Complex Organic Molecules Formation in Cold Cores

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International Symposium and Workshop on Astrochemistry
Campinas, SP, Brazil
July 4, 2016

Complex Organic Molecules

- Almost 200 interstellar molecules have been found.
- Carbon containing molecules with at least 6 atoms are called interstellar complex organic molecules(COMs).
- Found in almost all astronomical sources in the early phases of star formation including protoplanetary disks.

  CH_3CN, MWC480, Öberg et al 2015 Nature,

  CH_3OH, TW Hya, Walsh et al. 2016 APJL

COMs Formation Mechanism(1)

- COMs were initially found in hot cores. Rubin et al 1971 Apj.
- Two-step formation mechanism(Millar et al, Apj 1991).

1. Mother species were formed during the cold star formation process. Single atoms addition.

2. As molecular clouds warm up, mother species evaporate into gas phase and react with each other to form COMs.

- Challenge from laboratory experiments(Horn et al 2004 Apj).

COMs Formation Mechanism(2)

- Garrod & Herbst 2006, 2008, A&A.
- Radicals are formed by UV radiation of ice mantle on grain surface.
- Radicals recombine to form COMs.

  H_2CO ->HCO + H

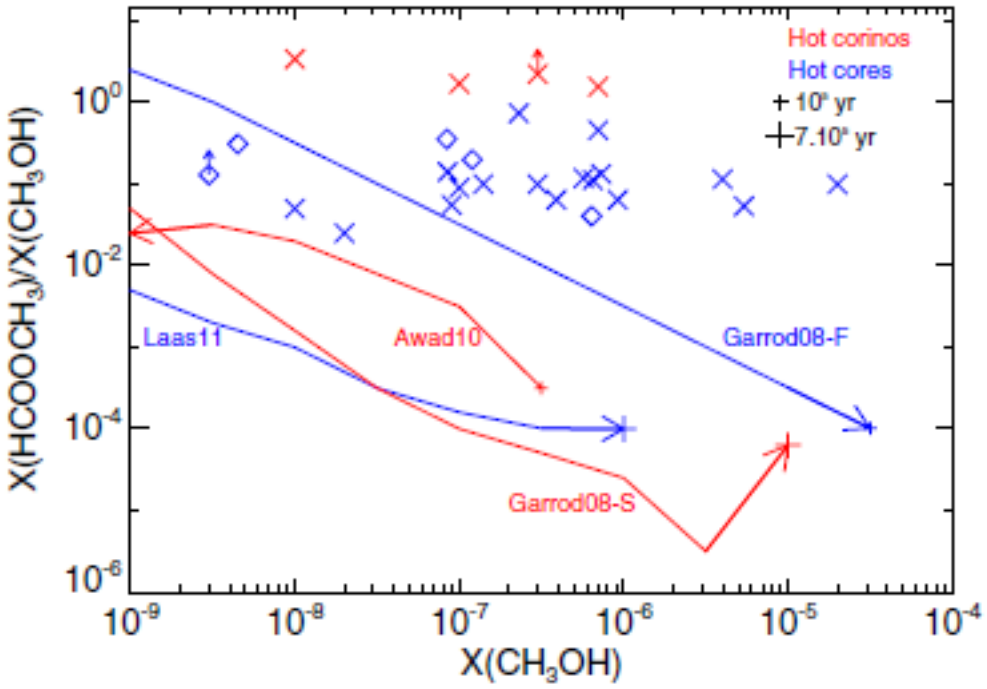
  CH_3OH ->CH_3O + H

  HCO + CH_3O ->$HCOOCH_3$

  Narrow temperature range (30-40K).

  Radicals have be able to diffuse on grain surface.

Methyl Formate ($HCOOCH_3$)



Taquet et al. A&A 2012

COMs in Cold Clouds (10K)

MF: $HCOOCH_3$ DM: CH_3OCH_3

- L1689b: MF: 7.4(-10), DM: 1.3(-10), Bacmann et al, A&A 2012
- B1-b: MF: 2.0(-11), DM: 2.0(-10) Cernicharo et al, ApJL, 2012
- L1544: MF: <1.5(-9), DM:<2.0(-10) Vastal et al, ApJ, 2014

Models

Reactive desorption (RD).

