The Big, the Small and the Heavy: Chemistry in protoplanetary disks

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Exochemistry & Astromaterials series
2008

Collaborator: Karen Willacy (JPL)

Outline

1. Introduction
   - Disks around T Tauri stars
2. Small molecules
   - Disk observations
   - Recent observations – AA Tau
   - Comparison with the model
   - Recent observations – GV Tau
   - Comparison with the model
3. Large molecules
   - Benzene
4. Heavy molecules

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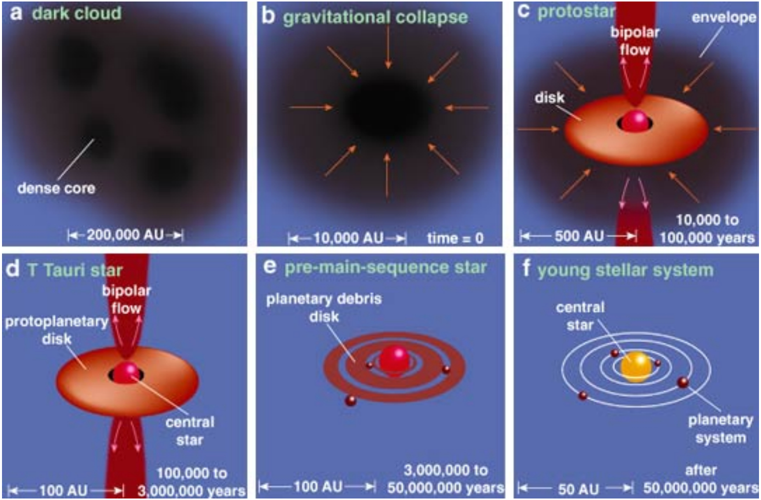
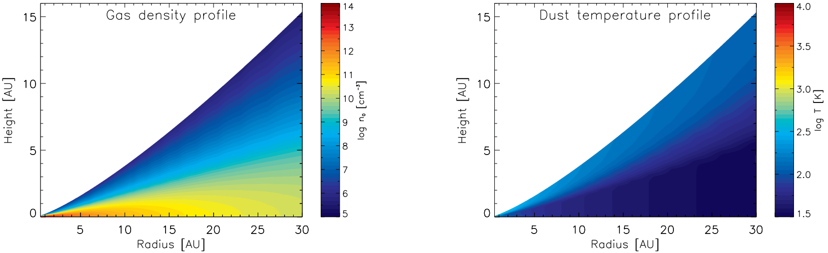
The low-mass star formation scenario



Disk structure

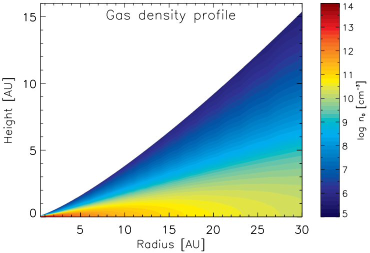
Hydrostatic disk model: D'Alessio et al. (1999, 2001)

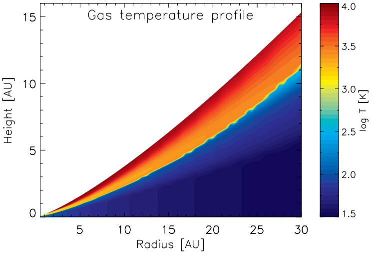


$T_\star$=4 000 K, $M_\star$=0.7 $M_\odot$, $L_\star$=0.9 $L_\odot$,
$R_\star$=2.5 $R_\odot$, $\dot{M}_\star=10^{-8}\,M_\odot\,yr^{-1}$, α=0.01

Disk structure

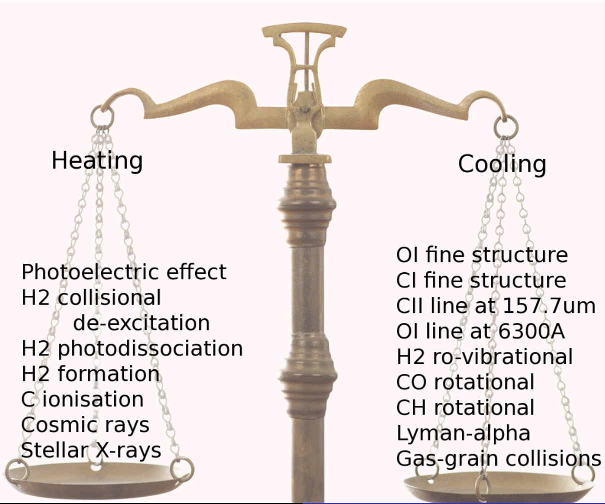
Hydrostatic disk model: D'Alessio et al. (1999, 2001)



