The chemical evolution in the early phases of massive star formation

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Abstract: Understanding the chemical evolution of young (high-mass) star-forming regions is a central topic in star formation research. The chemistry is employed as a unique tool: 1) to investigate the underlying physical processes and 2) to characterize the evolution of the chemical composition. With these aims in mind, we observed a sample of 59 high-mass star-forming regions at different evolutionary stages varying from the early starless phase of Infrared Dark Clouds (IRDC) to High Mass Protostellar Objects (HMPO) to Hot Molecular Cores (HMC) and, finally, Ultra Compact HII regions (UCHII) at 1mm and 3mm with the IRAM 30m telescope. We determined their large-scale chemical abundances and column densities and found that the chemical composition evolves along with the evolutionary stages.
We modeled the chemical evolution in these environments, using a 1D physical model where density and temperature vary from stage to stage coupled with an advanced gas-grain chemical model. By varying the density structure the best-fit chi-square values of all the relevant parameters were derived. A satisfying overall agreement between observed and modeled column densities for most of the molecules in all evolutionary stages was obtained. In addition the best-fit model provided chemical ages for each phase.

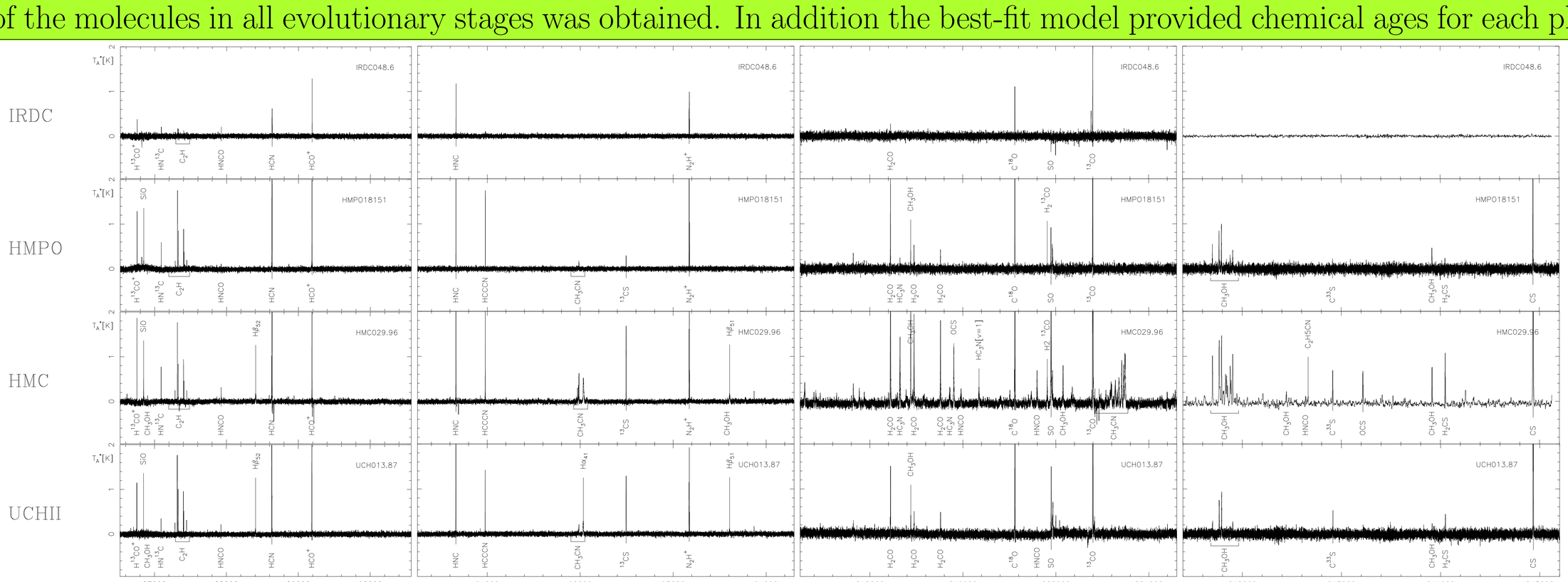


Fig. 1: From top to bottom the characteristic example spectra of the four sources IRDC048.6, HMPO18151, HMC029.96 and UCH013.87 for each of the four evolutionary stages in high-mass star formation in a total bandpass of 16 GHz are shown. The intensity of the molecular lines and diversity of molecules strongly increases with time and reaches its peak at the Hot Molecular Core phase with the formation of complex hydrocarbons.

