H_2CO	H_2NCN	C_5H			
NH	HNO	H_2CN	HNC_3	HC_2CHO			
NO	MgCN	H_2CS	SiH_4	CH_2CNH			
NS	MgNC	H_3O^+	H_2COH^+				
NaCl	N_2H^+	NH_3	C_4H^-				
OH	N_2O	SiC_3					
PN	NaCN	C_4					
SO	OCS	C_3N^-					
SO^+	SO_2	H_2CN^+		CH_3C_5N?	HC_9N	$CH_3OC_2H_5$	$HC_{11}N$
SiN	c-SiC_2			$(CH_3)_2CO$	CH_3C_6H	C_6H_6	$C_{10}H_8^-$
SiO	CO_2			NH_2CH_2COOH?			
SiS	NH_2			CH_3CH_2CHO			
CS	H_3^+						
HF	SiCN						
SH	AlNC						
FeO(?)	SiNC						

Chemical modelling

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{M} + \mathrm{N}$$

$$\frac{d}{dt}n(\mathrm{M}) = kn(\mathrm{A})n(\mathrm{B}) - \beta n(\mathrm{M})$$

$$\frac{d}{dt}n(\mathrm{N}) = kn(\mathrm{A})n(\mathrm{B}) - \beta_1 n(\mathrm{N})$$

$$\frac{d}{dt}n(\mathrm{A}) = k_1 n(\mathrm{X})n(\mathrm{Y}) - \beta_2 n(\mathrm{A})$$

$$\frac{d}{dt}n(\mathrm{B}) = k_2 n(\mathrm{J})n(\mathrm{K}) - \beta_3 n(\mathrm{B})$$

Chemical modelling

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{M} + \mathrm{N}$$

$$\frac{d}{dt} n(\mathrm{M}) = k n(\mathrm{A}) n(\mathrm{B}) - \beta n(\mathrm{M})$$

$$\frac{d}{dt} n(\mathrm{N}) = k n(\mathrm{A}) n(\mathrm{B}) - \beta_1 n(\mathrm{N})$$

$$\frac{d}{dt} n(\mathrm{A}) = k_1 n(\mathrm{X}) n(\mathrm{Y}) - \beta_2 n(\mathrm{A})$$

$$\frac{d}{dt} n(\mathrm{B}) = k_2 n(\mathrm{J}) n(\mathrm{K}) - \beta_3 n(\mathrm{B})$$

Chemical modelling

In addition to neutral-neutral processes, one must consider:

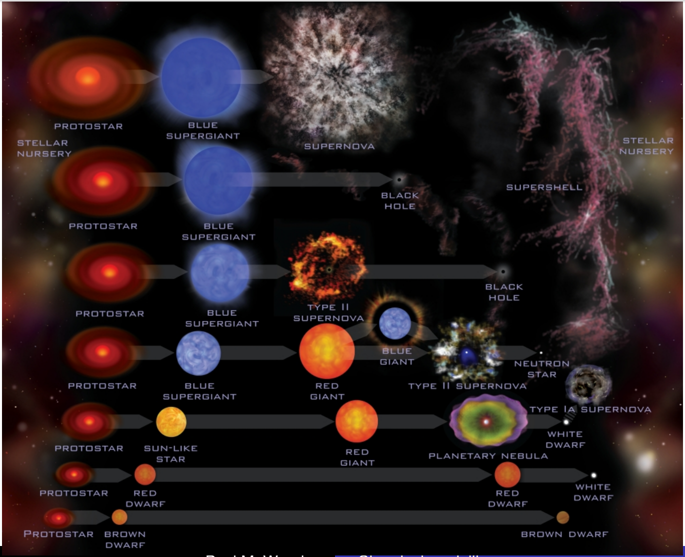
Ion-molecule reactions
Charge transfer reactions
Radiative associations
Radiative recombinations
Dissociative recombinations
Cosmic-ray ionisations
Photoionisation
Photodissociation
X-ray ionisation
Ionisation due to active radionucleides
Grain-surface reactions
etc. etc.