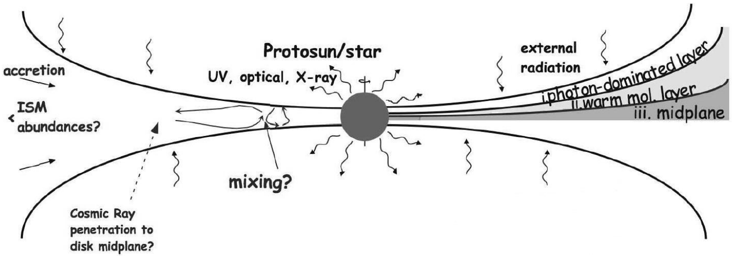


$T_\star$=4 000 K, $M_\star$=0.7 $M_\odot$, $L_\star$=0.9 $L_\odot$,
$R_\star$=2.5 $R_\odot$, $\dot{M}_\star=10^{-8}\,M_\odot\,yr^{-1}$, α=0.01

Heating/cooling balance



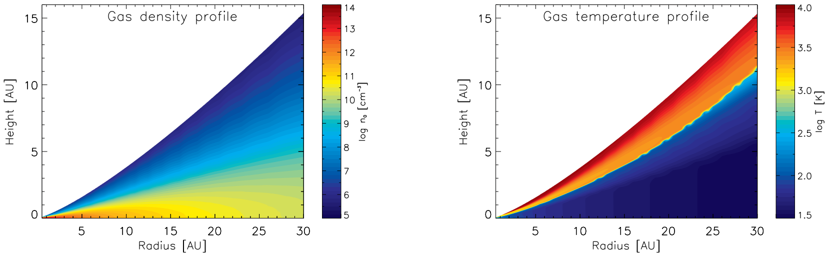
A chemical view of disks



Bergin, PPV

Disk structure

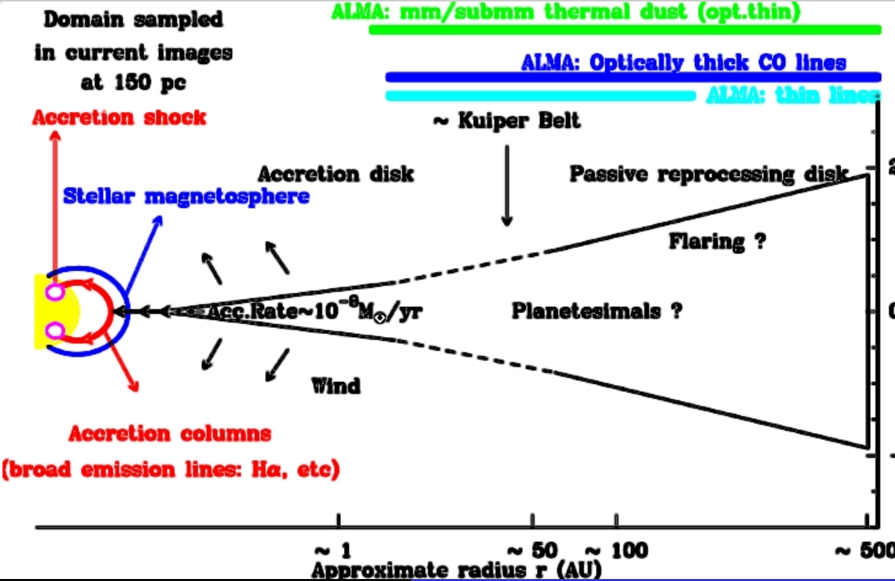
Hydrostatic disk model: D'Alessio et al. (1999, 2001)



Chemical model

A subset of the UMIST Ratefile
(www.udfa.net)
+ grain surface reactions
+ X-ray ionisation reactions
= around 8000 reactions
between 475 species
incorporating 6 elements
Interstellar initial abundances
3 or 4 days to run...

Outline


Domain sampled
in current images
at 150 pc
ALMA: mm/submm thermal dust (opt.thin)
ALMA: Optically thick CO lines
ALMA: thin lines
Accretion shock
~ Kuiper Belt
Accretion disk
Passive reprocessing disk
Stellar magnetosphere
Flaring ?
Acc.Rate~10^-8 M⊙/yr
Planetesimals ?
Wind
Accretion columns
(broad emission lines: Hα, etc)
~ 1
~ 50
~ 100
~ 500
Approximate radius r (AU)

Outer disk observations

CONTINUUM AND CO/HCO$^+$ EMISSION FROM THE DISK AROUND THE T TAURI STAR LkCa 15

CHUNHUA QI,[1,2] JACQUELINE E. KESSLER,[3] DAVID W. KOERNER,[4] ANNEILA I. SARGENT,[5] AND GEOFFREY A. BLAKE[1,3]

Letter to the Editor

Chemistry of Protosolar-like nebulae:

