Improving the quality of chemical model predictions for the interstellar medium

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2 atoms

H_2
AlF
AlCl
C_2**
CH
CH^+
CN
CO
CO^+
CP
SiC
HCl
KCl
NH
NO
NS
NaCl
OH
PN
SO
SO^+
SiN
SiO
SiS
CS
HF
SH
HD
FeO (?)
O_2 (?)
CF^+
SiH (?)
PO
AlO

3 atoms

C_3
C_2H
C_2O
C_2S
CH_2
HCN
HCO
HCO^+
HCS^+
HOC^+
H_2O
H_2S
HNC
HNO
MgCN
MgNC
N_2H^+
N2O
NaCN
OCS
SO_2
c-SiC_2
CO_2
NH_2
H_3^+
H_2D+, HD_2+
SiCN
AlNC
SiNC
HCP
CCP

4 atoms

c-C_3H
l-C_3H
C_3N
C_3O
C_3S
C_2H_2
NH_3
HCCN
$HCNH^+$
HNCO
HNCS
$HOCO^+$
H_2CO
H_2CN
H_2CS
H_3O^+
c-SiC_3
CH_3*
C_3N^-
HCNO

5 atoms

C_5
C_4H
C_4Si
l-C_3H_2
c-C_3H_2
H_2CCN
CH_4
HC_3N
HC2NC
HCOOH
H2CNH
H2C2O
H2NCN
HNC_3
SiH_4
H_2COH^+
C_4H^-
CNHCO

6 atoms

C_5H
l-H_2C_4
C_2H_4*
CH_3CN
CH_3NC
CH_3OH
CH_3SH
HC_3NH+
HC_2CHO
NH_2CHO
C_5N
l-HC_4H (?)
l-HC_4N
c-H_2C_3O
H_2CCNH (?)
C_5N^-

7 atoms

C_6H
CH_2CHCN
CH_3C_2H
HC_5N
CH_3CHO
CH_3NH_2
c-C_2H_4O
H_2CCHOH
C_6H^-

8 atoms

CH_3C_3N
$HCOOCH_3$
CH_3COOH
C_7H
H_2C_6
CH_2OHCHO
l-HC_6H (?)
CH_2CHCHO (?)
CH_2CCHCN
NH_2CH_2CN

9 atoms

CH_3C_4H
CH_3CH_2CN
$(CH_3)_2O$
CH_3CH_2OH
HC_7N
C_8H
$CH_3C(O)NH_2$
C_8H^-
CH_2CHCH_3

10 atoms

CH_3C_5N
$(CH_3)_2CO$
$(CH_2OH)_2$
CH_3CH_2CHO

11 atoms

HC_9N
CH_3C_6H

12 atoms

C_6H_6 (?)
$C_2H_5OCH_3$ (?)