An example

To model the carbon isotope chemistry in a protoplanetary disk, with species up to C_4 in size:

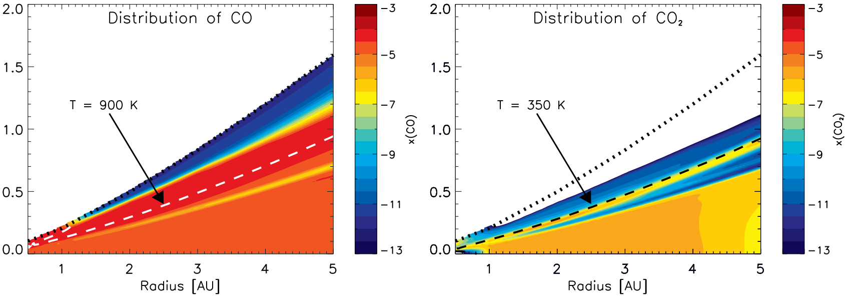
8172 reactions
479 species
6 elements
$\Rightarrow$ around four days runtime on a single processor

The big picture



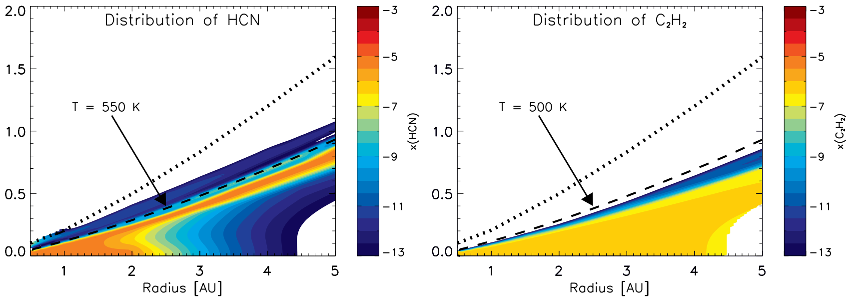
Outline

AA Tau results



Woods & Willacy (2008)
temperature: Carr & Najita (2008)

AA Tau results



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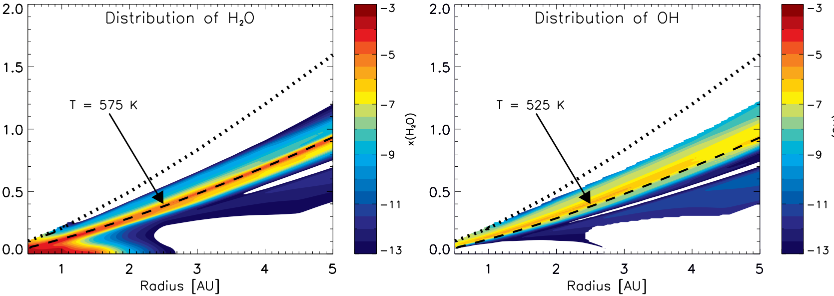
AA Tau results



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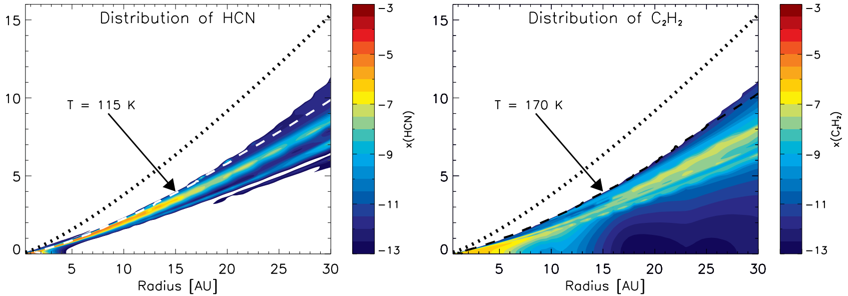
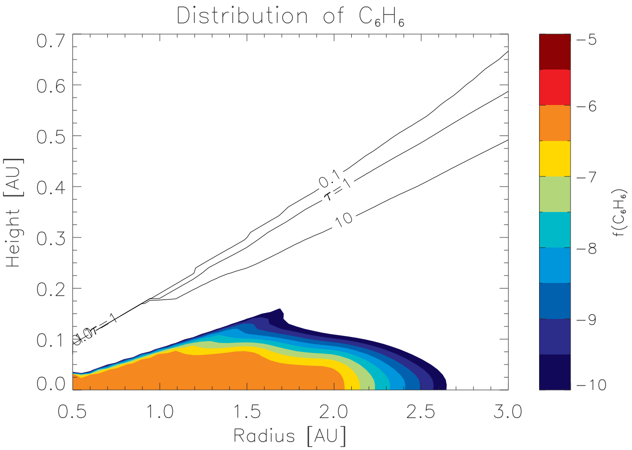
GV Tau results



Woods & Willacy (2008)
temperature: Gibb et al. (2007)

Outline

Benzene in protoplanetary disks



Benzene in protoplanetary disks

$$\begin{aligned}
HCO^{+} + C_2H_2 &\longrightarrow C_2H_3^{+} + CO \\
C_2H_3^{+} + CH_4 &\longrightarrow C_3H_5^{+} + H_2 \\
C_3H_5^{+} + e^{-} &\longrightarrow C_3H_4 + H \\
C_3H_4^{+} + C_3H_4 &\longrightarrow c - C_6H_7^{+} + H \\
c - C_6H_7^{+} + grain &\longrightarrow g - C_6H_6 + H
\end{aligned}$$