The molecular content of the DM Tau and GG Tau disks

A. Dutrey, S. Guilloteau, and M. Guélin

Institut de Radio Astronomie Millimétrique, 300 Rue de la Piscine, F-38406 Saint Martin d'Hères, France

Received 26 September 1996 / Accepted 1 November 1996

Abstract. We report the detection of CN, HCN, HNC, CS, HCO$^+$, C_2H and H_2CO (ortho and para) in the protoplanetary disks of DM Tau and GG Tau. For the first time organic molecules are observed in objects representative of the protosolar nebula. These molecules are underabundant with respect to the standard dense clouds. The depletions in the "outer" disk of DM Tau (100 < r < 900 AU) derived from the line intensities ≃ 5 (for CO) to 100 (for ... nces of CN and C_2H are ... stry.

... close – circumstellar mat- ... s: stars

L 1551 core, in a region devoid ... evidence of outflowing molecular ... est T Tauri stars in the Taurus reg... its mass $M_* = 0.65 M_\odot$, accordin... An extended disk of molecular ... loteau & Dutrey 94 (GD94). Its r... Continuum and ^{12}CO J=1→0 m... terferometer at angular resolution ... et al. 1996,G96), show a compact ... (80 AU) at the center of the CO di... with the dust disk is $M_d \sim 0.03$ M... cross section $\kappa_d(\nu) = 0.1 \times (\nu/1$... GG Tau is a young binary

Organic molecules in protoplanetary disks around T Tauri and Herbig Ae stars★

W.-F. Thi[1,2,3], G.-J. van Zadelhoff[1,4], and E. F. van Dishoeck[1]

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e-mail: ewine@strw.leidenuniv.nl
[2] Depar...
[3] Sterre...
[4] Konin...

Receive...

Abstrac... disks are... Simple r... star LkC... SO and ... (10^6–10^8... and the u...

W... spec... cont... 57° ... with... fairl... subs... char... ity fi... that

MILLIMETER OBSERVATIONS AND MODELING OF THE AB AURIGAE SYSTEM

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Max-Planck-Institut für Astronomie, Königstuhl 17, D-69117 Heidelberg, Germany; henning@mpia.de, ...

AND

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Received 2004 July 29; accepted 2004 November 23

ABSTRACT

We present the results of millimeter observations and a suitable chemical and radiative tra... Aurigae (HD 31293) circumstellar disk and surrounding envelope. The integral molecular c... studied by observing CO, C^{18}O, CS, HCO$^+$, DCO$^+$, H_2CO, HCN, HNC, and SiO rotationa... 30 m antenna, while the disk is mapped in the HCO$^+$ (1–0) transition with the Plateau d... Using a flared disk model with a vertical temperature gradient and an isothermal spherical ...

REPORTS

X-ray and Molecular Emission from the Nearest Region of Recent Star Formation

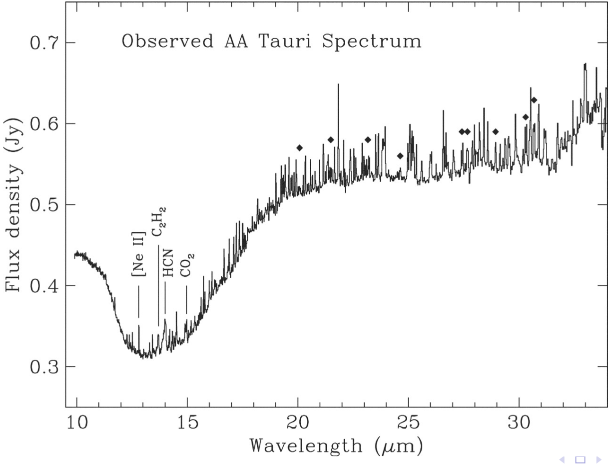
J. H. Kastner,* B. Zuckerman, D. A. Weintraub, T. Forveille

The isolated, young, sunlike star TW Hya and four other young stars in its vicinity are strong x-ray sources. Their similar x-ray and optical properties indicate that the stars make up a physical association that is on the order of 20 million years old and that lies (between about 40 and 60 parsecs (between about 130 and 200 light years) from Earth. TW Hya itself displays circumstellar CO, HCN, CN, and HCO$^+$ emission. These molecules probably orbit the star in a solar-system–sized disk viewed more or less face-on, whereas the star is likely viewed pole-on. Being at least three times closer to Earth than any well-studied region of star formation, the TW Hya Association serves as a test-bed for the study of x-ray emission from young stars and the formation of planetary systems around sunlike stars.

Outline

Inner disk observations

Carr & Najita (2008): HCN, C_2H_2, CO_2, H_2O, OH detected with Spitzer.