13 atoms

$HC_{11}N$

Massive star formation region

Dense cloud

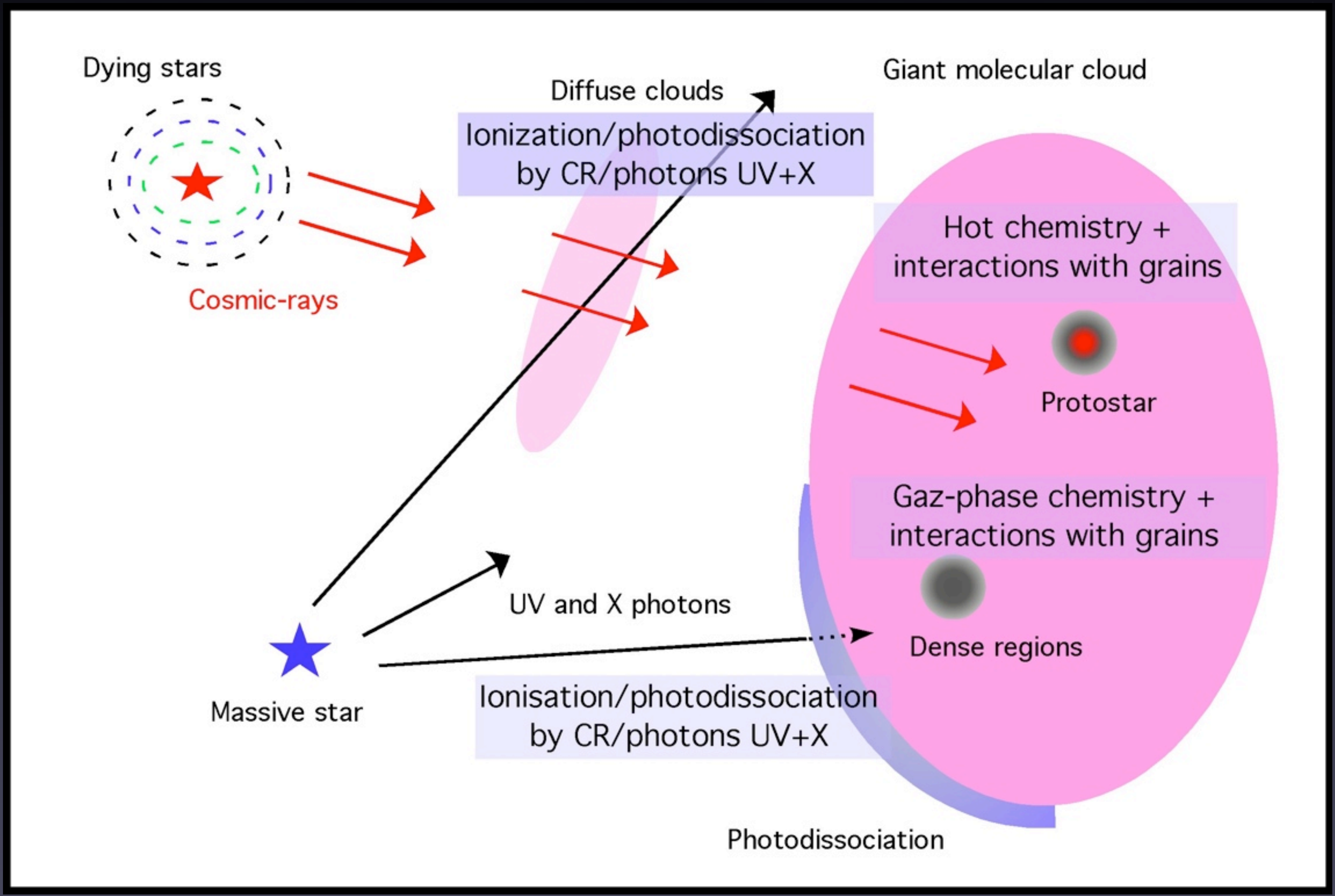
Evolved star

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms
H_2	C_3	c-C_3H	C_5	C_5H	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N	HC_9N
AlF	C_2H	l-C_3H	C_4H	l-H_2C_4	CH_2CHCN	$HCOOCH_3$	CH_3CH_2CN	$(CH_3)_2CO$	CH_3C_6H
AlCl	C_2O	C_3N	C_4Si	C_2H_4*	CH_3C_2H	CH_3COOH	$(CH_3)_2O$	$(CH_2OH)_2$	
C_2**	C_2S	C_3O	l-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH	CH_3CH_2CHO	
CH	CH_2	C_3S	c-C_3H_2	CH_3NC	CH_3CHO	H_2C_6	HC_7N		
CH^+	HCN	C_2H_2	H_2CCN	CH_3OH	CH_3NH_2	CH_2OHCHO	C_8H		
CN	HCO	NH_3	CH_4	CH_3SH	c-C_2H_4O	l-HC_6H (?)	$CH_3C(O)NH_2$		
CO	HCO^+	HCCN	HC_3N	HC_3NH+	H_2CCHOH	CH_2CHCHO (?)			
CO^+	HCS^+	$HCNH^+$	HC2NC	HC_2CHO	C_6H^-	CH_2CCHCN	C_8H^-		
CP	HOC^+	HNCO	HCOOH	NH_2CHO		NH_2CH_2CN	CH_2CHCH_3		
SiC	H_2O	HNCS	H2CNH	C_5N					
HCl	H_2S	$HOCO^+$	H2C2O	l-HC_4H (?)					
KCl	HNC	H_2CO	H2NCN	l-HC_4N					
NH	HNO	H_2CN	HNC_3	c-H_2C_3O					
NO	MgCN	H_2CS	SiH_4	H_2CCNH (?)					
NS	MgNC	H_3O^+	H_2COH^+	C_5N^-					
NaCl	N_2H^+	c-SiC_3	C_4H^-						
OH	N2O	CH_3*	CNHCO						
PN	NaCN	C_3N^-							
SO	OCS	HCNO							
SO^+	SO_2								
SiN	c-SiC_2								
SiO	CO_2								
SiS	NH_2								
CS	H_3^+								
HF	H_2D+, HD_2+								
SH	SiCN								
HD	AlNC								
FeO (?)	SiNC								
O_2 (?)	HCP								
CF^+	CCP								
SiH (?)									
PO									
AlO									

12 atoms	13 atoms
C_6H_6 (?)	$HC_{11}N$
$C_2H_5OCH_3$ (?)	

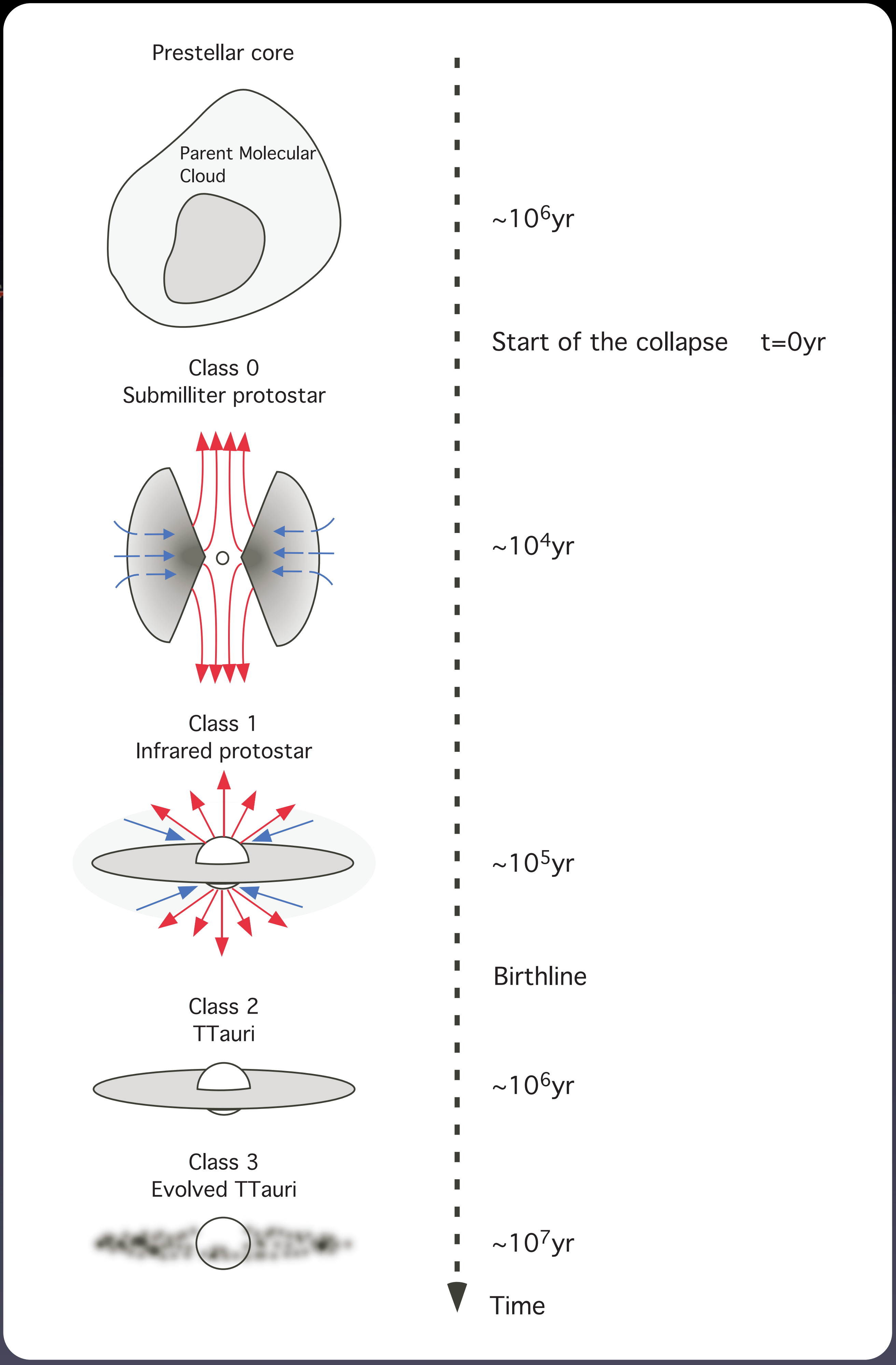
(circle) Molecules detected in dense clouds

