Models of individual sources

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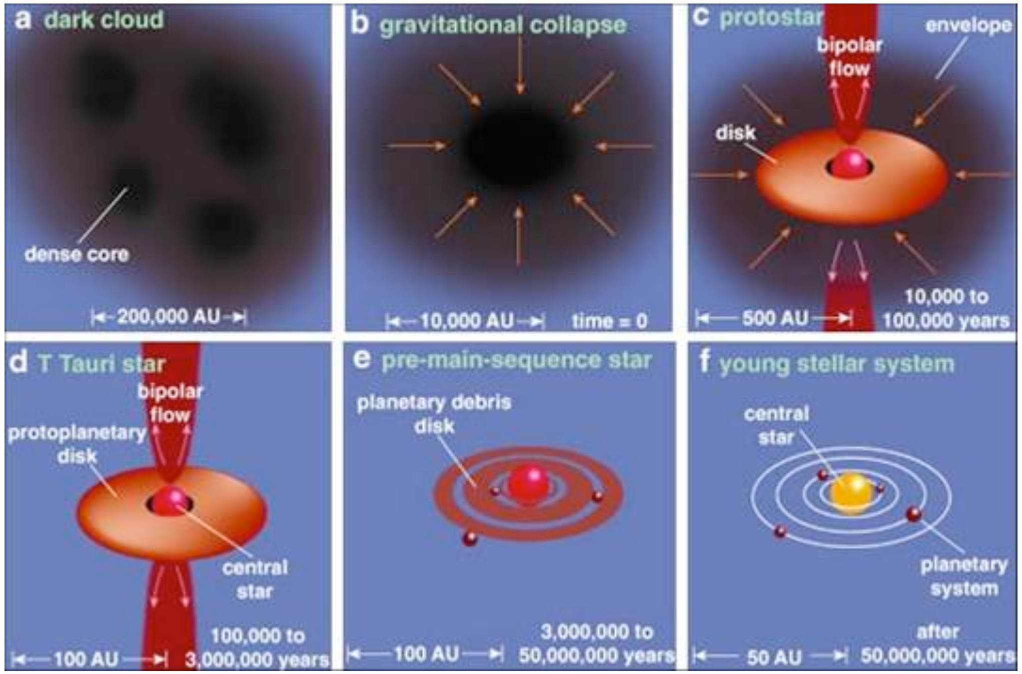


The UMIST Database for Astrochemistry 2006

UMIST udfa 06

The UMIST Database for Astrochemistry

Woodall, Agúndez, Markwick-Kemper, Millar

Astronomy & Astrophysics, 466, 1197-1204 (2007)

www.udfa.net

Summary

23 new species

577 new reactions

450 rate coefficients updated since RATE99

Experimental data on just over one-third of reactions

Temperature range given for applicability of rate coefficient

(some have different behaviours in different temperature ranges)

Historical data provided (and often links to original papers) for previous versions of the UMIST Database

RATE06-Dipole – also provided

If the reaction does not have a rate coefficient measured at low temperature and if the neutral molecule has a dipole moment > 0.9 Debye, the rate coefficients for ion-neutral reactions are taken to be proportional to $T^{-1/2}$

Updates

Ion-neutral reactions: 2950 binary reactions – 1160 measured – Anicich (2004)

Neutral-neutral reactions: 549 binary reactions – increase of about 100 - 275 measured
NIST, IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry, Smith, Herbst & Chang (2004)

Dissociative recombination: 500 product channels – 100 measured – Geppert et al.

Radiative association: 91 reactions – CH_3^+ + H_2O --> $CH_3OH_2^+$ - Luca et al. (2002)

Photoprocesses: 216 product channels

Cosmic ray photon reactions: 156 reactions – probabilities decreased by a factor of two (S Doty)

Fluorine chemistry – detection of interstellar HF and CF^+

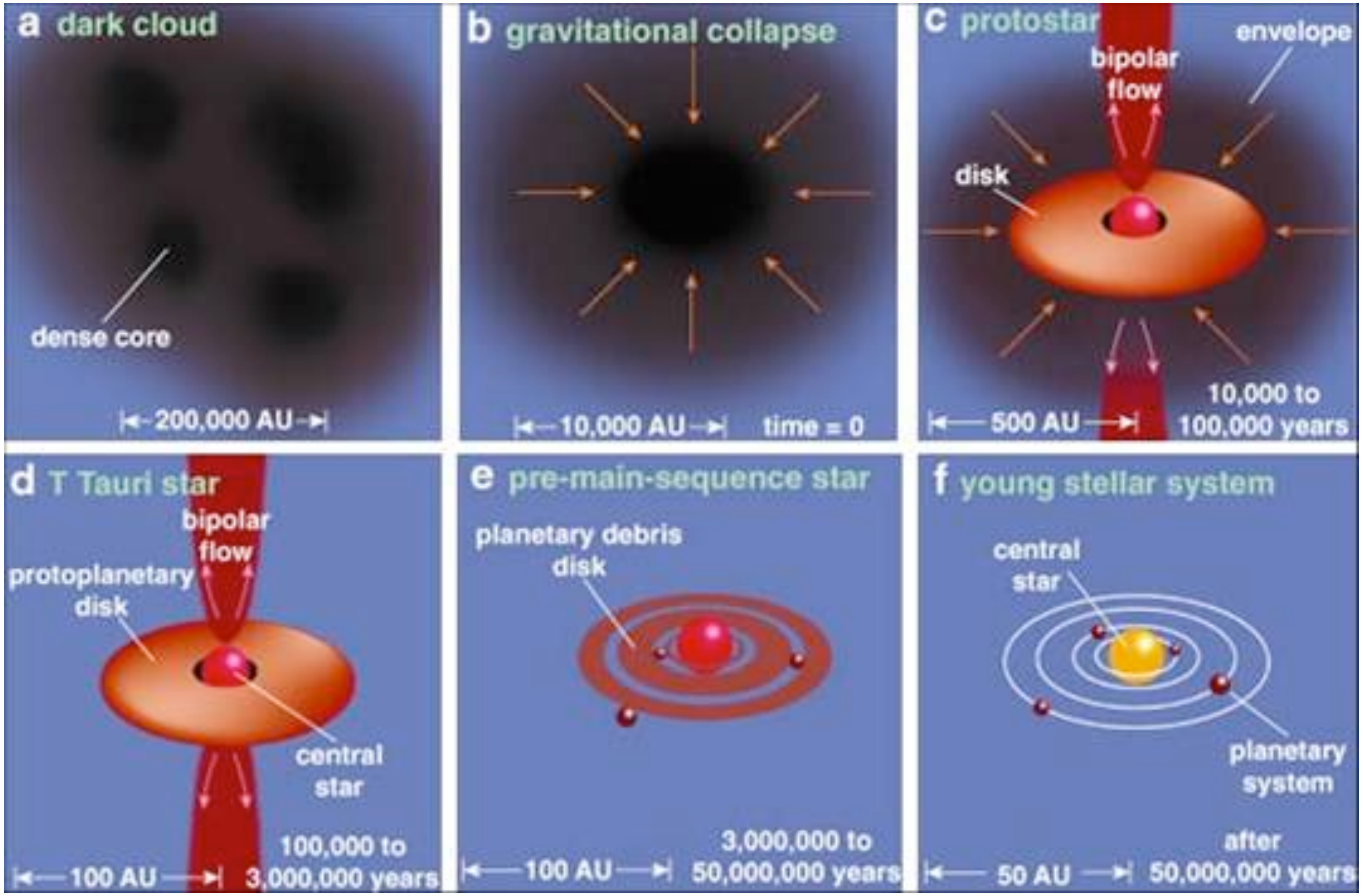
Modelling molecular anion chemistry

- Three different environments:
  - CSE – IRC+10216
  - PDR – Horsehead Nebula
  - Dense molecular cloud – TMC-1