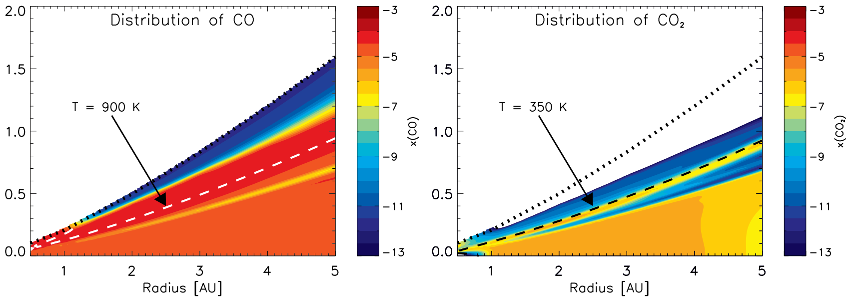
Outline

AA Tau molecules

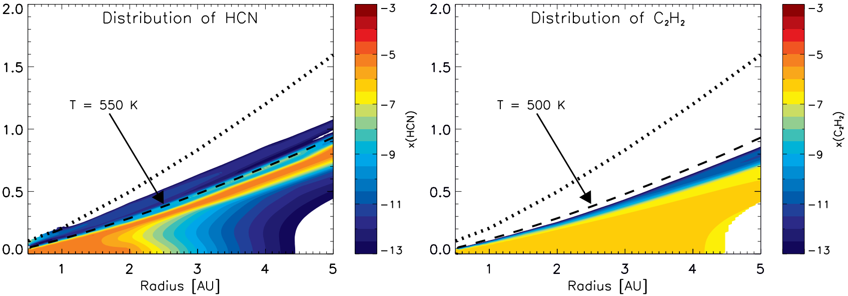
Species	Temperature	Obs'd abundance	Calc'd abundance
CO	900±100 K	1.0	1.0
CO_2	350±100 K	0.004-0.26	0.06
C_2H_2	650±150 K	0.016	0.03
HCN	650±100 K	0.13	0.23
H_2O	575±50 K	1.3	6.2
OH	525±50 K	0.18	6×10^{-5}

Carr & Najita (2008)

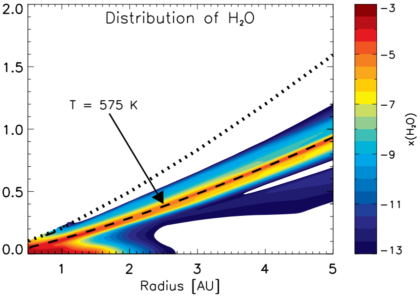
AA Tau results

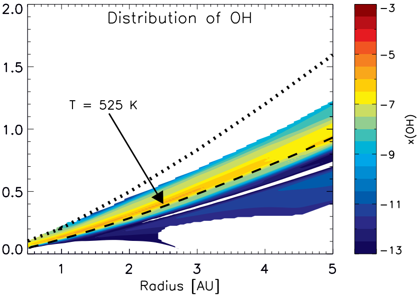


AA Tau results



AA Tau results





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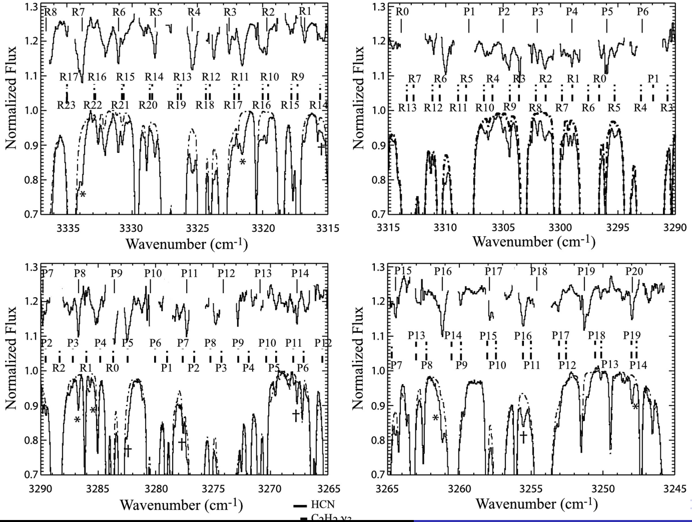
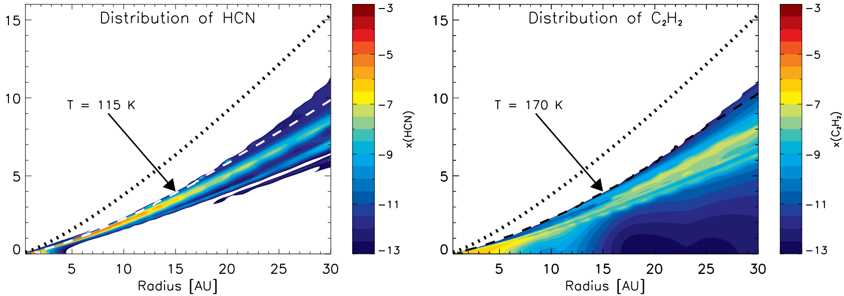
Inner disk observations