The chemistry of the interstellar medium



Importance of chemical composition

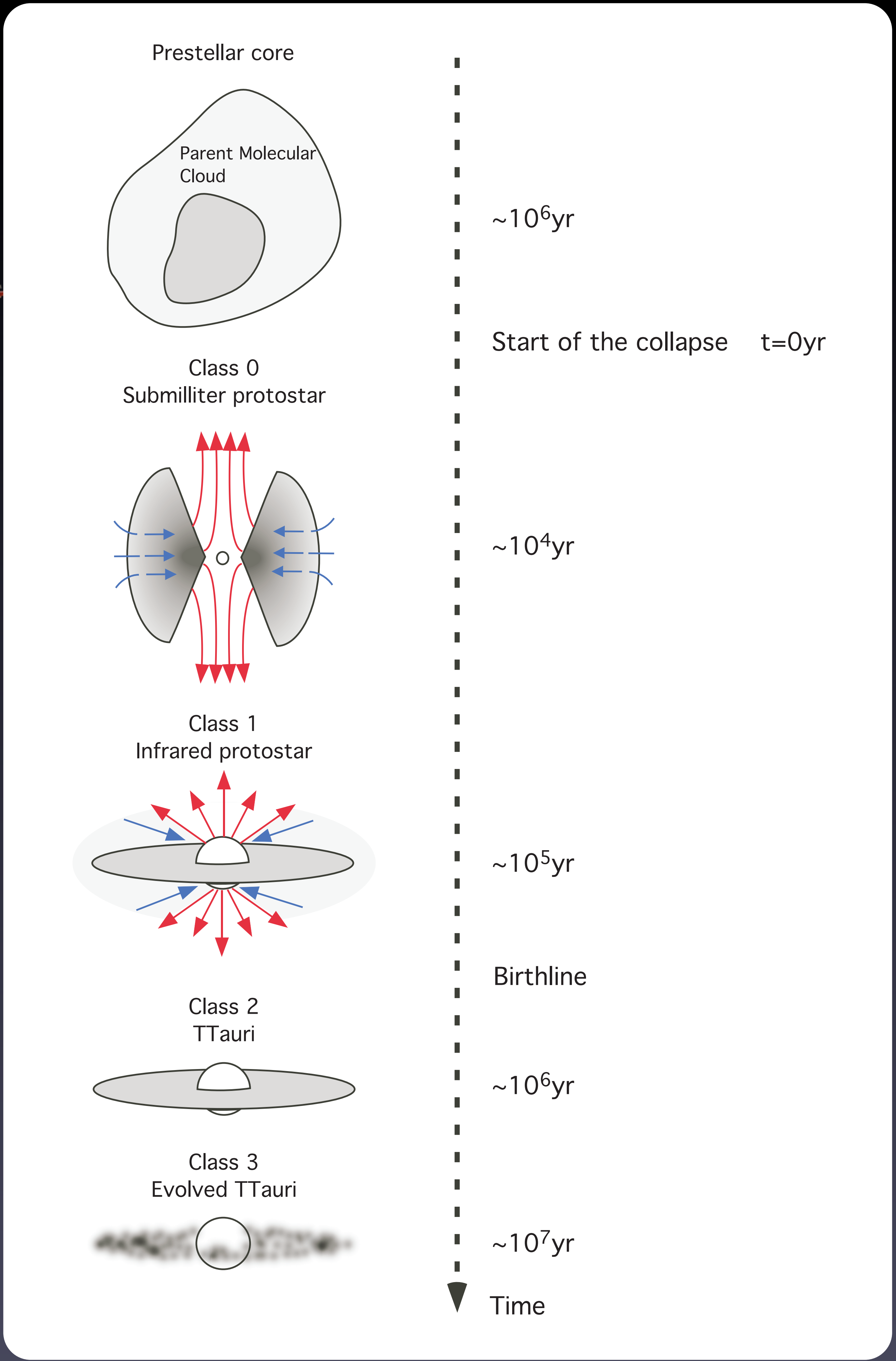
Star formation



Importance of chemical composition

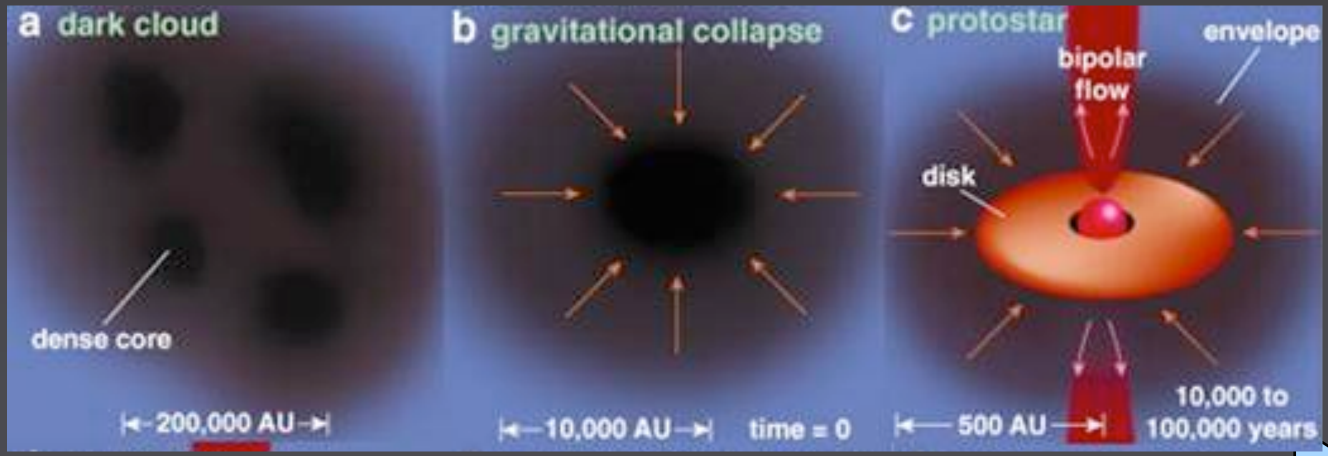
Star formation

- Pressure of radiation (gas cooling)
- Magnetic field coupling (ionization fraction)



Importance of chemical composition

Chemical clocks



Temps

Evolution chimique

t=0
Conditions initiales

Observation

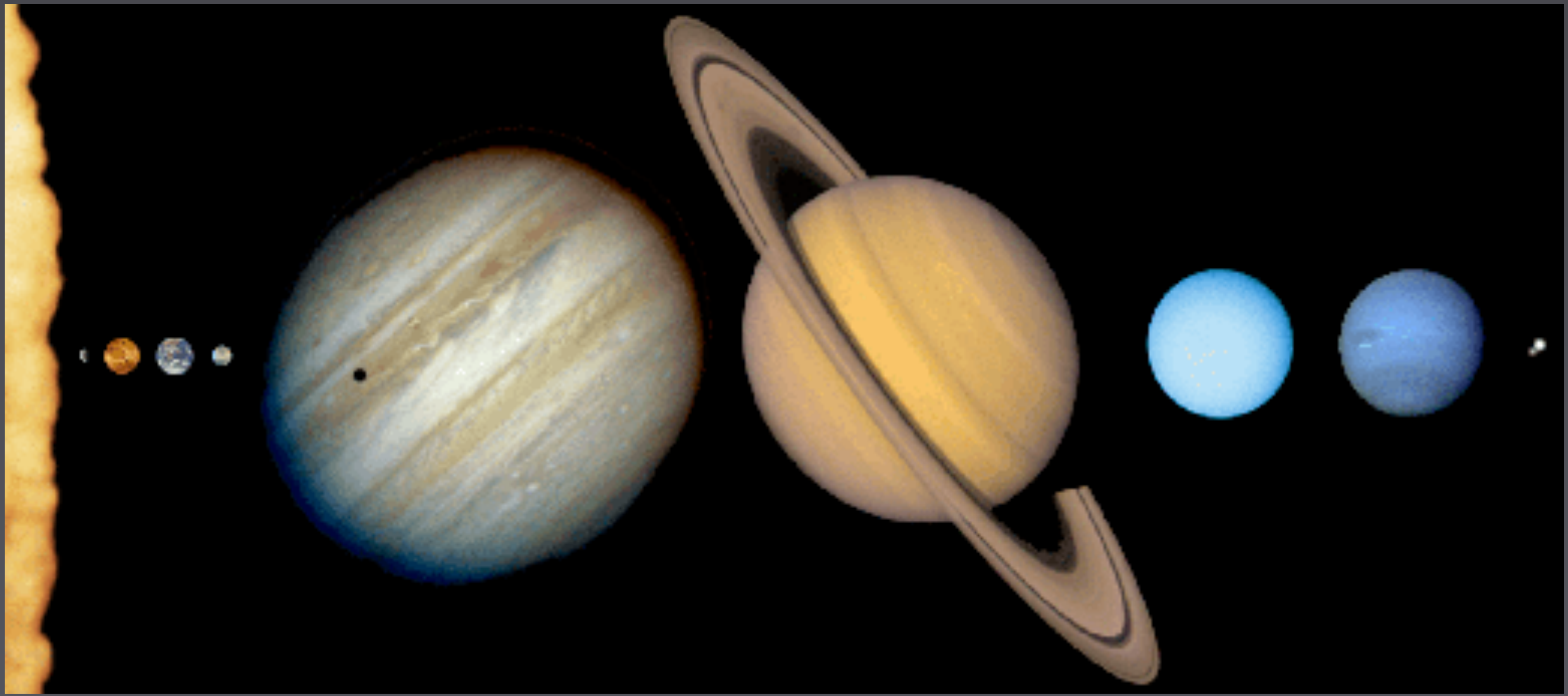
Observed abundances + Time dependent chemical models → Time between initial conditions and the observations