- New chemical reactions and rates added to current successful models
  - Formation: Radiative electron attachment
    - $C_6H + e^- \rightarrow C_6H^- + \text{photon}$
  - Destruction: Photodetachment
    - $C_6H^- + \text{photon} \rightarrow C_6H + e^-$

    Reaction with most abundant species
    - $C_6H^- + H \rightarrow C_6H_2 + e^-$
    - $C_6H^- + C \rightarrow C_7H + e^-$
    - $C_6H^- + C^+ \rightarrow C_6H + C$
    - $C_6H^- + C_2H_2^+ \rightarrow C_6H + C_2H_2$ (IRC+10216)

Low mass star formation



Greene (2001)

TMC-1

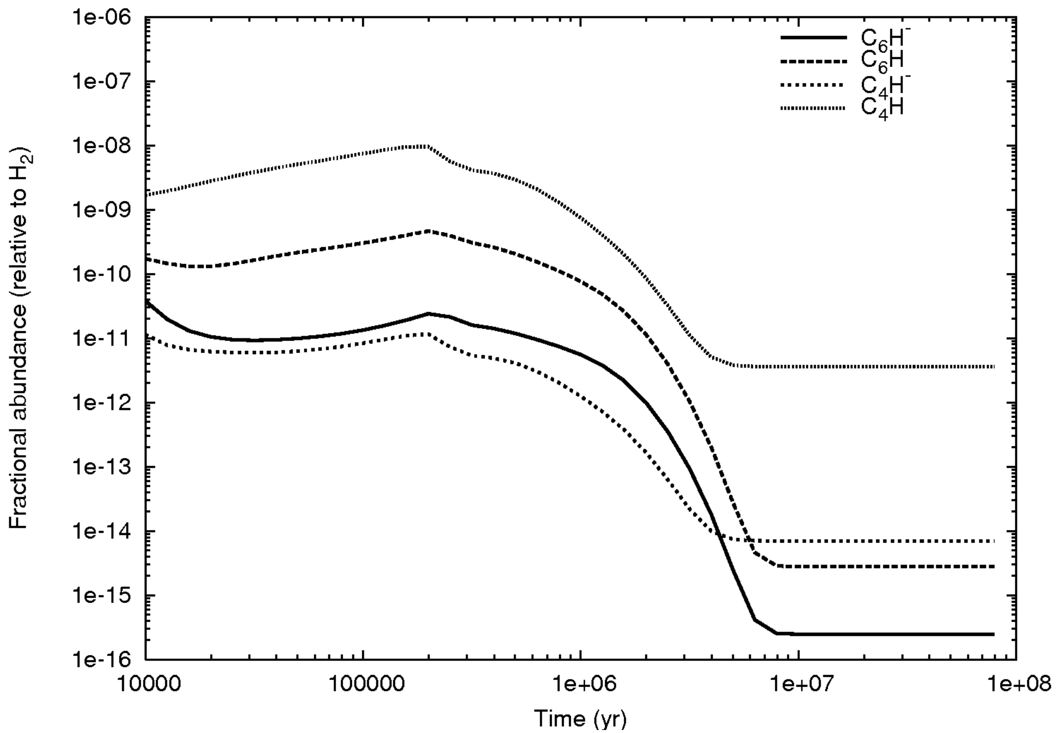
- Giant, 20 solar-mass, quiescent molecular cloud about 140 pc away
- Cold (10K), dense (10^5 cm^{-3})
- Relatively young ~ 10^5 years
- >60 molecules detected; Carbon chains, cyanopolyynes, carbon rings, deuterated molecules, largest identified interstellar molecule $HC_{11}N$, positive ions
- Anions! C_6H^-, C_8H^-

TMC-1- Results

- Pseudo-time-dependent gas-phase models
- Chemical evolution under fixed physical conditions
- Wakelam, Herbst, Selsis (2006) compared with model output with abundances of 52 molecules at TMC-1 CP – 60% agreement to within factor of 3
- However, if CP is C-rich ($C/O > 1$), 76% agree to within 3, 86% to within 5 at 10^5 yr
- L134N – 80% to within 3, 87% within 5 ($C/O < 1$)