- Vasyunin & Herbst, ApJ 2013, (VH)

Critical species were formed on grain surface and then ejected into gas phase by RD. COMs are formed in gas phase.

$CH_3O + CH_3 \rightarrow DM$

$H_2COH^+ + H_2CO \rightarrow H_5C_2O_2^+$

$H_5C_2O_2^+ + e \rightarrow MF + H$

- Balucani et al, MNRAS, 2015, (BCT)

Methanol were formed on grain surface and then ejected into gas phase by RD. Methanol starts the COMs formation processes.

$CH_3OH + OH \rightarrow CH_3O + H_2O$, $CH_3O + CH_3 \rightarrow DM$,

$DM \rightarrow CH_3OCH_2 \rightarrow MF$

- Ruaud et al, MNRAS, 2015, (RW)

COMs are formed on grain surface. Eley-Rideal and complex induced reaction.

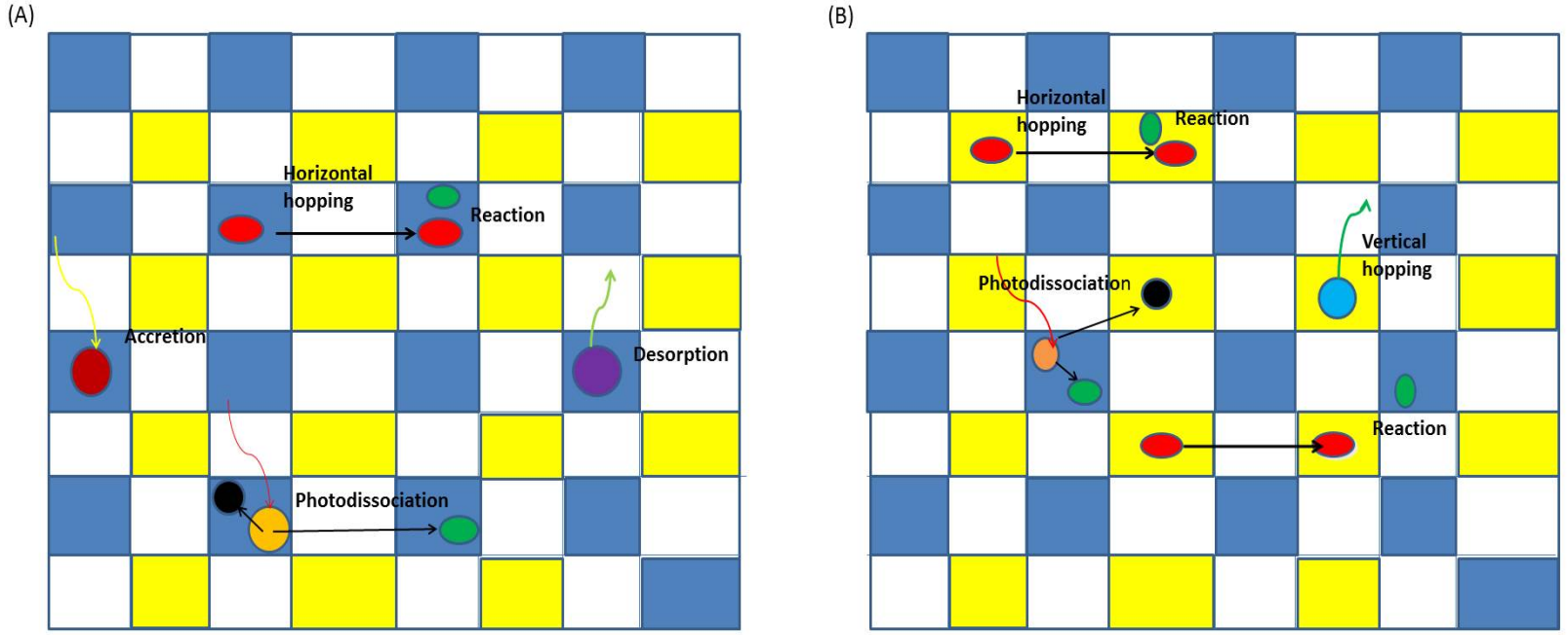
CO_2 Formation

- Is the discovery of COMs in cold cores a new challenge to astrochemical modeling?
- Not really. We had problem to explain the formation of CO_2 on grain surface.

$$CO + OH \rightarrow CO_2 + H$$

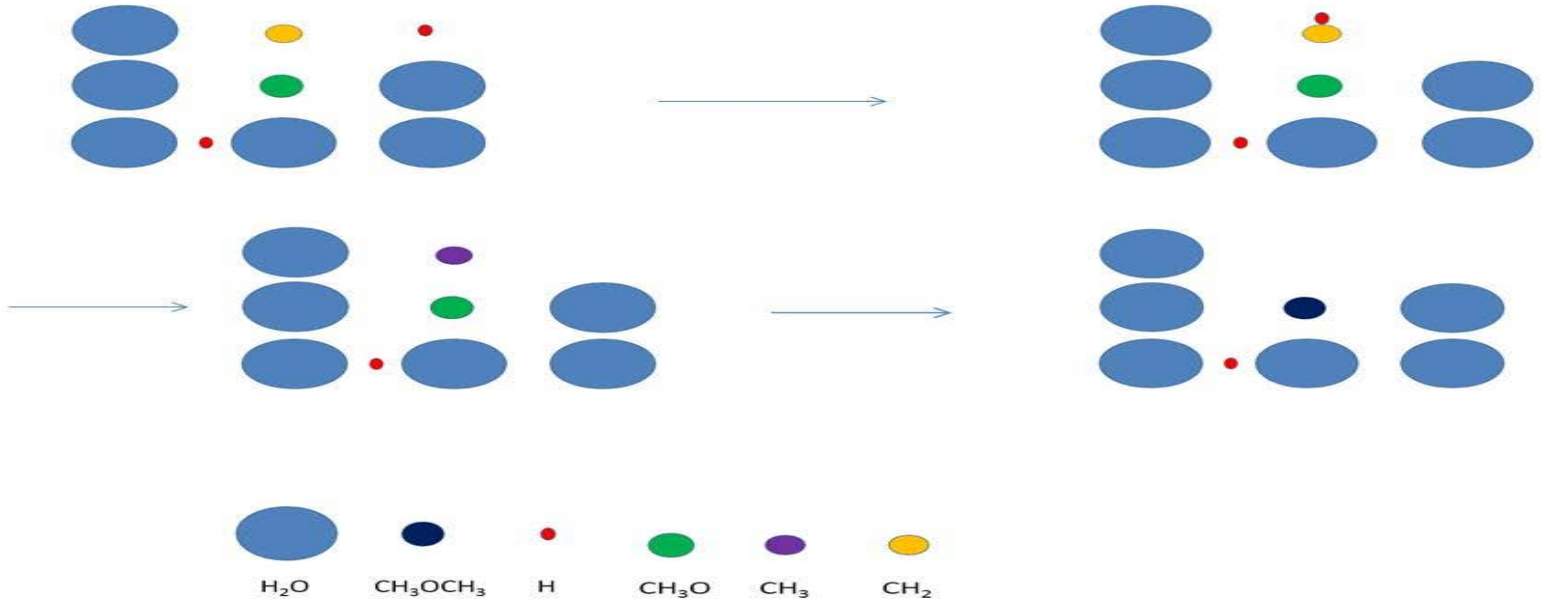
Unified Microscopic-Macroscopic Monte Carlo Simulation Method

- Surface Processes(Chang & Herbst, ApJ. 2012, 2014）



Chain Reactions

- Non-diffusive surface chemical reactions. Smallest scale chemical explosion? Chang & Herbst, ApJ 2016