Importance of chemical composition

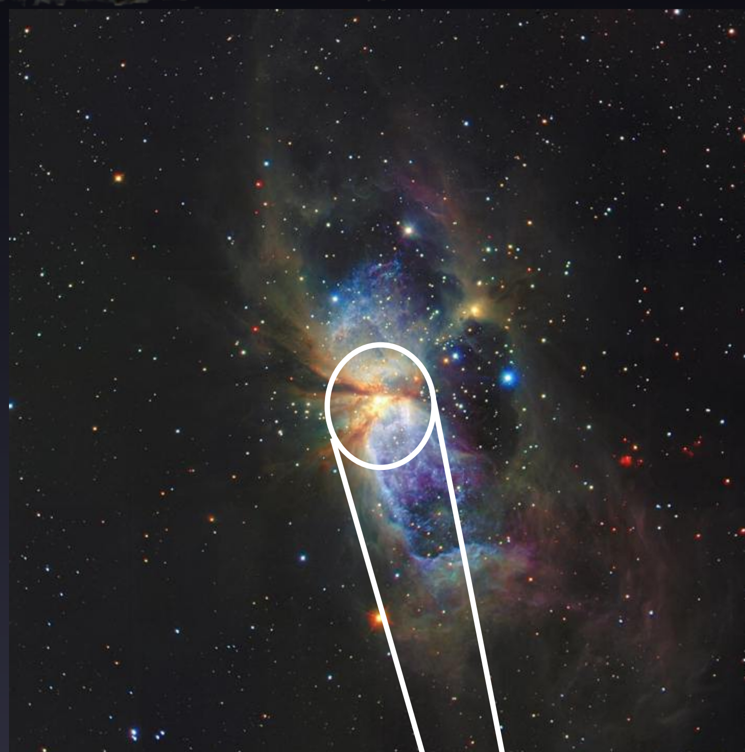
Planet formation

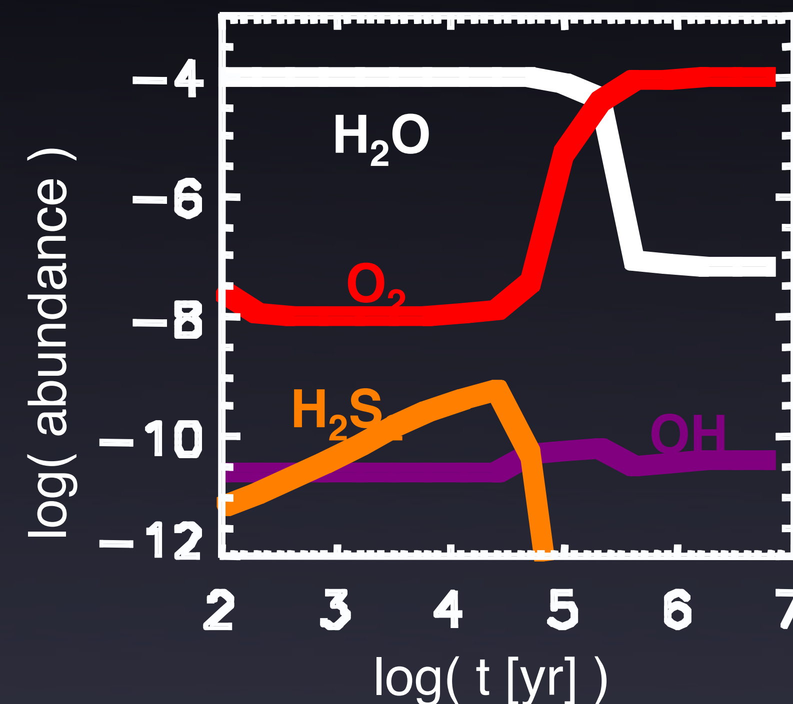
Distribution of species in the protoplanetary disk → Composition of system solar bodies (H_2O, N_2, CO_2, CH_4 etc)

C/O elemental ratio in the disk → presence of water in the system or not



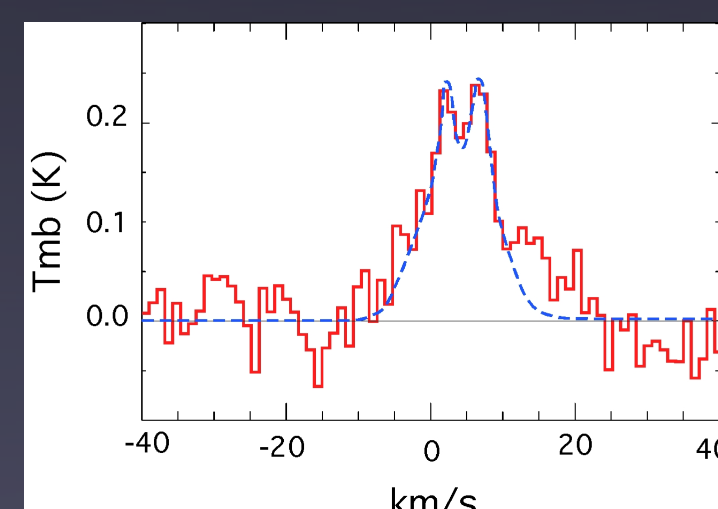
Modeling the chemistry / testing those models





Theoretical abundances

Comparisons



Observed abundances

Gas-Phase chemical models

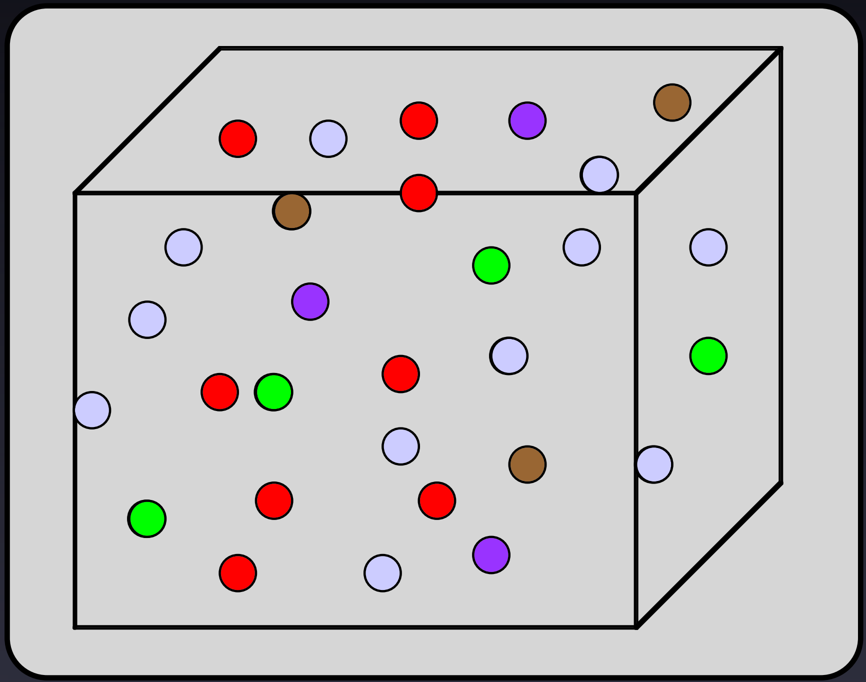
Description of processes

- ✓ Mainly ion-molecule reactions with atoms (C^+, O, N and S^+) and radicals (OH, CH, CH_2, H_3^+ etc)
- ✓ Ionization and dissociation by cosmic-rays, UV and X photons (source of ionization, $H_2 + \gamma \rightarrow H_2^+ + e^-$)
- ✓ Electronic recombinations ($H_3O^+ + e^- \rightarrow H_2O + H$)
- ✓ Neutral-neutral reactions mainly with atoms and radicals (Smith, Herbst & Chang 2004)
- ✓ Radiative associations ($C + H_2 \rightarrow CH_2$ + photon)
- ✓ Electron attachment ($C_4 + e^- \rightarrow C_4^-$ -- $PAH + e^- \rightarrow PAH^-$)