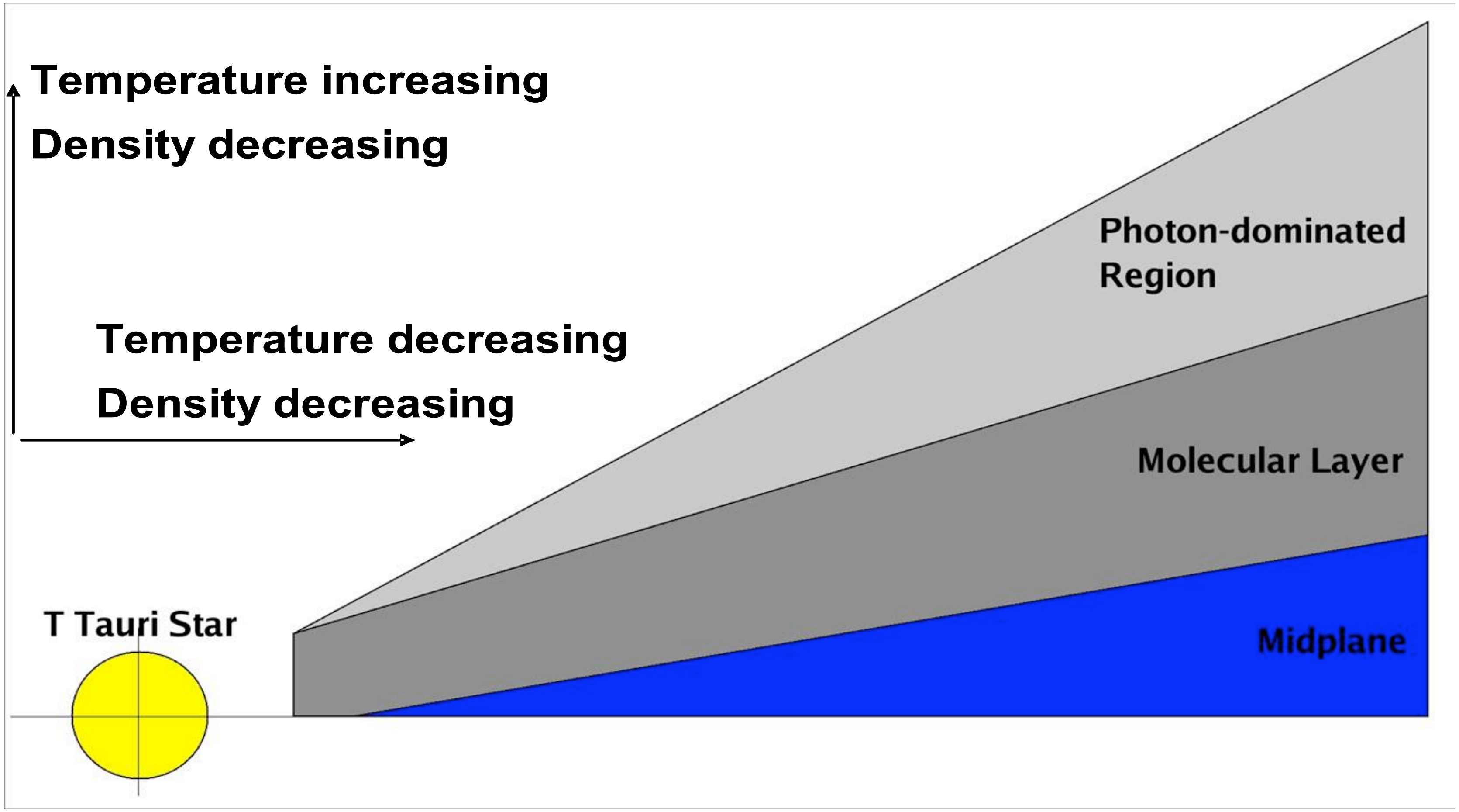
TMC-1 results

- Model:
  - $N(C_6H^-) = 1.4 \times 10^{11}$ cm^{-2}
  - $N(C_6H) = 2.6 \times 10^{12}$ cm^{-2}
  - Ratio = 0.05
- Observation:
  - $N(C_6H^-) = 1.0 \times 10^{11}$ cm^{-2}
  - $N(C_6H) = 4.1 \times 10^{12}$ cm^{-2}
  - Ratio = 0.03
- Prediction:
  - $N(C_4H^-) = 5.6 \times 10^{10}$ cm^{-2}
  - $N(C_8H^-) = 3.7 \times 10^{10}$ cm^{-2}
  - C8H-/C8H = 0.04

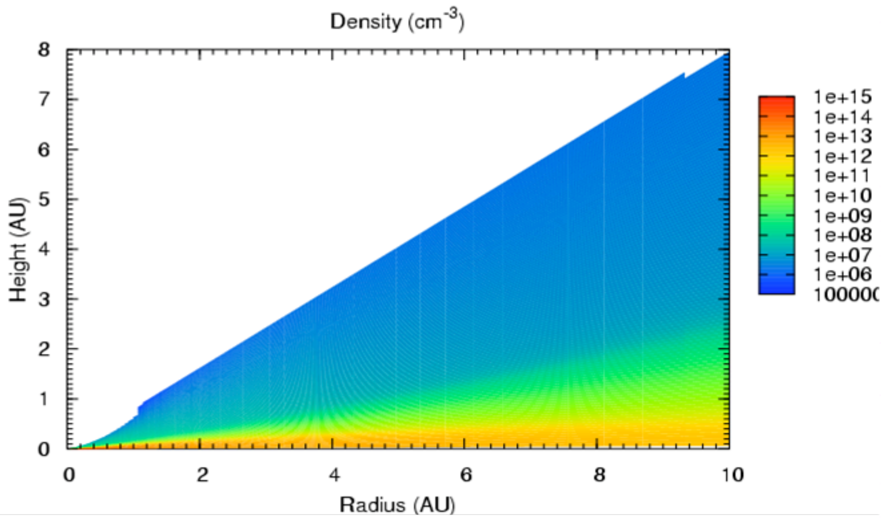


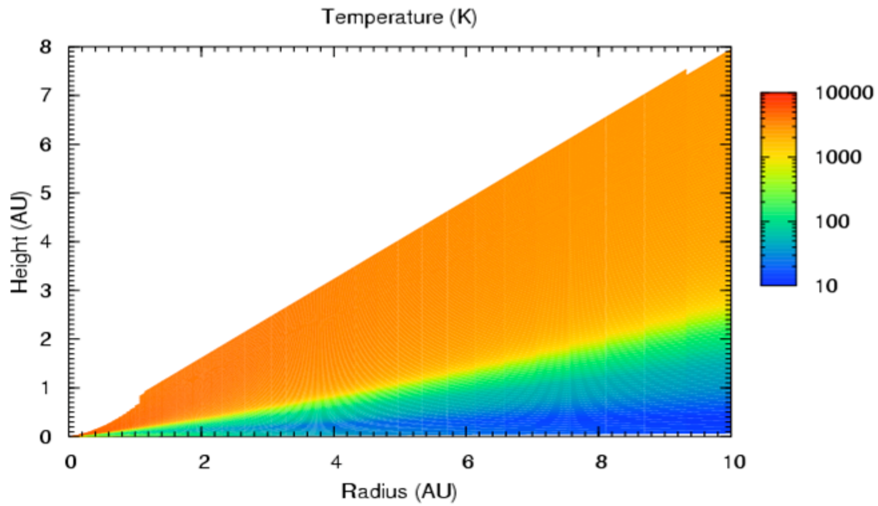
Millar et al. ApJ, 662, L87 (2007)