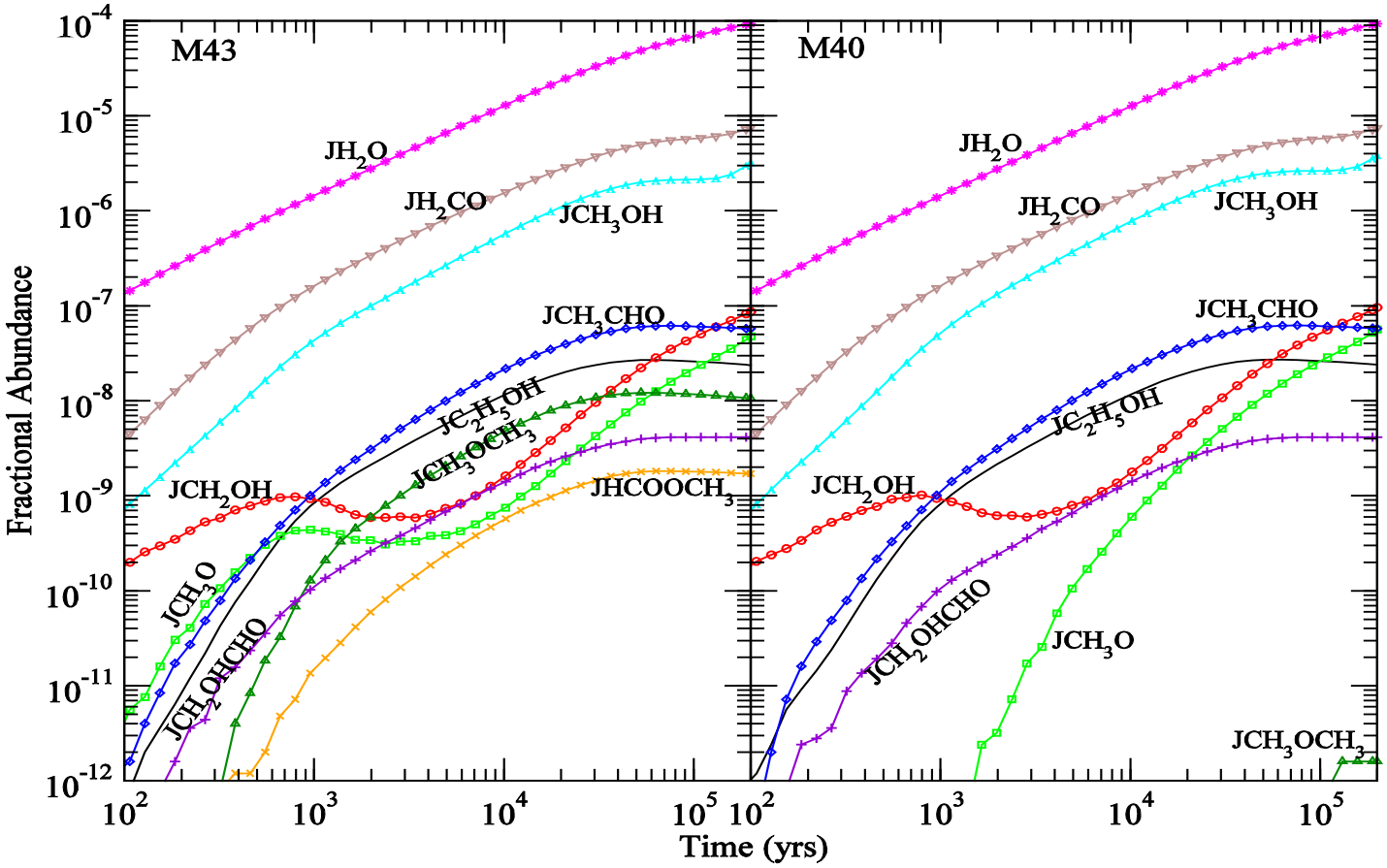
Surface CH_3O

- CO + H -> …-> CH_3OH
- CH_3OH + photon -> CH_3O + H

- CH_3O -> CH_2OH ?
- CH_3OH + OH ->CH_3O + H_2O
- Two Models, M40 and M43

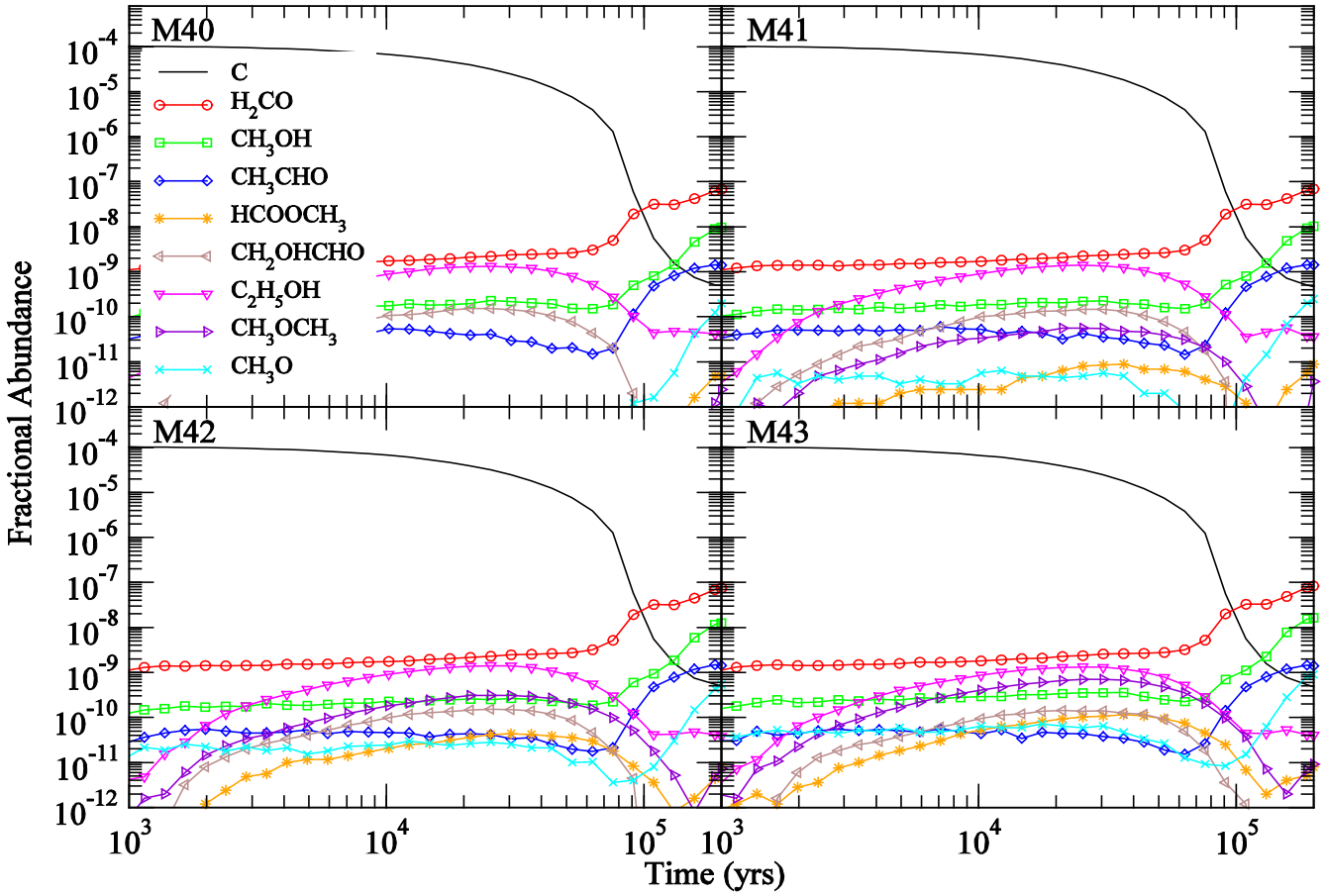
Results

- Surface COMs



Results

- Gas Phase COMs



L1689b

	DM	CH_3O	MF	H_2CO
Observation:	1.3(-10)	…	7.4(-10)	1.3(-9)