Gas-Phase chemical models

Description of models

Compute species abundances as a function of time:



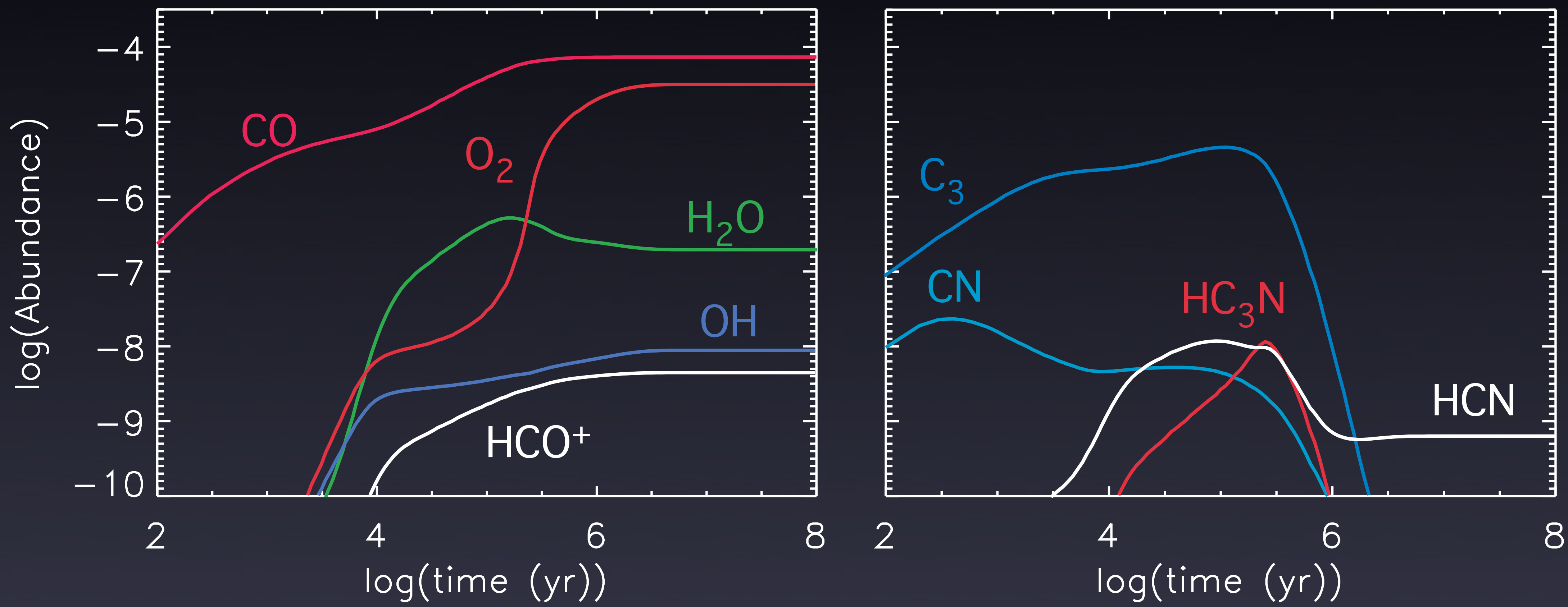
$$\frac{dn_i}{dt} = \underbrace{\sum k_{ij}\, n_i n_j}_{\text{Production}} - \underbrace{n_i \sum k_{ij}\, n_j}_{\text{Destruction}}$$

Parameters of the models:

- Gas and grain temperatures (K)
- Density (cm-3)
- Elemental abundances
- UV, X-ray and Cosmic-ray fields
- Chemical networks

Current models follow around 400 gas-phase species through more than 4500 gas-phase reactions

Gas-Phase chemical models



Initial conditions
Set of parameters describing your object

↓

Evolution of abundances as a function of time

↔

Observations

↓

Constraints on the age and/or chemical processes

Gas-Phase chemical models

Sensitivity analysis

Parameter uncertainties for a 0D gas-phase model:

Gas temperature and density, elemental abundances, initial conditions, cosmic-ray ionization rate (ζ), reaction rate coefficients

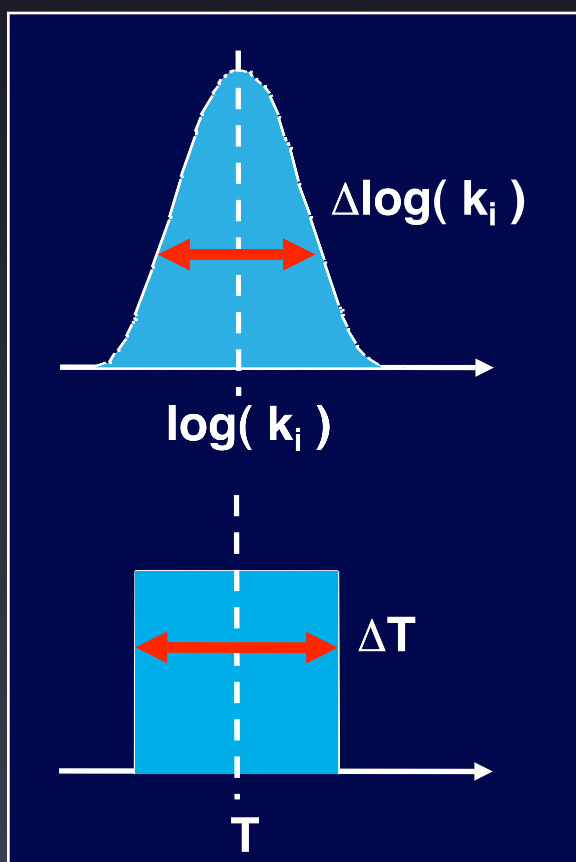
Sensitivity analysis

Theoretical error bars - Comparison with observations

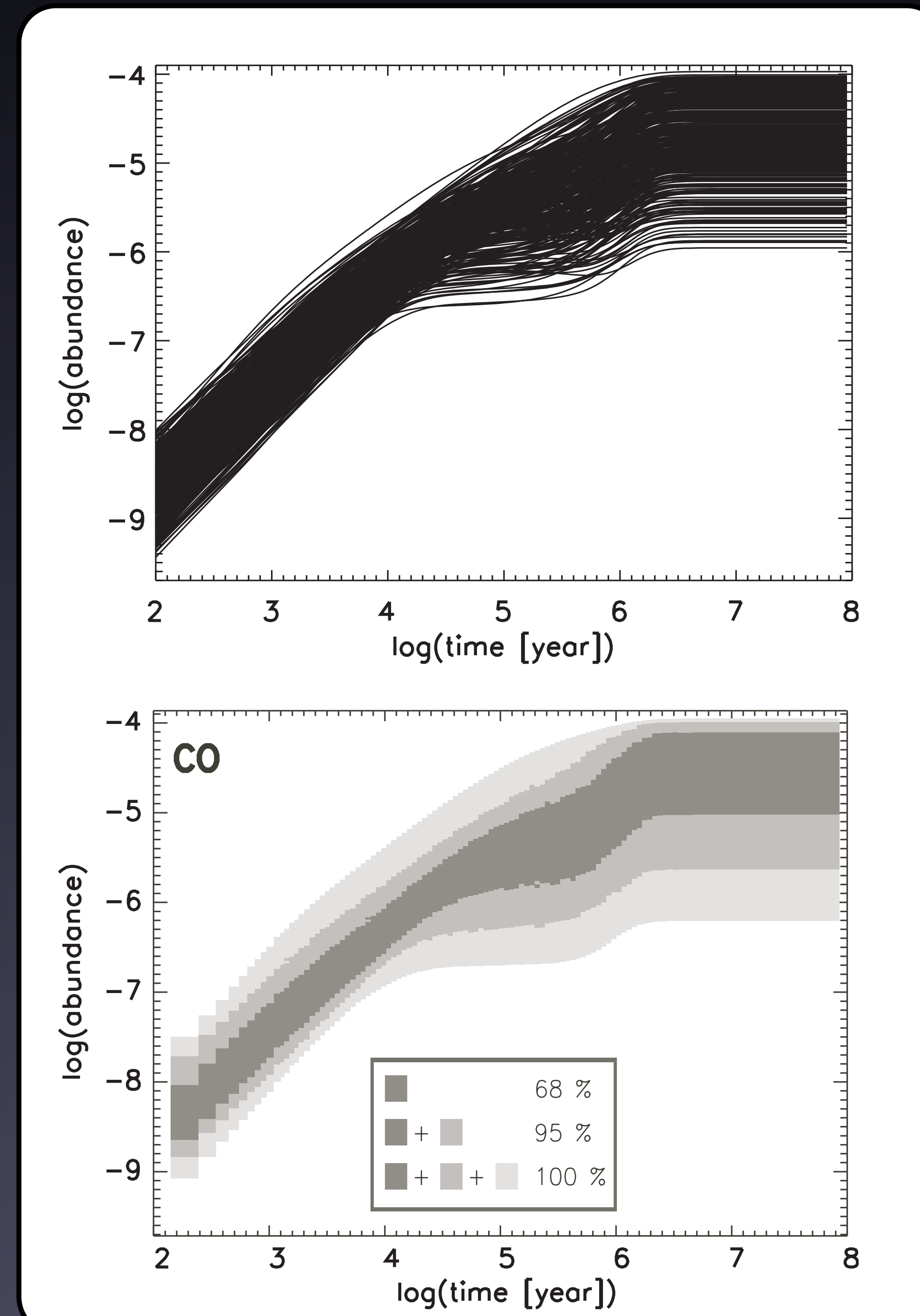
Reliability of the models Improvements / complexification