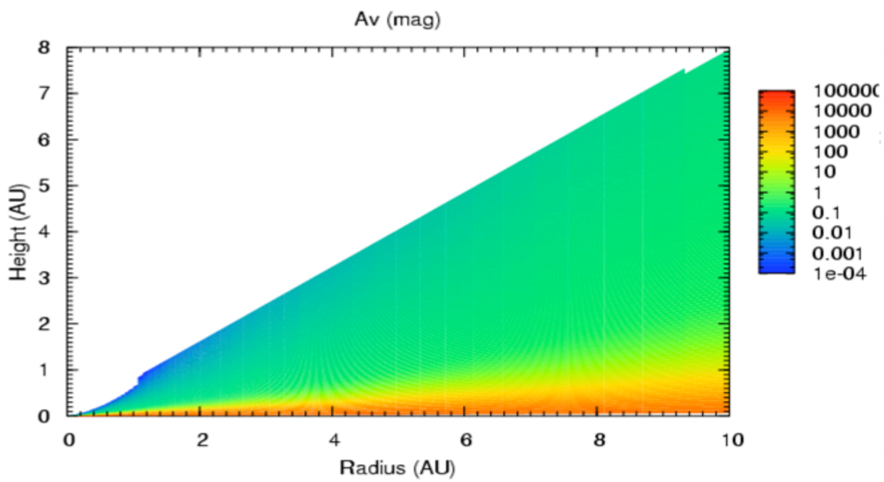
PPD Schematic

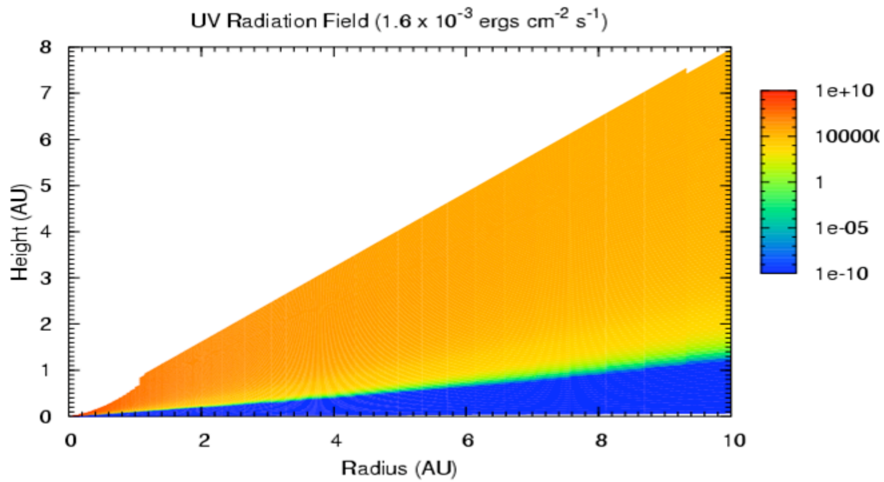


PPD Structure

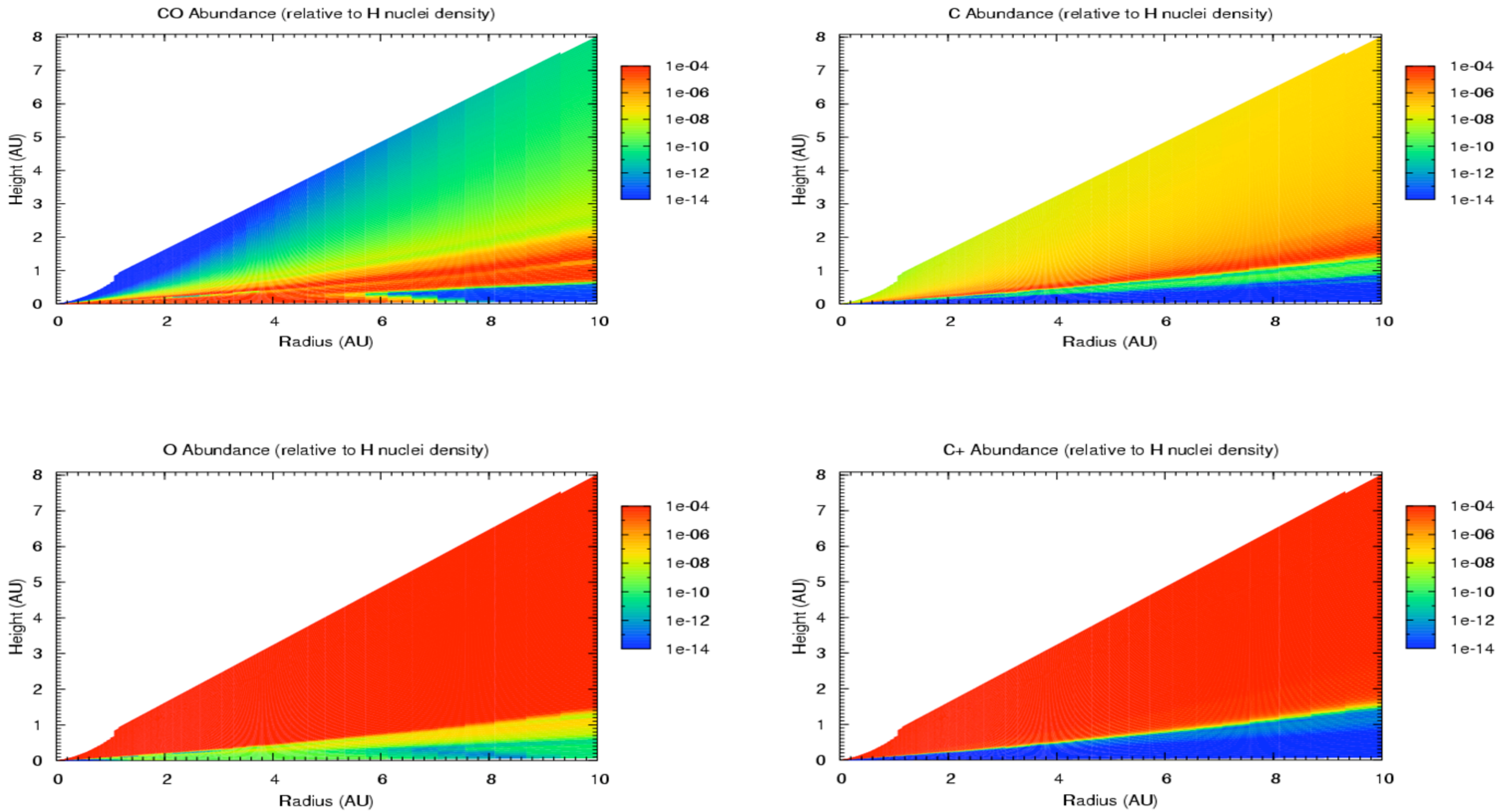






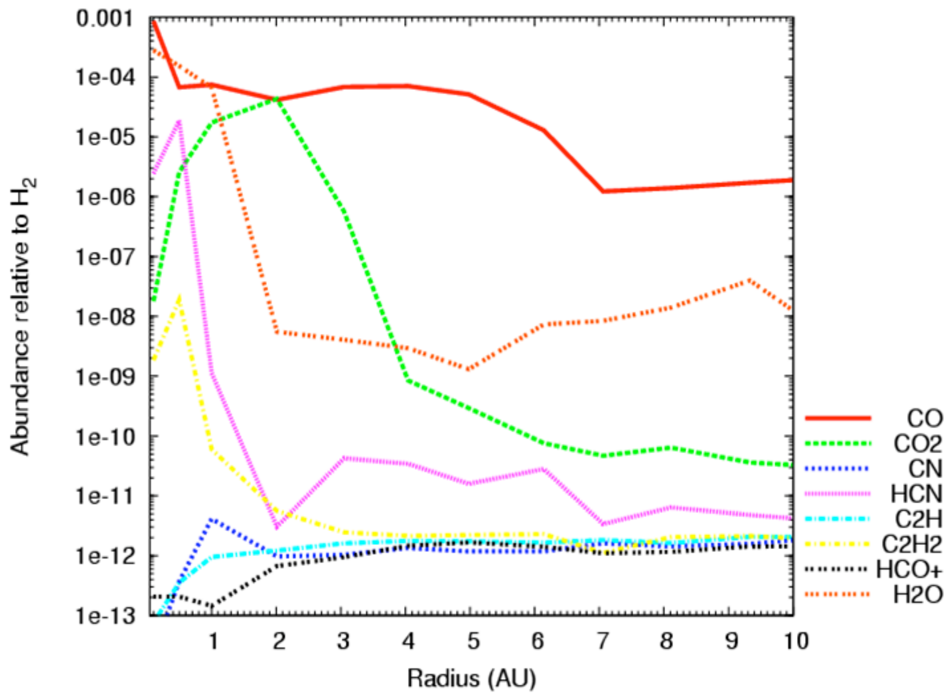


Molecular distributions

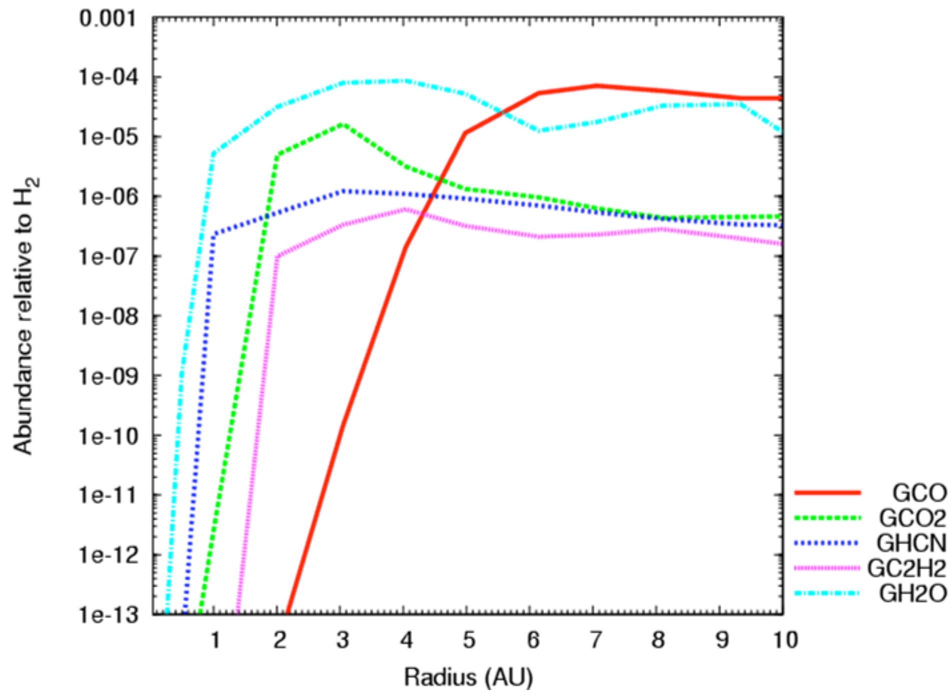


Walsh, Nomura & Millar, in preparation

Column Densities rel. to H2



Gas Phase

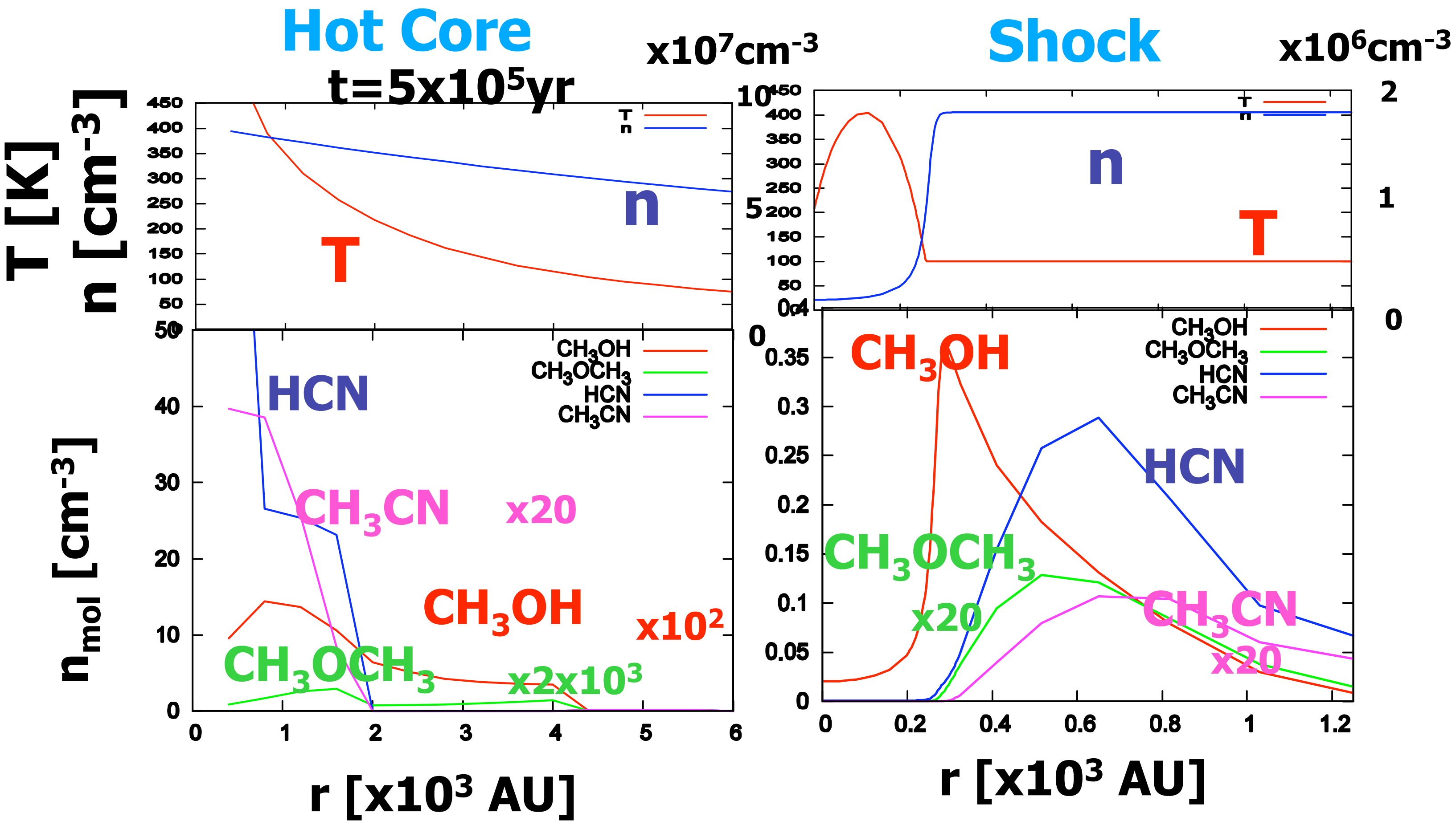


Grain mantle

Hot Cores

- Hot, dense, compact regions in areas of massive star formation
- Observed kinetic temperatures of 100-300K
- Observed densities ~ 10^6 – 10^8 cm^{-3}
- Large abundances of saturated molecules (H_2O, NH_3, H_2S, CH_3OH, C_2H_5OH, CH_3OCH_3, ..)
- Enhanced fractionation in some molecules (DCN, HDS)
- Gas-phase species thought to be the result of grain mantle evaporation, either directly (parents) or indirectly (daughters)
- Evaporation – thermal (stellar heating) or non-thermal (shock waves from outflows)
- Knowledge about surface chemistry (initial conditions)
- Accurate rate coefficients from 10-2000K