Gibb et al. (2007)
GV Tau

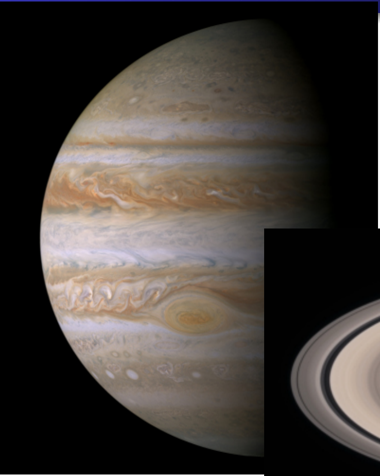
Outline

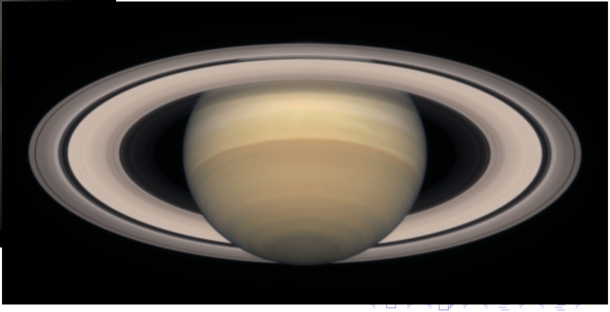
GV Tau results



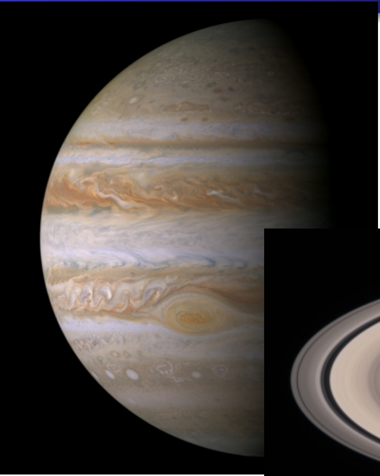
Outline

Benzene in the universe





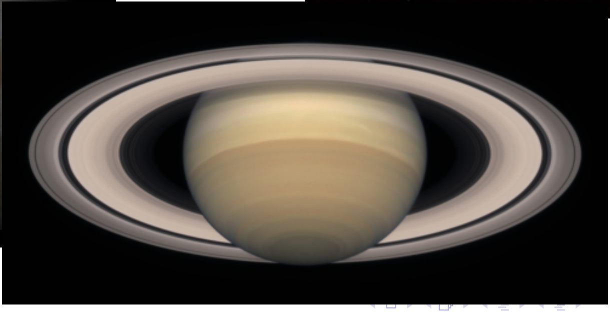
Benzene in the universe



CRL618 ⟶

⟵ Jupiter

Saturn



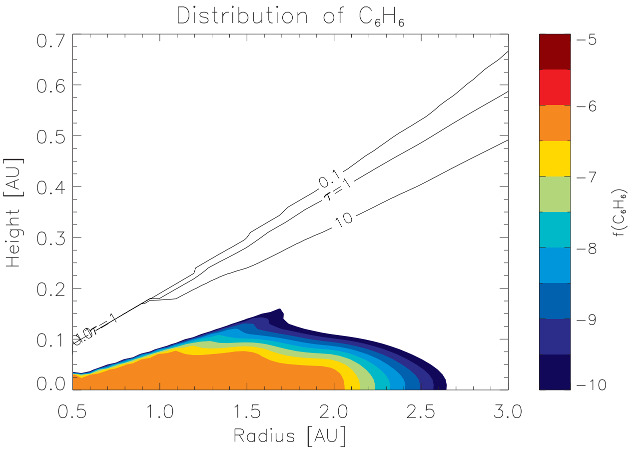
Also the PPN, SMP LMC 11

Benzene in the disks of evolved stars

$$\begin{aligned}
HCO^+ + C_2H_2 &\longrightarrow C_2H_3^+ + CO \\
C_2H_3^+ + C_2H_2 &\longrightarrow C_4H_3^+ + H_2 \\
C_4H_3^+ + C_2H_2 &\longrightarrow c-C_6H_5^+ + h\nu \\
c-C_6H_5^+ + H_2 &\longrightarrow c-C_6H_7^+ + h\nu \\
c-C_6H_7^+ + e^- &\longrightarrow c-C_6H_6 + h\nu
\end{aligned}$$

Woods et al. (2002)