Sensitivity analysis

Parameter uncertainties
(k, T, n etc)



Monte-Carlo
simulations (thousands)



Wakelam, Selsis, Herbst & Caselli (2005)

Wakelam, Herbst & Selsis (2006)

Sensitivity analysis

Parameter uncertainties for a 0D gas-phase model:

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Theoretical error bars - Comparison with observations

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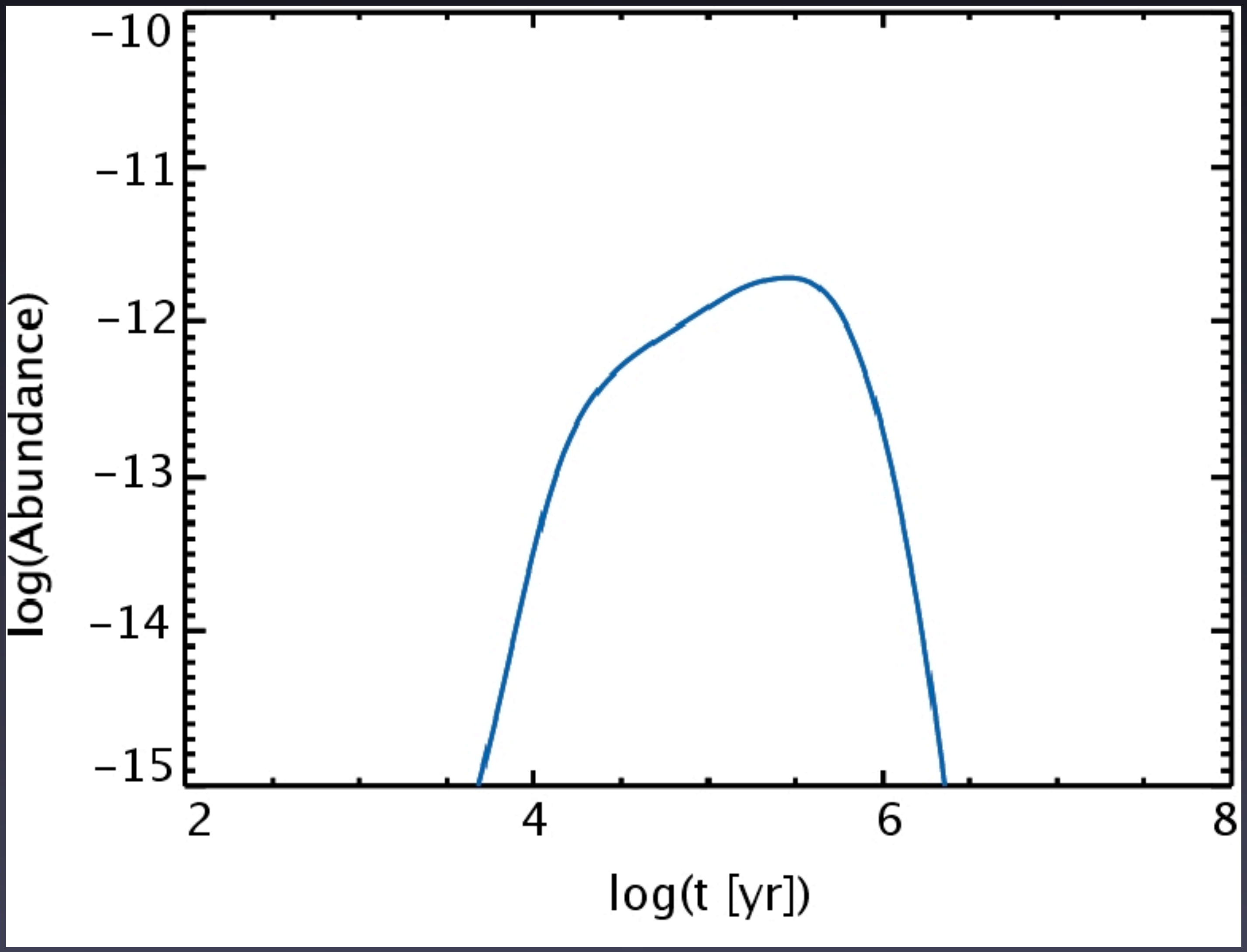
Theoretical error bars - Comparison with observations