Hot Core vs. Shock



Hot core: HCN, CH_3CN: abundant

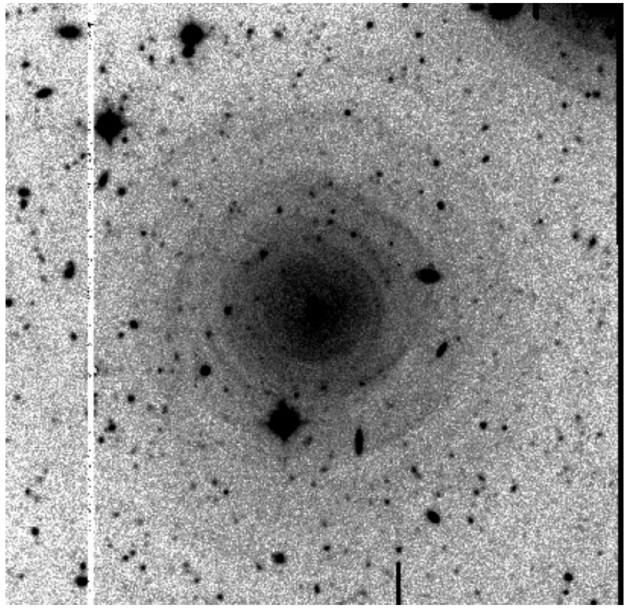
Shock: CH_3OH, CH_3OCH_3: abundant

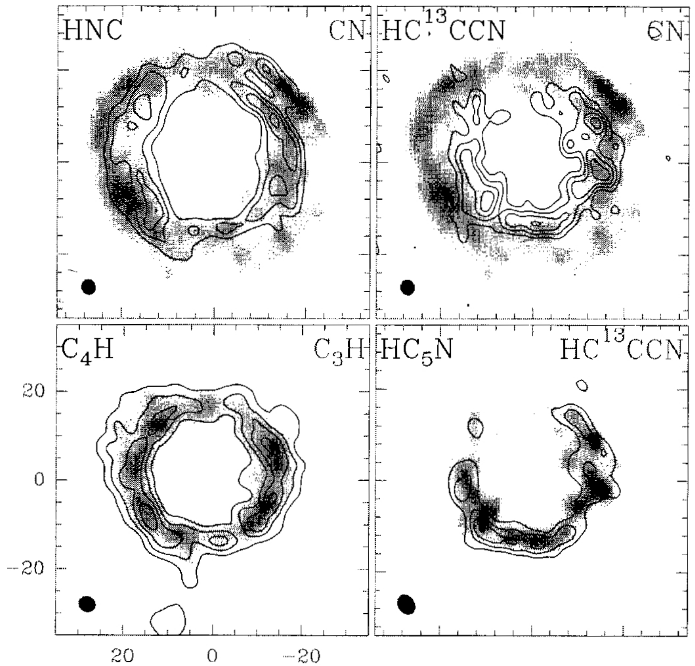
Orion KL like ?

(e.g., Charnley et al. '92, Rodgers & Charnley '01)

IRC+10216

- Nearby (~130 pc) high mass-loss carbon star (AGB)
- Dust envelope detected out to 200''
  = 25,000 AU
- Molecular shells at ~ 1000 - 4000 AU
- >60 molecules detected: CO, C_2H_2, HC_9N ...
- Newly discovered anions C_8H^-, C_6H^-, C_4H^-





Figures from Mauron & Huggins (2000) Lucas and Guelin et al. (1999)

IRC+10216

HC3N J + 5-4 emission in plane of sky shown as contours

Molecular shells/arcs shown as thick green lines

Contour is optical V-band image in false colour

Trung & Lim 2008, ApJ, in press

Molecular emission is correlated with dust shells/density enhancements

– 14 –

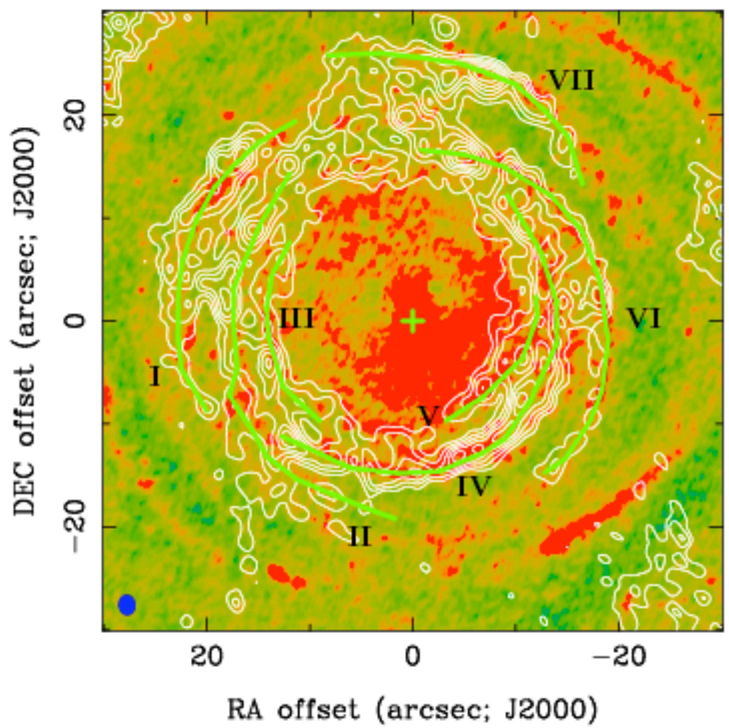


Fig. 3.— Location of the molecular shells (thick solid lines) traced by cyanopolyyne emissions around the systemic velocity, i.e close to the plane of the sky. The cross denotes the central stellar position. The shells are numbered I - VII. The HC_3N J=5−4 emission at the systemic velocity is shown in contours. Contour levels are (3, 5, 7, 9, 11, 13)σ with σ=3.6 mJy/beam

IRC+10216

Comparison of HC_3N J = 5-4 (greyscale) with HC_5N J = 9-8 (contours) using the VLA (Trung & Lim 2008, ApJ, in press)

Very close spatial correlation between HC_3N and HC_5N emission (and presumably abundances)

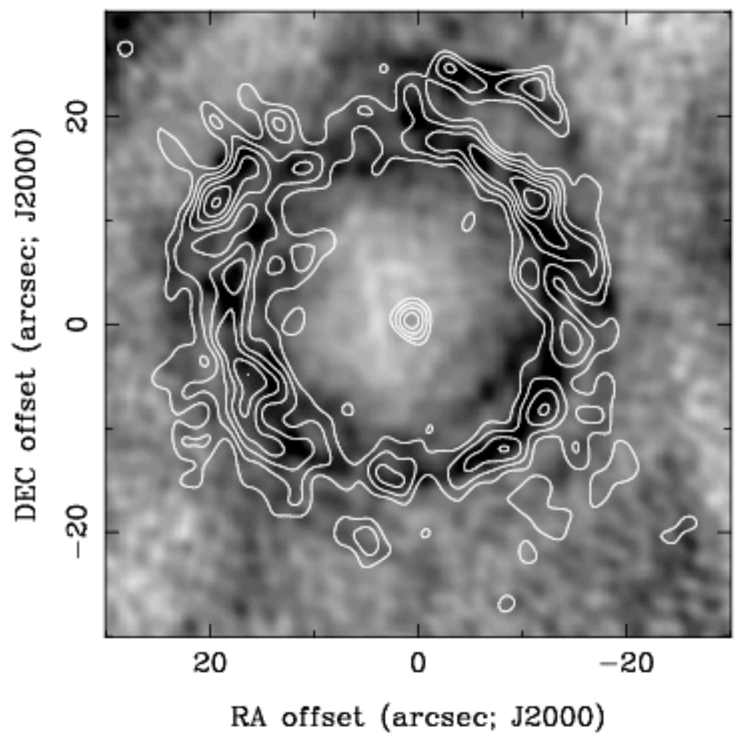
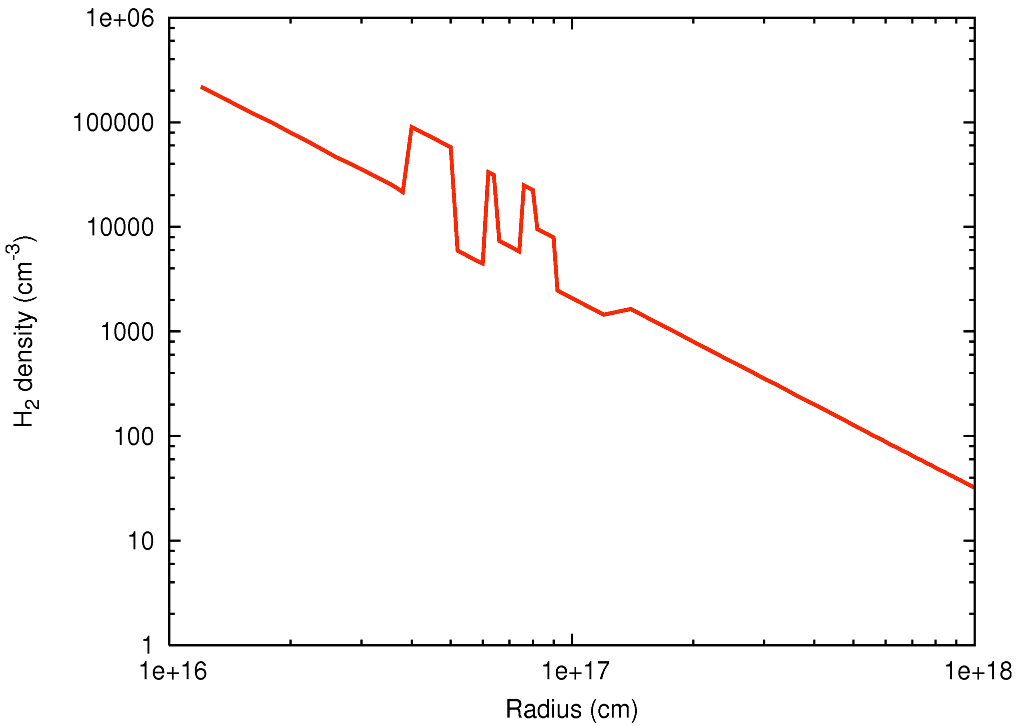