Benzene in protoplanetary disks



Benzene in the disks of evolved stars

$$HCO^+ + C_2H_2 \longrightarrow C_2H_3^+ + CO$$

$$\begin{aligned} C_2H_3^+ + C_2H_2 &\longrightarrow C_4H_3^+ + H_2 \\ C_4H_3^+ + C_2H_2 &\longrightarrow c-C_6H_5^+ + h\nu \\ c-C_6H_5^+ + H_2 &\longrightarrow c-C_6H_7^+ + h\nu \\ c-C_6H_7^+ + e^- &\longrightarrow c-C_6H_6 + h\nu \end{aligned}$$

Woods et al. (2002)

Benzene in the disks of T Tauri stars

$$HCO^+ + C_2H_2 \longrightarrow C_2H_3^+ + CO$$

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

Woods & Willacy (2007)

Benzene in protoplanetary disks

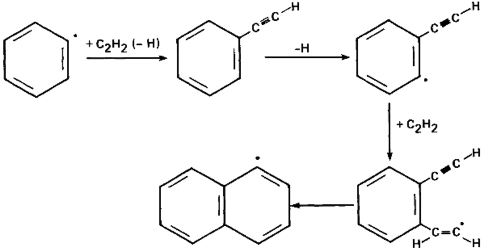
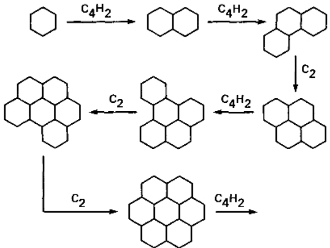
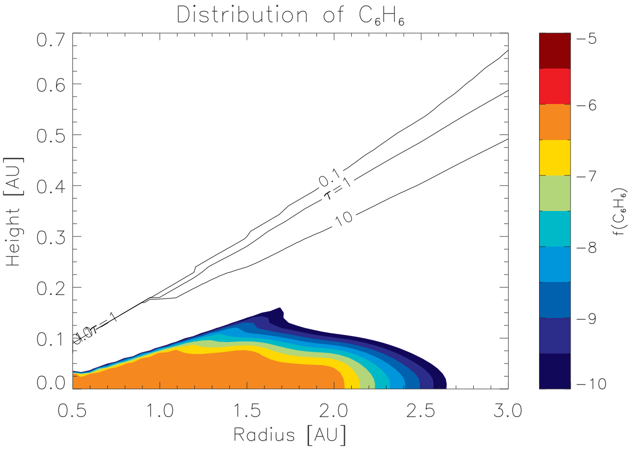


FIG. 23a



Allamandola et al. (1989)

Benzene in protoplanetary disks



PAHs in protoplanetary disks?

PAHs have been observed in T Tauri disks:
e.g., Geers et al. (2006)

PAHs may form in the gas phase in AGB stars:
e.g., Frenklach & Feigelson (1989), Cherchneff et al. (1992)

Regions of high density with long residency times occur in the inner regions of disks. Do the right ingredients (benzene, acetylene) mix at the right temperatures (700–1 100 K)?

Mini-summary

- Our model matches observations of small molecules very well!
- Benzene and similarly complex molecules could also be present in PPDs
- [CII] lines could give us a quick measure of $^{12}C/^{13}C$ ratios in PPDs
- $^{12}C/^{13}C$ ratios in PPDs do not tally with those in the Solar System

What can isotopes of C tell us?

- Trace the origin and evolution of molecules
  - Formation environment
  - Types of chemical processing
- Trace vertical temperature structure of disks (Pietu et al. 2007, Dartois et al. 2003)
- Allow us to trace molecules which may be optically thick (^{12}CO vs. ^{13}CO)
- Label various regions of the disk

Isotope exchange reactions

$$^{13}\mathrm{C}^{+} + ^{12}\mathrm{CO} \rightleftharpoons ^{13}\mathrm{CO} + ^{12}\mathrm{C}^{+} + \Delta E(35\,\mathrm{K})$$

Rate measured by Watson et al. (1976), Smith & Adams (1980)
Rate calculated by Langer et al. (1984), Lohr (1998)

$$\mathrm{H}^{12}\mathrm{CO}^{+} + ^{13}\mathrm{CO} \rightleftharpoons \mathrm{H}^{13}\mathrm{CO}^{+} + ^{12}\mathrm{CO} + \Delta E(9\,\mathrm{K})$$

Rate measured by Smith & Adams (1980)
Rate calculated by Langer et al. (1984), Lohr (1998)

Isotope exchange reactions

$$^{13}\mathrm{C}^+ + ^{12}\mathrm{CO} \rightleftharpoons ^{13}\mathrm{CO} + ^{12}\mathrm{C}^+ + \Delta E(35\,\mathrm{K})$$

$$k_{\mathrm{for}} = 3.3 \times 10^{-10}(T/300\,\mathrm{K})^{-0.448}$$
$$k_{\mathrm{rev}} = k_{\mathrm{for}} \exp(-35\,\mathrm{K}/T)$$