Reliability of the models
Improvements / complexification

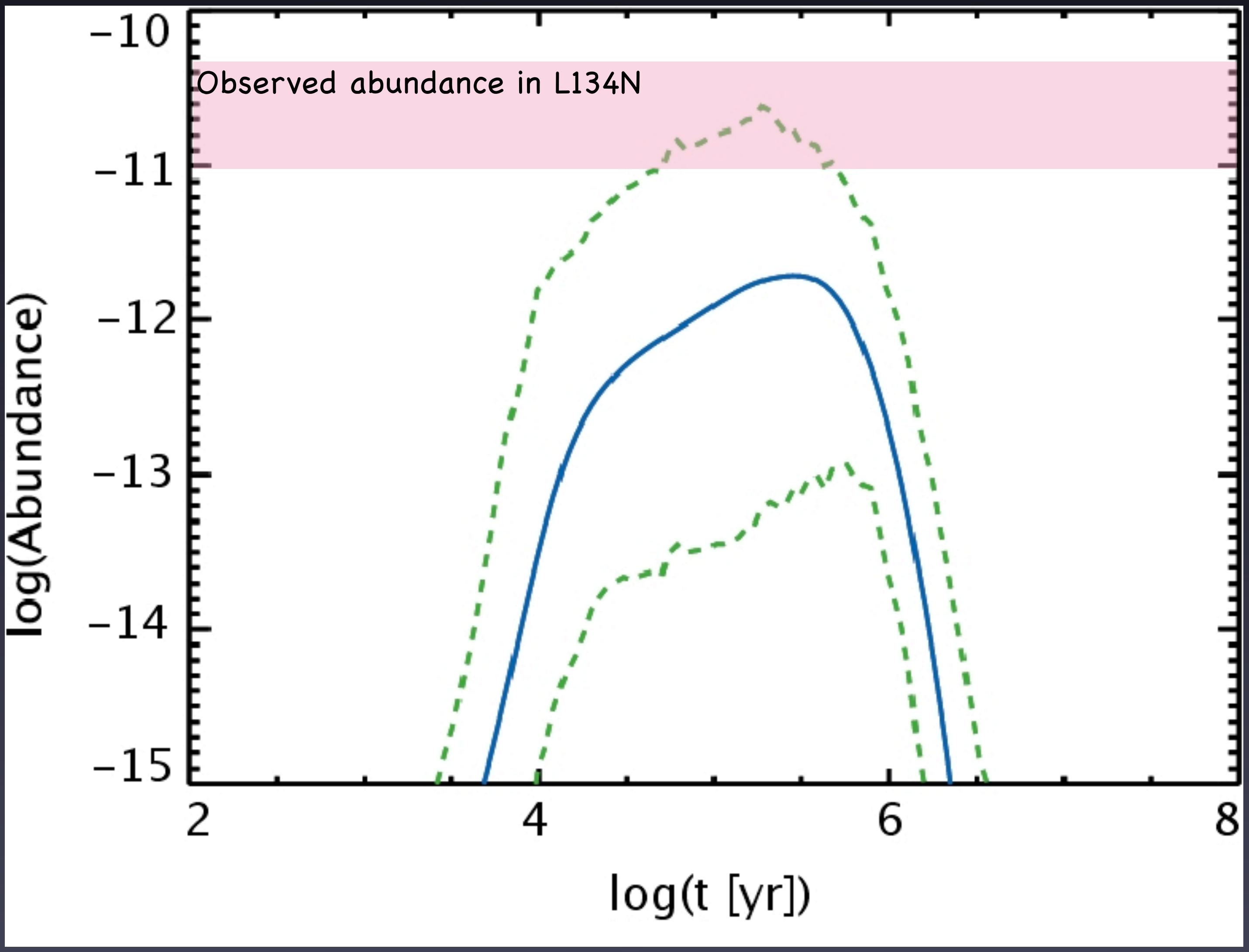
Error bars on model predictions

HC_7N abundance is a typical dense cloud



Error bars on model predictions

HC_7N abundance is a typical dense cloud -
with error bars dues to rate coefficient uncertainties



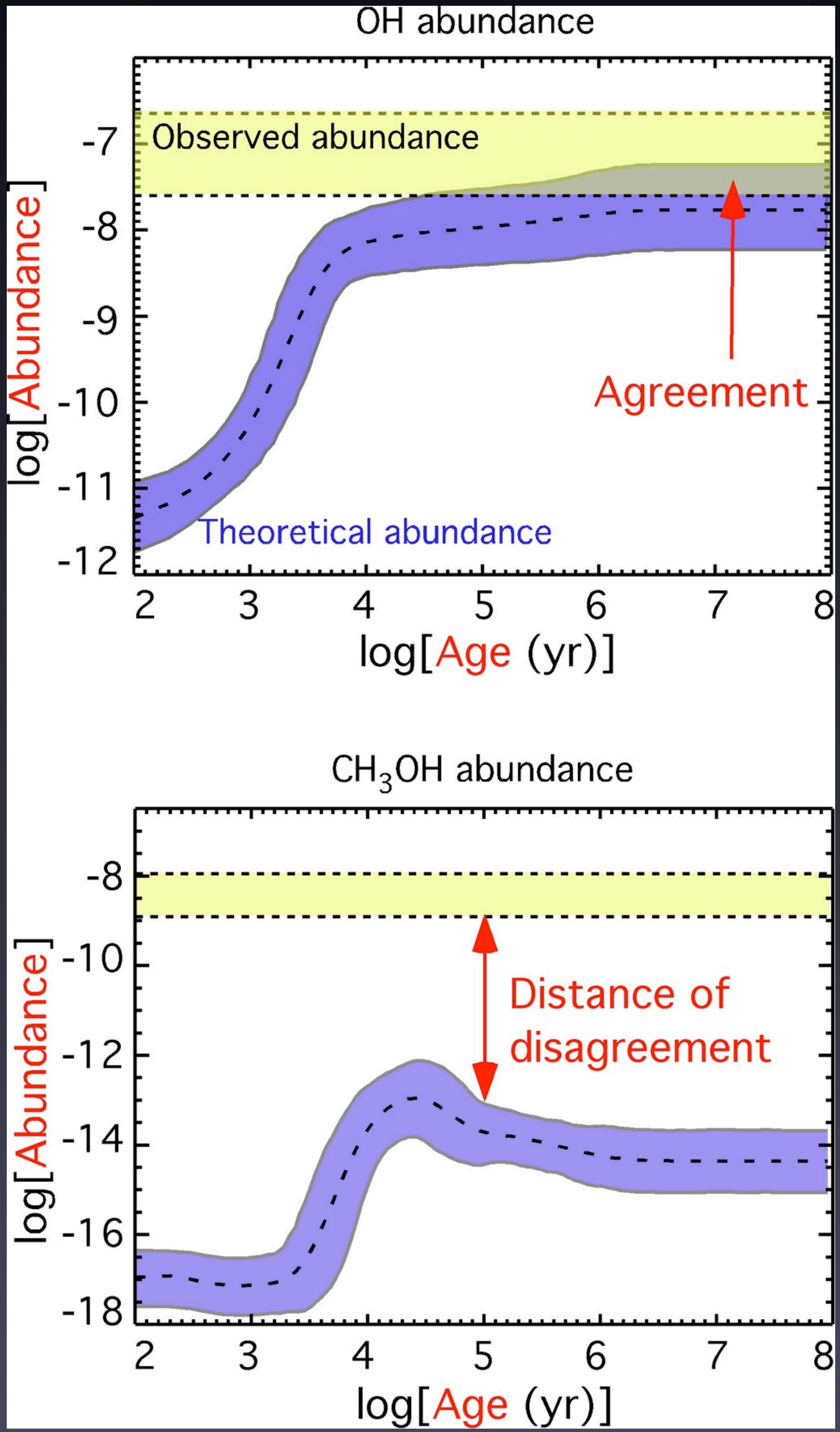
Wakelam, Herbst & Selsis (2006)

Error bars on model predictions

Objectives:

- Find which species are really not reproduced by the model to look for missing processes or wrong chemistry

- Constrain "best models" (i.e. sets of parameters)



Sensitivity analysis

Parameter uncertainties for a 0D gas-phase model:

Gas temperature and density, elemental abundances, initial conditions, cosmic-ray ionization rate (ζ), reaction rate coefficients

Sensitivity analysis

Theoretical error bars - Comparison with observations

Reliability of the models Improvements / complexification

Sensitivity analysis

Parameter uncertainties for a 0D gas-phase model:

Gas temperature and density, elemental abundances, initial conditions, cosmic-ray ionization rate (ζ), reaction rate coefficients