Observations vs. model

IRDC:

Species	N_{obs}[cm^{-2}]	N_{model}[cm^{-2}]
CO	1.9(18)	2.1(18)
HNC	1.5(14)	2.0(14)
HCN	9.1(13)	2.1(14)
HCO^+	1.2(14)	5.4(13)
HNCO	1.9(12)	5.3(11)
H_2CO	3.5(13)	7.2(13)
N_2H^+	2.2(13)	3.0(12)
CS	≤6.0(14)	1.4(15)
SO	≤8.4(12)	7.6(13)
OCS	≤2.7(15)	2.8(12)
C_2H	3.8(14)	1.9(14)
SiO	1.9(12)	6.0(12)
CH_3CN	≤5.2(12)	3.3(12)
CH_3OH	≤4.8(13)	2.0(12)
Chemical age:		∼ 10 000 years

HMC:

Species	N_{obs}[cm^{-2}]	N_{model}[cm^{-2}]
CO	4.2(19)	1.1(19)
HNC	2.4(15)	1.1(14)
HCN	1.3(15)	1.4(15)
HCO^+	2.6(15)	6.9(14)
HNCO	6.3(13)	5.9(13)
H_2CO	4.4(14)	5.6(14)
N_2H^+	7.3(13)	7.4(13)
CS	2.4(16)	1.5(15)
SO	8.6(14)	7.8(15)
OCS	8.8(14)	1.2(15)
C_2H	1.0(16)	1.8(14)
SiO	5.0(13)	2.2(13)
CH_3CN	1.2(14)	7.6(13)
CH_3OH	2.2(15)	5.1(14)
Chemical age:		∼ 40 000 years:

HMPO:

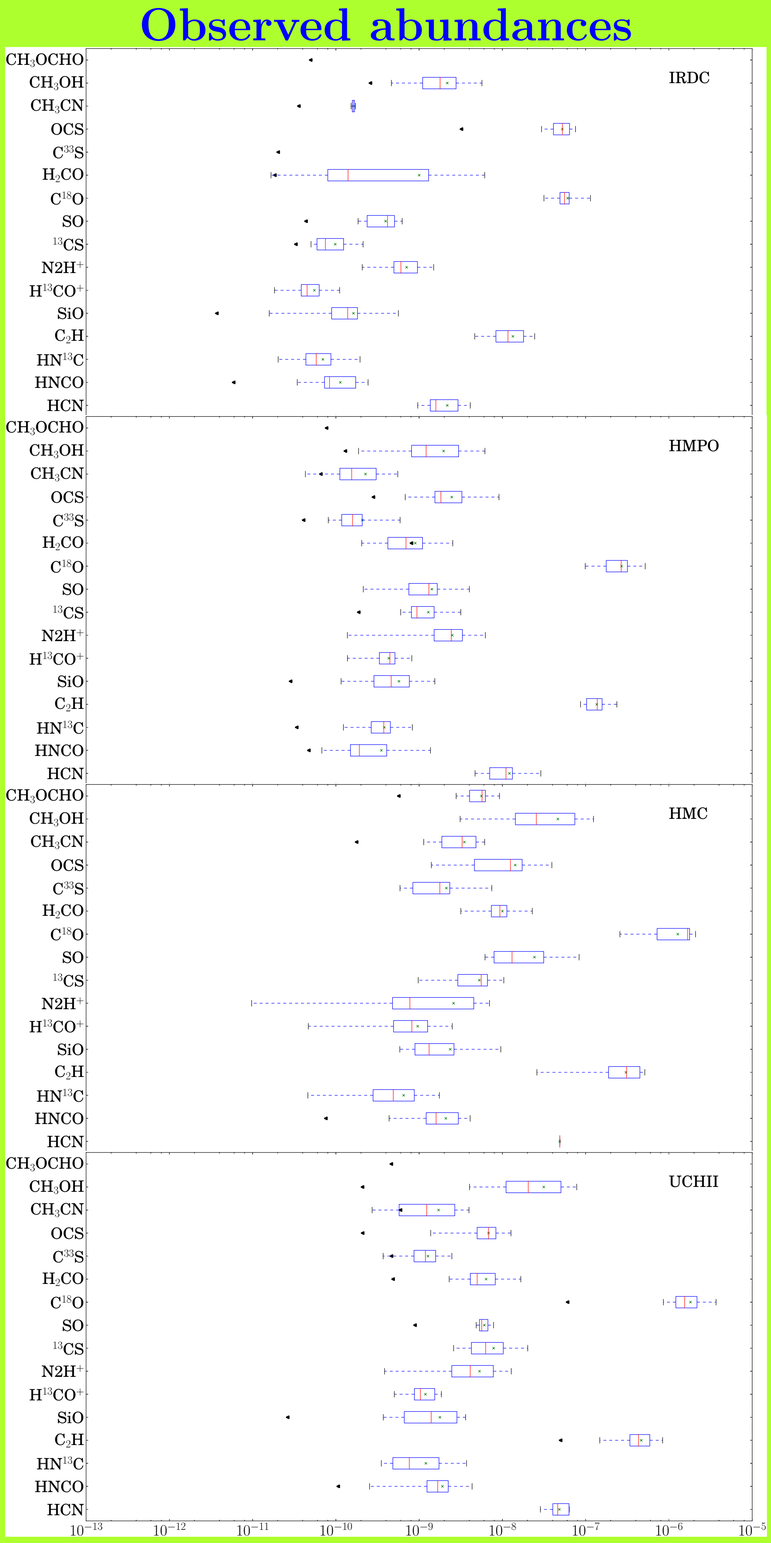
Species	N_{obs}[cm^{-2}]	N_{model}[cm^{-2}]
CO	6.7(18)	4.1(18)
HNC	7.0(14)	7.5(14)
HCN	2.2(14)	1.3(15)
HCO^+	9.6(14)	4.3(14)
HNCO	4.7(12)	3.5(12)
H_2CO	4.4(13)	7.2(15)
N_2H^+	4.8(13)	4.1(13)
CS	1.3(15)	1.2(15)
SO	9.1(13)	7.9(14)
OCS	≤6.9(13)	2.2(14)
C_2H	2.8(15)	6.8(14)
SiO	9.1(12)	9.4(12)
CH_3CN	2.4(12)	2.2(13)
CH_3OH	7.3(13)	5.7(12)
Chemical age:		∼ 60 000 years