Woods & Willacy (2007)

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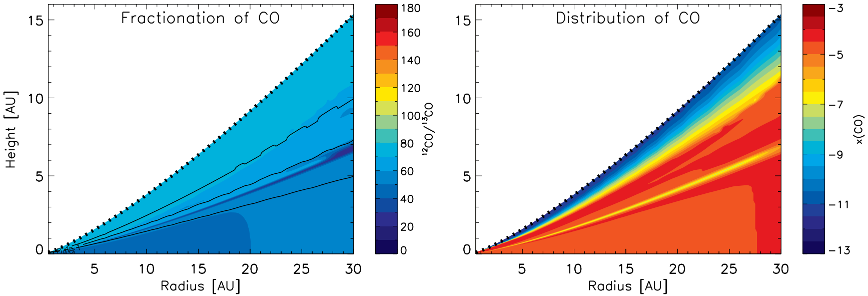
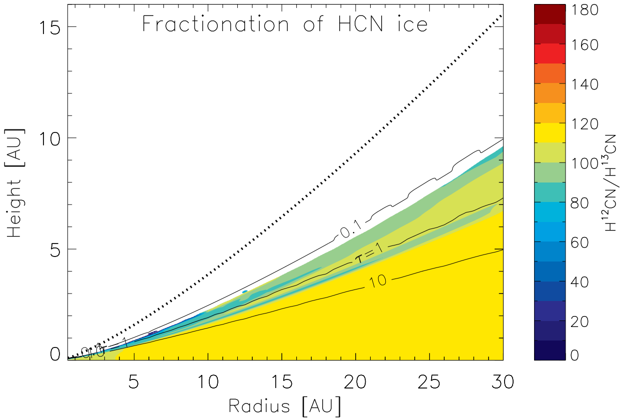
CO and ^{13}CO



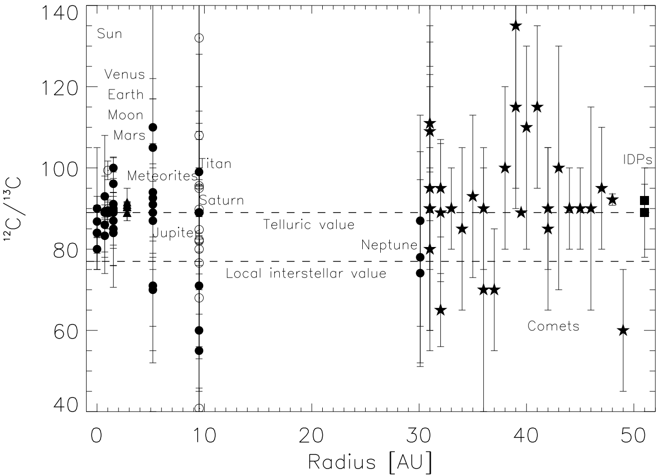
$$^{13}\mathrm{C}^{+} + ^{12}\mathrm{CO} \rightleftharpoons ^{13}\mathrm{CO} + ^{12}\mathrm{C}^{+} + \Delta E$$

HCN and $H^{13}CN$ ice

Woods & Willacy (2008)

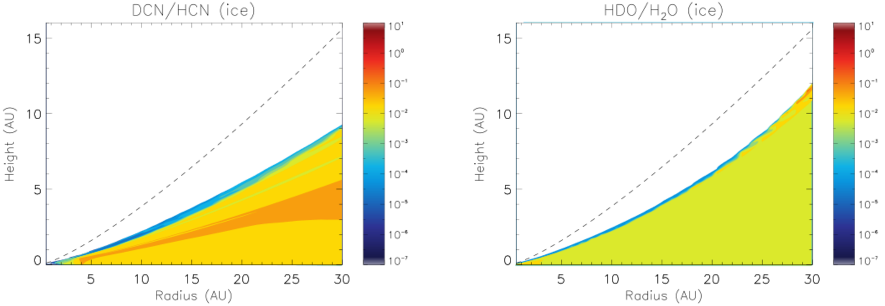


Solar System comparison - ^{13}C



Deuterium isotopes

Fig. 11.— The deuteration of HCN and H_2O ices in Model 2.



