AST393F **Spring 2007**
Jaffe **February 14, 2007**

Class 11 Notes

Return first to equation 4.24

$$\frac{dn(i)}{dt} = -n(i)\sum_{j} n(j)k_{ij} + \sum_{j,k} n(j)n(k)k_{jk} + \sum_{j} n(j)k_{j} - n(i)\sum_{j} k_{j}$$

Last time, we talked about a steady-state solution where we set $\frac{dn(i)}{dt} = 0 \quad \forall\, i$.

This can be solved, iteratively using a convergence technique like Newton-Raphson, keeping in mind that we conserve each element and we conserve charge in steady-state.

The simplest time-dependent case looks at something like the atomic to molecular transition in a static cloud-constant T, n CR rate (i.e., ignore changes in cooling)

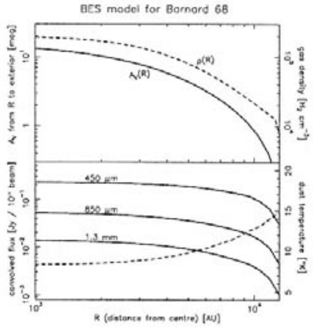
Question: Why is this at all relevant?
Timescales for chemical evolution are long dynamically – before considering the coupled effects, it is good to get a handle on what the chemistry above will do.

Question: How might you go about it?
You know initial conditions- assume pure atomic gas. Calculate $\frac{dn(i)}{dt}$ and move in small time steps.

One of the single biggest problems with this approach – both the steady-state and the time-dependent is that it leaves out dust chemistry.

- Dust can act as a sink by depleting molecules out of the gas phase
- Dust can produce critical molecules – notably H_2 but also others.
- Dust can act as a source – icy matter can sublimate if icy grains appear in warm regions

Figure 1 from Walmsey et. al 2002 shows a model based on observations of the core Barnard 68.



Walmsley et al. (2002)
ESO Astrophysics Symposia

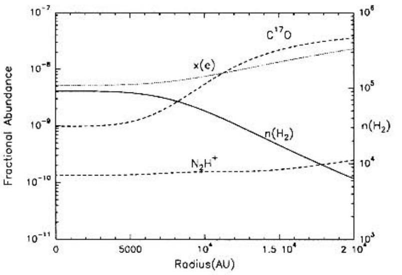
Model for the dust temperature distribution in the core B68 based on the results of Zucconi et al. (2001). In the top panel, we show the density distribution and distribution of visual extinction (from the center of the core) for the model used by Alves et al. (2001) to fit their NIR extinction data. In the bottom panel, we show the corresponding dust temperature distribution (dashed) computed using the mean interstellar radiation field proposed by Black (1994) and optical constants from Ossenkopf and Henning (1994). We also show the intensities as a function of offset which one would expect on the basis of this model at some typical millimeter and sub–millimeter frequencies

Question: Why does it look the way it does?

Question: Why is the submillimeter flux distribution flatter than ρ if it "traces" the dust?

Note density & A_v drop, temperature rises, different profiles at different wavelengths.

Figure 2 is a chemical model for the same core.



Walmsley et al. (2002)
ESO Astrophysics Symposia

Results from a model of the ionization and depletion in the nearby pre-protostellar core L1498. We show as a function of radius the density $n(H_2)$ and the fractional abundance of electrons $x(e)$, of N_2H^+ and of $C^{17}O$. The fall-off of the $C^{17}O$ abundance at small radii reflects the depletion of CO onto dust grains (in this model the $C^{17}O$ abundance is proportional to that of CO). The N_2H^+ abundance in contrast remains relatively constant with radius due partially to the fact that molecular nitrogen is less depleted than CO

Question: Why look at $C^{17}O$ rather than $^{12}C^{16}O$?
A1: optically thin A2: no self-shielding

Note $C^{17}O$ abundance is down by 30X at center.

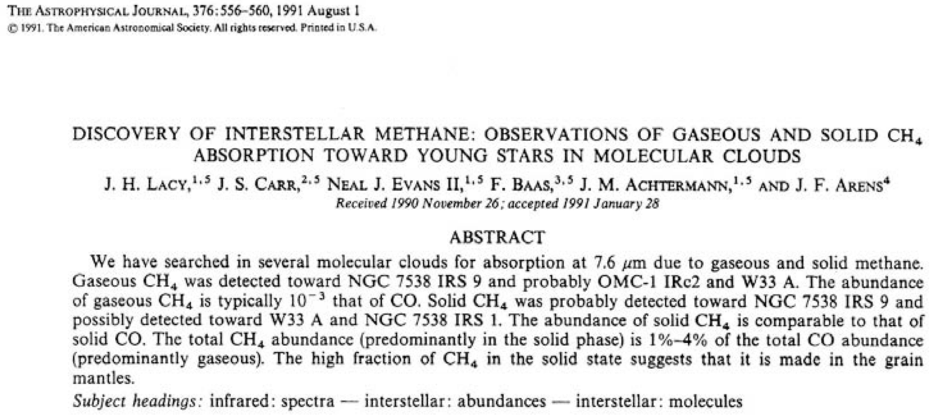
Question: Where did it go?