UCHII:

Species	N_{obs}[cm^{-2}]	N_{model}[cm^{-2}]
CO	2.8(19)	6.4(18)
HNC	1.1(15)	9.0(13)
HCN	3.7(14)	4.0(14)
HCO^+	1.8(15)	4.8(14)
HNCO	1.1(13)	1.8(13)
H_2CO	1.2(14)	2.4(14)
N_2H^+	7.3(13)	5.4(13)
CS	5.0(15)	5.3(14)
SO	1.3(14)	6.7(15)
OCS	≤1.9(13)	1.6(14)
C_2H	7.8(15)	8.0(13)
SiO	8.5(12)	1.7(13)
CH_3CN	2.0(13)	8.7(12)
CH_3OH	1.9(14)	1.2(14)
Chemical age:		∼ 10 000 years

Tables: The tables show the comparison between the median of the observed column densities (including 3σ-limits for non-detections) and values of the best-fit model for the 4 evolutionary stages. The model explains most of the molecules in all stages reasonably well. The total best-fit age of ∼ 120 000 years is consistent with the estimates obtained from other theoretic models of the formation of high-mass stars.

Observed abundances



Assumptions and model

Observations:
- Local Thermodynamic Equilibrium
- optically thin lines (only N_2H^+ and HCN corrected for τ)
- characteristic temperature for each stage

Model:
- 1D physical model with time-dependent gas-grain chemistry (from D. Semenov)
- best-fit molecular abundances ⇒ input for next stage
- χ^2-fitting of column densities for all time steps

Outlook

- include deuterated species to put constrains on thermal history
- study single sources by interferometric means to derive filling factors
- extend model to 2D and include additional physics (e.g., UV-penetration, shocks)

Left Figures: Abundances (wrt to the total H) of the analyzed molecules calculated for $T_{kin} = T_{ex}$ and assuming T_{kin} = 15 K for IRDCs, T_{kin} = 50 K for HMPOs and T_{kin} = 100 K for HMCs and UCHIIs. The red line shows the median, the green cross is the mean, the bar indicates the inner 25%-75% range around the median and the whiskers mark the total range of all calculated values. The black arrows give the minima of all calculated upper limits. The median column densities increase in general with evolutionary stage.