Fig. 5.— Comparison between HC_3N J=5−4 emission (shown in greyscale) and HC_5N J=9−8 emission (shown in contours) at the systemic velocity $V_{LSR} = -26$ kms^{-1}. The contour levels are (2, 3, 4, 5, 6, 7, 9, 11)σ for HC_5N J=9−8 (σ=1.0 mJy/beam).

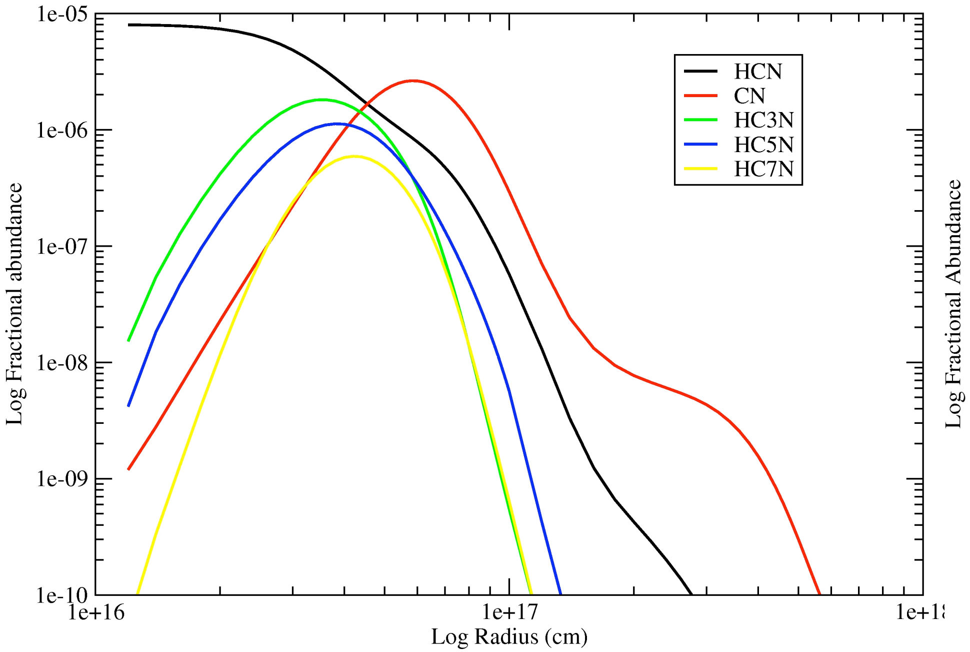
IRC+10216 with rings

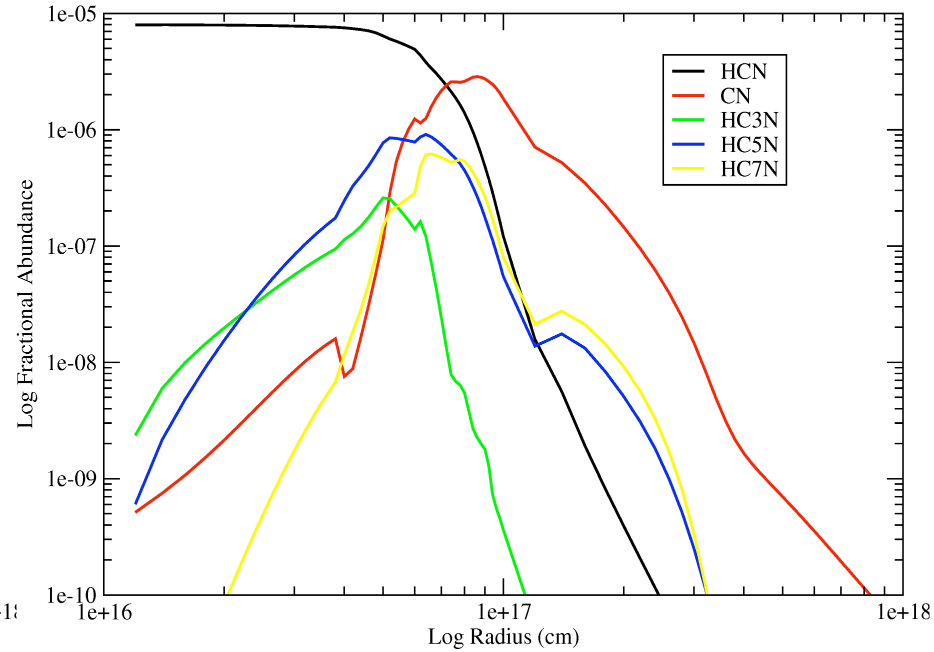
- **Data on shells from Mauron & Huggins**
- Placed on top of r^{-2} distribution
- Assume shells increase dust density (additional extinction of external UV photons)
- Assume shells increase gas density (increases the collisional rates)



Cordiner & Millar, in preparation

IRC+10216 – Standard vs Rate06 + Rings





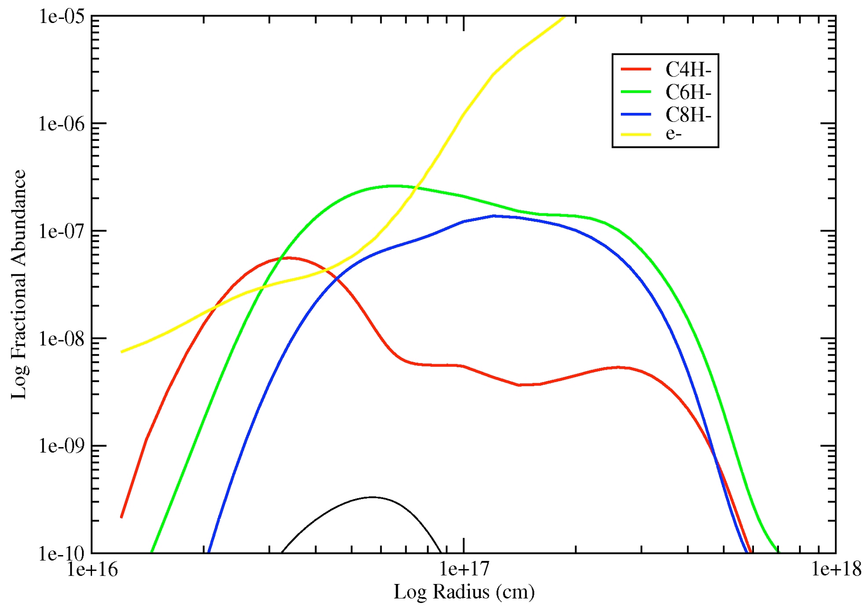
Rings provide additional extinction – so parents are destroyed further out