M43 :	4.7(-10)	2.7(-11)	9.4(-11)	2.8(-9)
VH model:	1.3(-10)	8.5(-10)	3.3(-12)	5.4(-8)
RW model:	2.4(-10)	7.6(-12)	3.6(-13)	1.1(-8)

B1-b

	DM	CH_3O	MF	H_2CO
Observation:	2.0(-11)	4.7(-12)	2.0(-11)	4.0(-10)
M43 :	9.8(-11)	8.4(-12)	2.5(-11)	2.0(-8)
VH model:	3.7(-12)	1.5(-10)	2.0(-12)	4.8(-8)
RW model:	5.5(-12)	1.2(-11)	1.7(-13)	8.5(-9)

Future COMs Formation Models

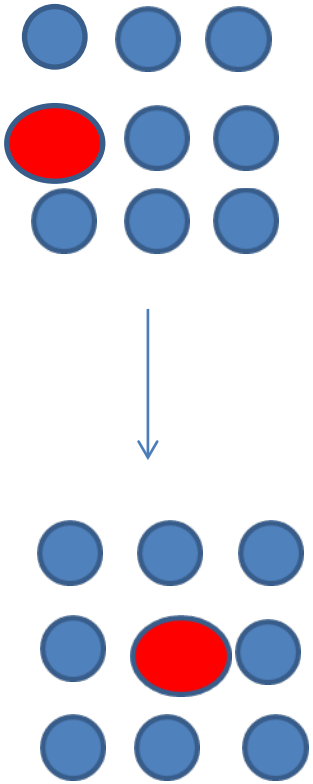
- Progress driven by observation.
- Gas phase chemistry.
- Chemical reactions in ice.

  Three phase model with bulk diffusion(Chang & Herbst 2014).
- Missing physical processes.

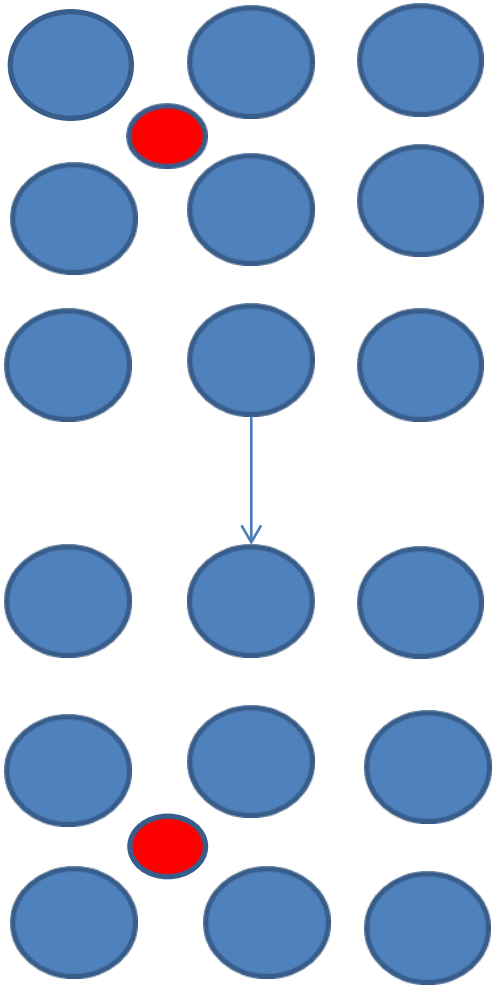
  e.g. stochastic heating of smaller dust grains.

Bulk diffusion

- Substitutional



- Interstitial



Thank you!