Note also that N_2H^+ - it is not depleted which is why if it is here

Question: What would a trace species like N_2H^+ with its uncertain abundance be good for?
Answer: As a dynamical tracer.

Question: What is the observational evidence for depletion?

1) Existence of solid features of some molecules (Figure 3 - Lacy, et. al)



THE ASTROPHYSICAL JOURNAL, 376:556–560, 1991 August 1

DISCOVERY OF INTERSTELLAR METHANE: OBSERVATIONS OF GASEOUS AND SOLID CH_4 ABSORPTION TOWARD YOUNG STARS IN MOLECULAR CLOUDS

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Received 1990 November 26; accepted 1991 January 28

ABSTRACT

We have searched in several molecular clouds for absorption at 7.6 μm due to gaseous and solid methane. Gaseous CH_4 was detected toward NGC 7538 IRS 9 and probably OMC-1 IRc2 and W33 A. The abundance of gaseous CH_4 is typically 10^{-3} that of CO. Solid CH_4 was probably detected toward NGC 7538 IRS 9 and possibly detected toward W33 A and NGC 7538 IRS 1. The abundance of solid CH_4 is comparable to that of solid CO. The total CH_4 abundance (predominantly in the solid phase) is 1%–4% of the total CO abundance (predominantly gaseous). The high fraction of CH_4 in the solid state suggests that it is made in the grain mantles.

Subject headings: infrared: spectra — interstellar: abundances — interstellar: molecules

Question: How do you tell a solid feature from a gas feature? - Depth + λ

2) Spatial correlations. Dust peaks in dark clouds can occur where there is no peak in a CO isotopomer.

Question: What is an isotopomer?

Now to the grains.
-First you have to get molecules onto the grains.

$$k_{ac} = \underbrace{n_d \sigma_d v}_{\text{Probability of hitting a grain}} \underbrace{S(T, T_d)}_{\text{“sticking” coefficient}} \simeq 10^{-17} \left(\frac{T}{10K} \right)^{\frac{1}{2}} n\ s^{-1}$$

Analogy for S

The $T^{1/2}$ just comes from the gas particle velocity.

Tielens' book gives a polynomial expansion for S
S = 0.8 at 10K 0.5 at 100K for H on bare grains.

What are depletion timescales?

$$\tau_{d\rho p\ell} = 4 \times 10^9 / n \qquad \text{yrs.} \Rightarrow$$

less than the dynamical timescales, so depletion effects are important
viz. the B68 model.

Binding energies small for physisorbed atoms

-van der Waals interaction, large for chemisorbed (sharing electrons).

H_2 or surface lowers binding energy for other H_2's until equilibrium is reached.

Reactions: Langmuir-Hinshelwood – surface-surface *
Eley- Riedel - hit something on the surface.

Evaporation: Partial pressures not really relevant because its not in equilibrium.

$$\tau_{eV} = \nu_0^{-1} \exp\left(\frac{E_b}{kT_d} \right)$$

$$\nu_0 = \frac{kT}{h} f_z^{-1}$$ f_z Depends on characteristics of substrate an on E_b

$$\tau_{eV} \simeq 3\times10^2 \ \frac{\mathrm{n}}{10^4\,\mathrm{cm}^{-3}}\ \mathrm{S} \ \text{ for H}$$

i.e. on and off all the time. Reactions depend on surface migration.

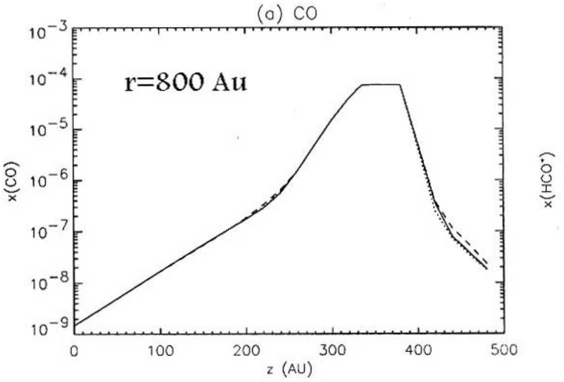
H, or C, O – Sticks and bops about. Scans whole surface in a time comparable to next hit.

Tendency to saturate radicals in these interactions many in gas-phase more in equilibrium at high density – dust reduces.

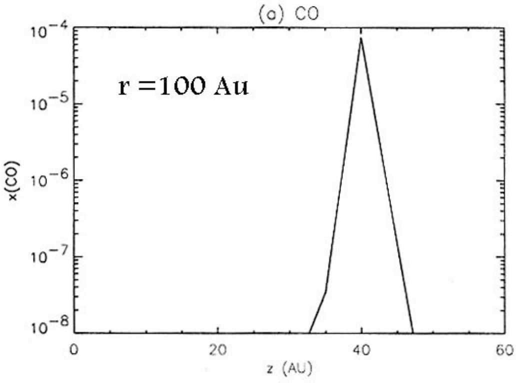
Models
Bergin & Langer – gas-phase chemistry plus depletion into grains during collapse.

Willacy & Langer –
Protoplanetary disks
- Freezeout in mid-plane
- Destruction in top layer
- "photoabsorption" in middle layer

Look at Figures 4 and 5 vertical distributions.



Willacy & Langer (2000)



Doty et al. high temperature version of Bergin & Langer – Look at Figure 4