HC3N no longer most abundant cyanopolyyne – effect of Rate06

IRC+10216 results - standard

- Model:
  - $N(C_6H^-) = 2.7 \times 10^{13}$ cm^{-2}
  - $N(C_6H) = 1.3 \times 10^{13}$ cm^{-2}
  - Ratio = 2.1
- Observation:
  - $N(C_6H^-) = 7.0 \times 10^{12}$ cm^{-2}
  - $N(C_6H) = 7.7 \times 10^{13}$ cm^{-2}
  - Ratio = 0.10

- Predictions:
  - $N(C_4H^-) = 6.4 \times 10^{12}$ cm^{-2}
  - $N(C_8H^-) = 6.1 \times 10^{12}$ cm^{-2}
  - $N(C_8H) = 2.5\ 10^{12}$ cm^{-2}



C_4H^- and C_8H^- detected with column densities within 3-10 of those predicted

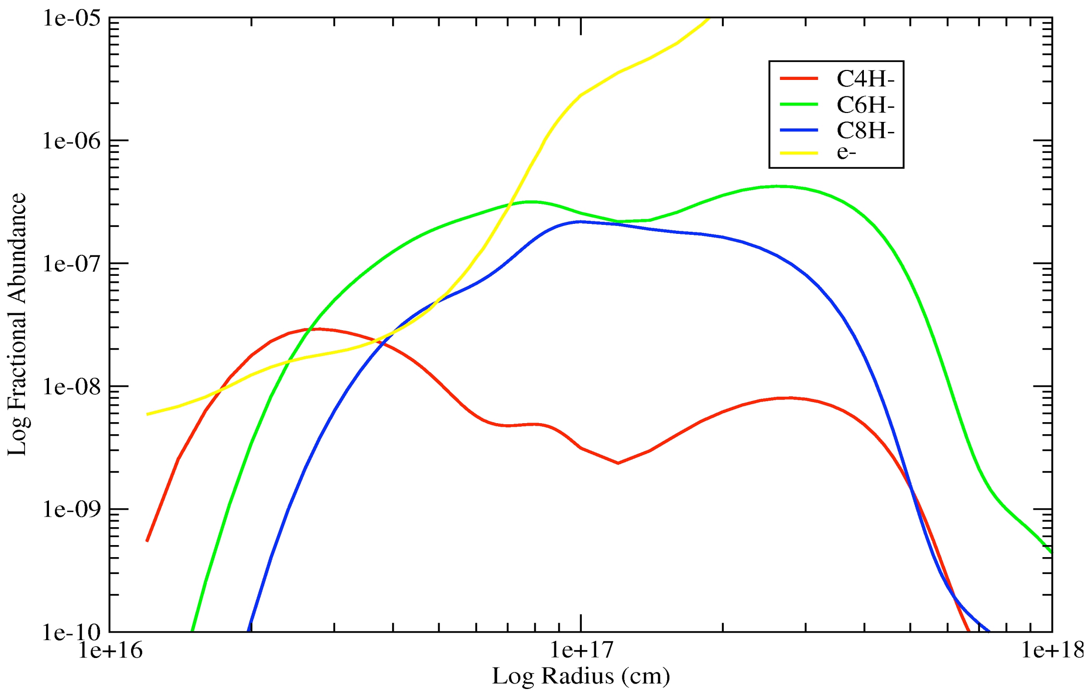
In parts of the envelope, anions are more abundant than free electrons

IRC+10216 - Rate06

Rate06 decreases the peak abundances of many of the carbon-chain species including the anions.

Note the anion abundance is still larger than that of the free electrons in part of the envelope.

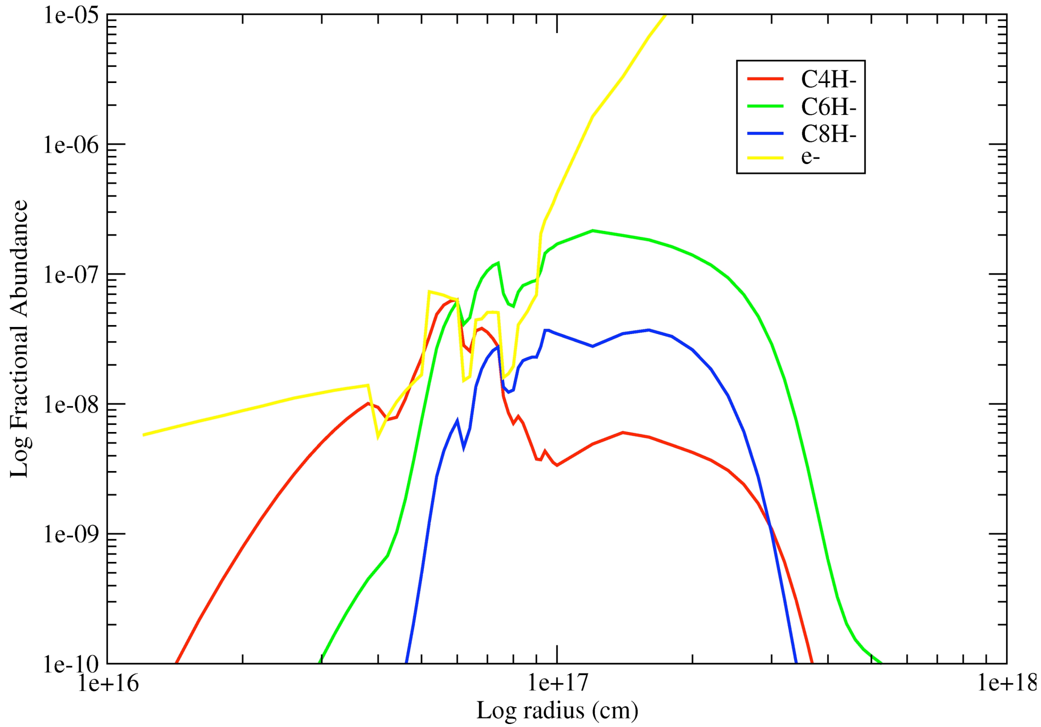
Radial distributions are broader so that column densities are hardly changed.



IRC+10216 – Rate06 + Rings

The presence of rings causes additional extinction at small radii and prevents photo-dissociation of parents occurring until farther out in the envelope.

The result is that molecular distributions tend to be more 'shell-like'.



IRC+10216 – Rate06 + Rings Intensity

We plot the product of the H2 density and the species density (per cm3) as a function of radial distance to show 'relative intensity' assuming collisional excitation.
The effect of the rings is clearly visible.