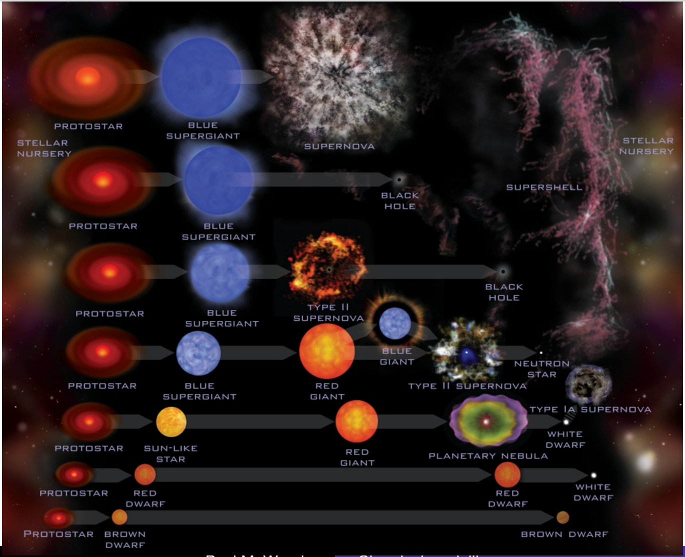
Willacy & Woods (2009)

Oxygen isotopes

Work in progress...

Woods & Willacy (2009?)

The big picture



Outline

IRC+10216

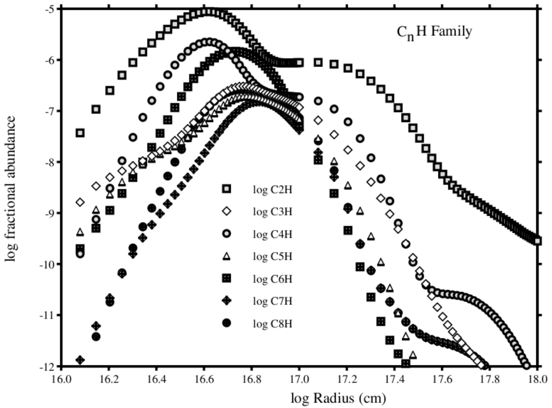
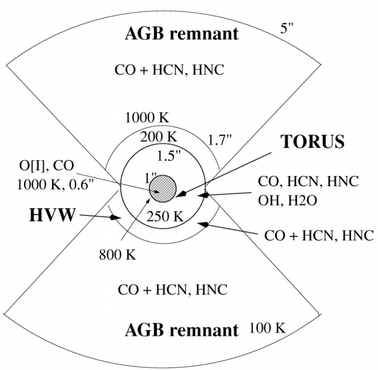


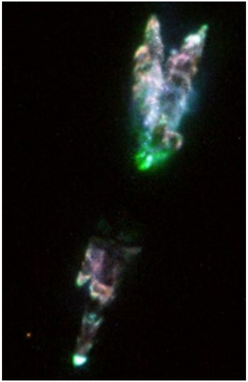
Figure 5. A plot of fractional abundance versus the log of radius (cm) for assorted C_nH radicals.

Millar et al. (2000)

Outline

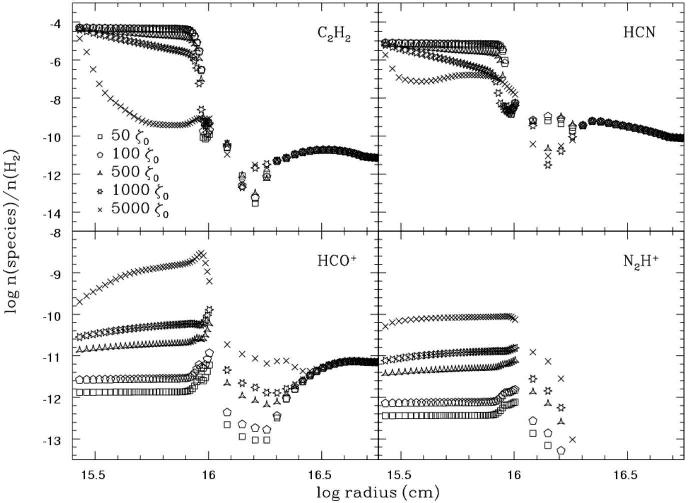
CRL 618





Herpin & Cernicharo (2000); ESA/Tielens

The radiation catastrophe



Woods et al. (2003)

Summary

- The chemistry of simple molecules is complex!
- The chemistry of complex molecules is ~~simple~~ more complex!
- Despite the complexities, chemical models work pretty well whether applied to young stellar environments or old.
- Chemical models allow us to understand what we see with our telescopes, and they allow us to predict what we could see (for instance, with ALMA)

- Future work
  - SAGE-Spec: an infrared survey of the LMC (w/ Ciska et al.)
  - Dust condensation modelling (w/ Andrew & Ciska)
  - Oxygen isotopes in the protosolar nebula (w/ Karen Willacy)
  - etc. etc.

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