Woods & Willacy (2008, in review)

$$\mathrm{H}^{12}\mathrm{CO}^+ + ^{13}\mathrm{CO} \rightleftharpoons \mathrm{H}^{13}\mathrm{CO}^+ + ^{12}\mathrm{CO} + \Delta E(9\,\mathrm{K})$$

$$k_{\mathrm{for}} = 2.6 \times 10^{-10}(T/300\,\mathrm{K})^{-0.277}$$
$$k_{\mathrm{rev}} = k_{\mathrm{for}} \exp(-9\,\mathrm{K}/T)$$

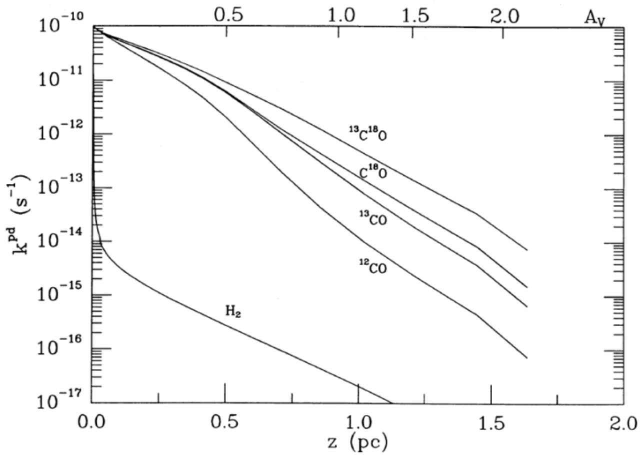
Woods & Willacy (2008, in review)

Isotope exchange reactions

$$
\begin{aligned}
HO^{13}C^{+} + {}^{12}CO &\rightleftharpoons {}^{13}CO + HO^{12}C^{+} + \Delta E(2.5\,K) \\
{}^{13}C^{+} + {}^{12}CN &\rightleftharpoons {}^{13}CN + {}^{12}C^{+} + \Delta E(34\,K) \\
{}^{13}C^{+} + {}^{12}CS &\rightleftharpoons {}^{13}CS + {}^{12}C^{+} + \Delta E \\
{}^{13}C^{+} + {}^{12}CH_3 &\rightleftharpoons {}^{13}CH_3 + {}^{12}C^{+} + \Delta E
\end{aligned}
$$

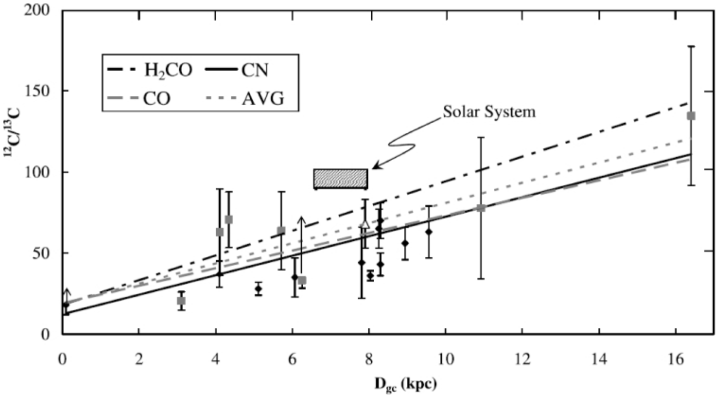
$\Longrightarrow$ Rates unknown?

Selective photodissociation



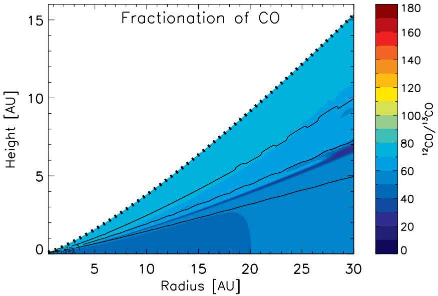
van Dishoeck & Black (1988)

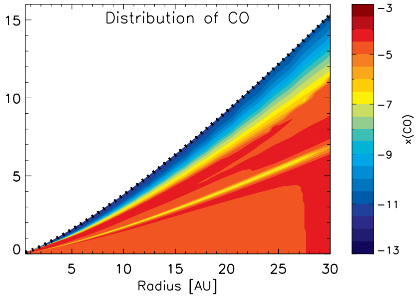
Galactic $^{12}C/^{13}C$ ratio



Milam et al. (2005)

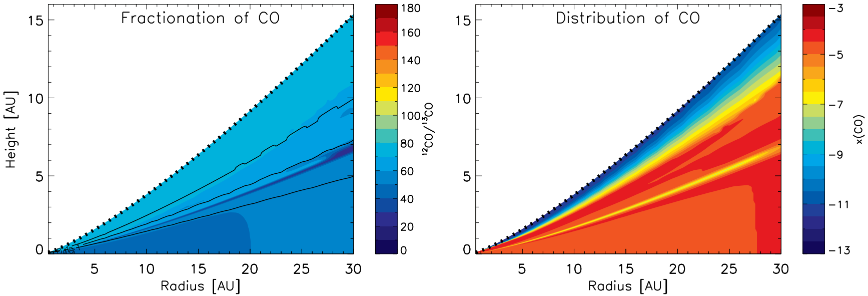
Results - CO





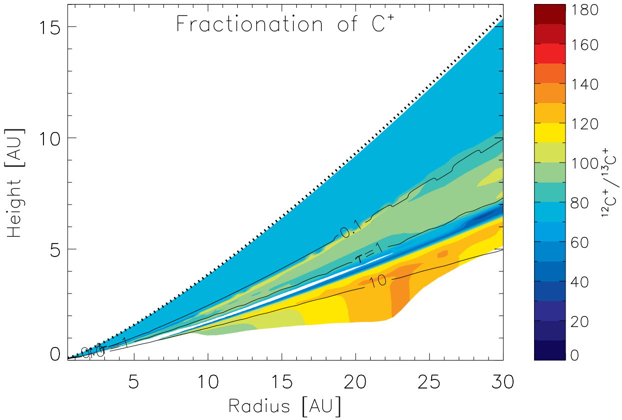
$$^{13}\mathrm{C}^+ + ^{12}\mathrm{CO} \rightleftharpoons ^{13}\mathrm{CO} + ^{12}\mathrm{C}^+ + \Delta E$$

Results - CO

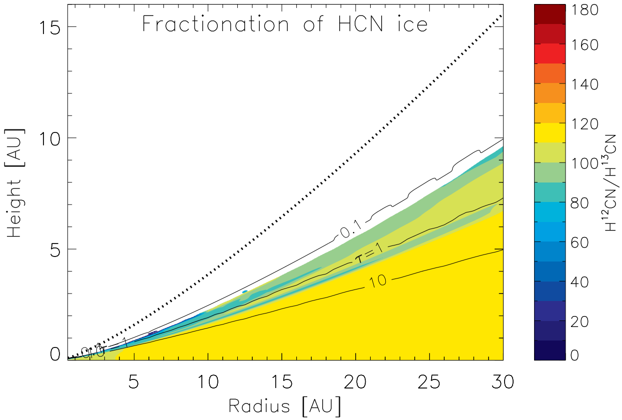


Gibb et al. (2007), GV Tau: $T(^{12}CO) \approx 240\,K$ $^{12}CO/^{13}CO = 54 \pm 15$
Brittain et al. (2005), HL Tau: $T(^{12}CO) \approx 100\,K$ $^{12}CO/^{13}CO = 76 \pm 9$

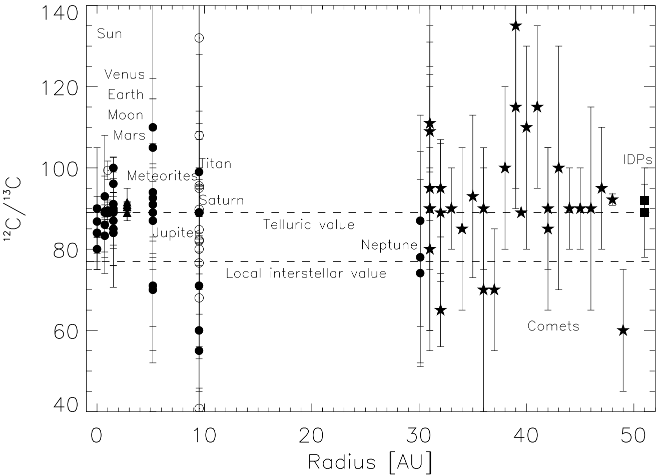
Results - C^+


Fractionation of C+
Height [AU]
Radius [AU]
15
10
5
0
5
10
15
20
25
30
0.1
τ=1
10
180
160
140
120
100
80
60
40
20
0
12C+/13C+

Results - HCN ice



Solar System comparison



Summary

- Our model matches observations of small molecules very well!
- Benzene and similarly complex molecules could also be present in PPDs
- [CII] lines could give us a quick measure of $^{12}C/^{13}C$ ratios in PPDs
- $^{12}C/^{13}C$ ratios in PPDs do not tally with those in the Solar System
- Future work
  - PAHs forming *in situ* in disks?
  - Oxygen isotopes in the protosolar nebula