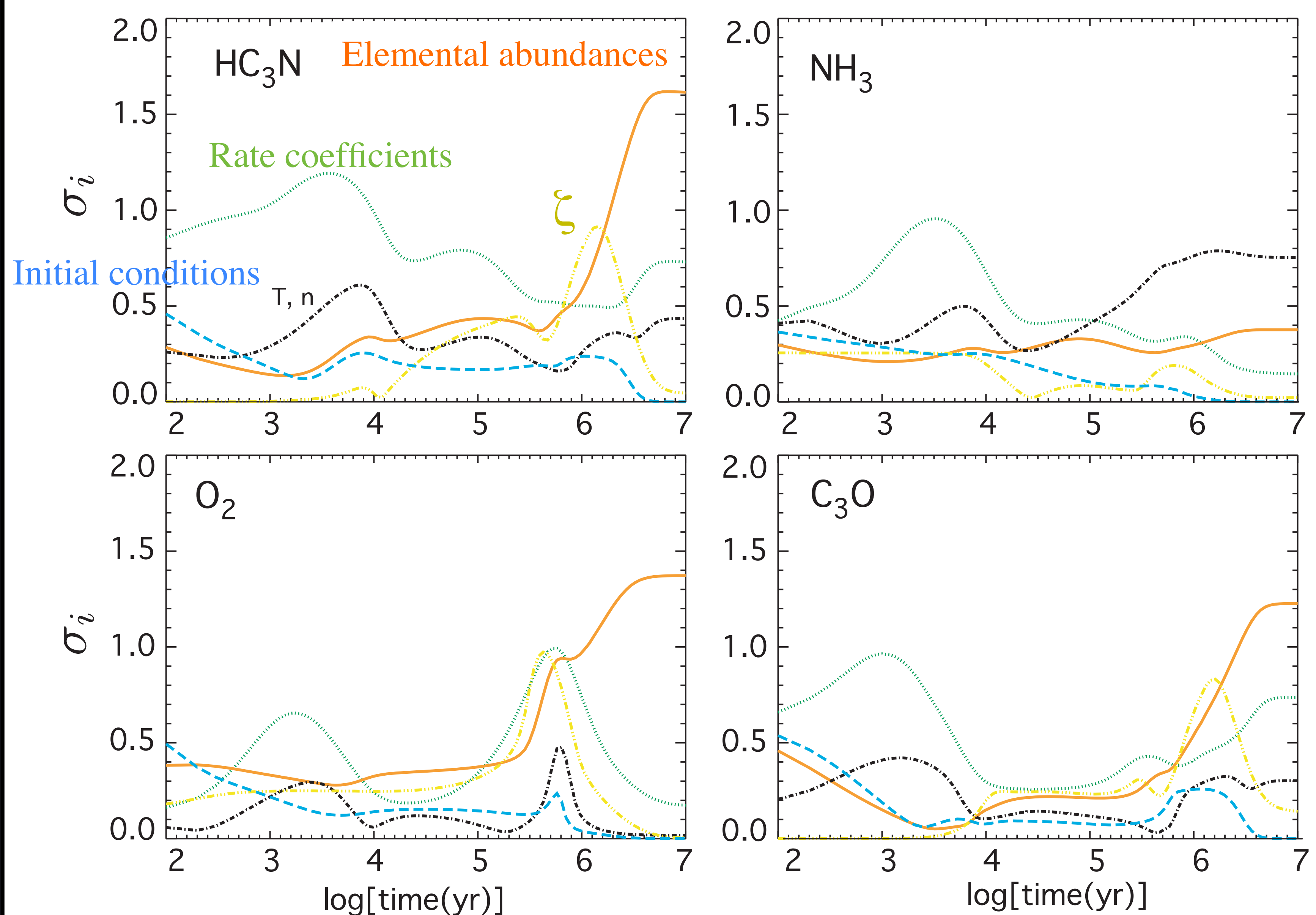
Sensitivity analysis

Theoretical error bars -
Comparison with observations

Reliability of the models
Improvements / complexification

Sensitivity analysis

Sum of the standard deviations on the abundance species obtained varying the parameters



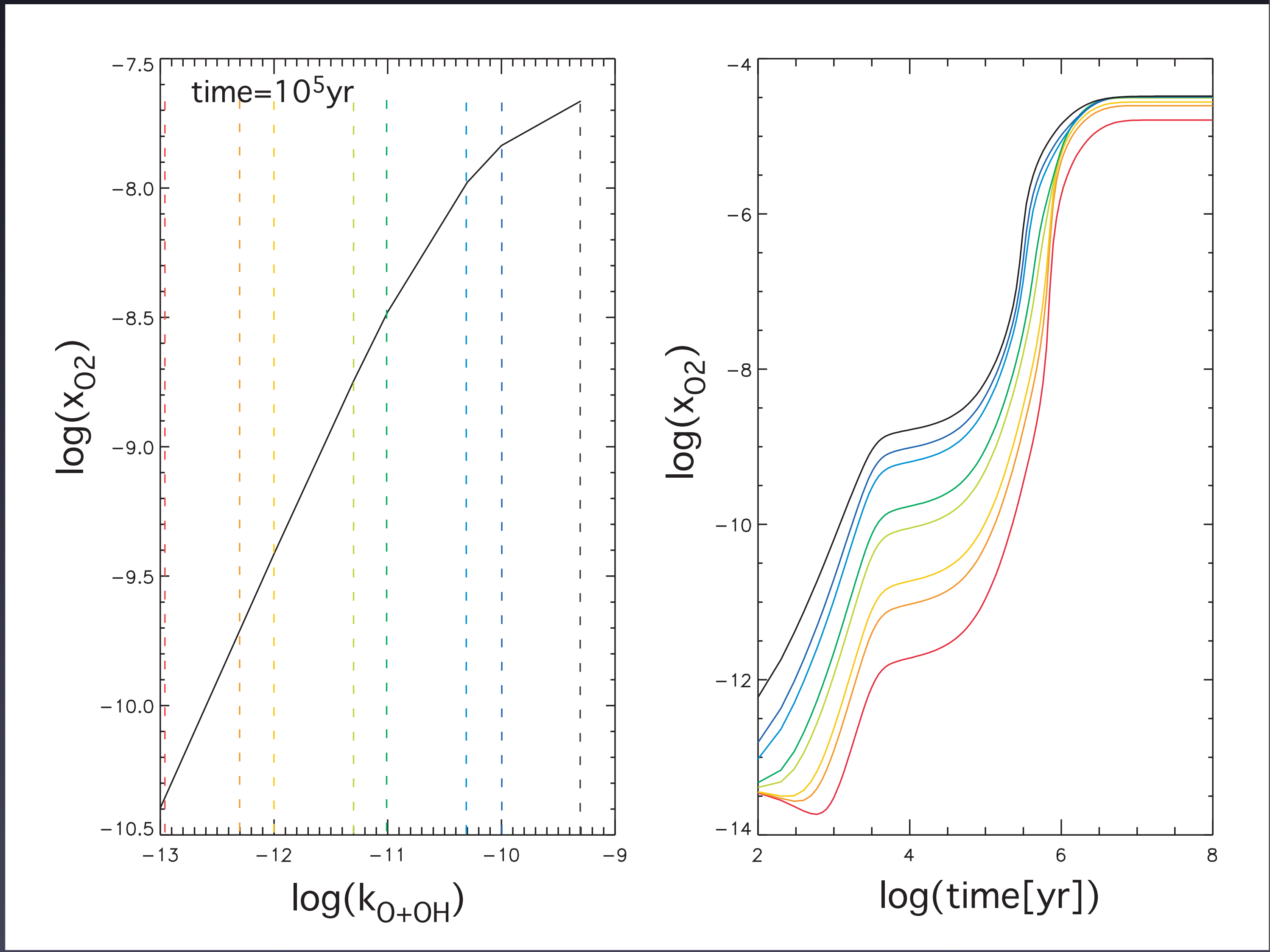
Wakelam et al. (2010)

What is a key reaction?

Answer 1 : A reaction that forms or destroys the most a species

Example of the main reaction forming O_2: O + OH -> O_2 + H

O2 abundance is not much changed if the rate coefficient is changed.



Dark cloud conditions see also Quan, Herbst et al. (2008)

What is a key reaction?

Answer 2: A reaction which rate coefficient quantitatively changes the model predictions

Two philosophies:
- Important for specific species
- Important for the model in general (reactions affecting many species)

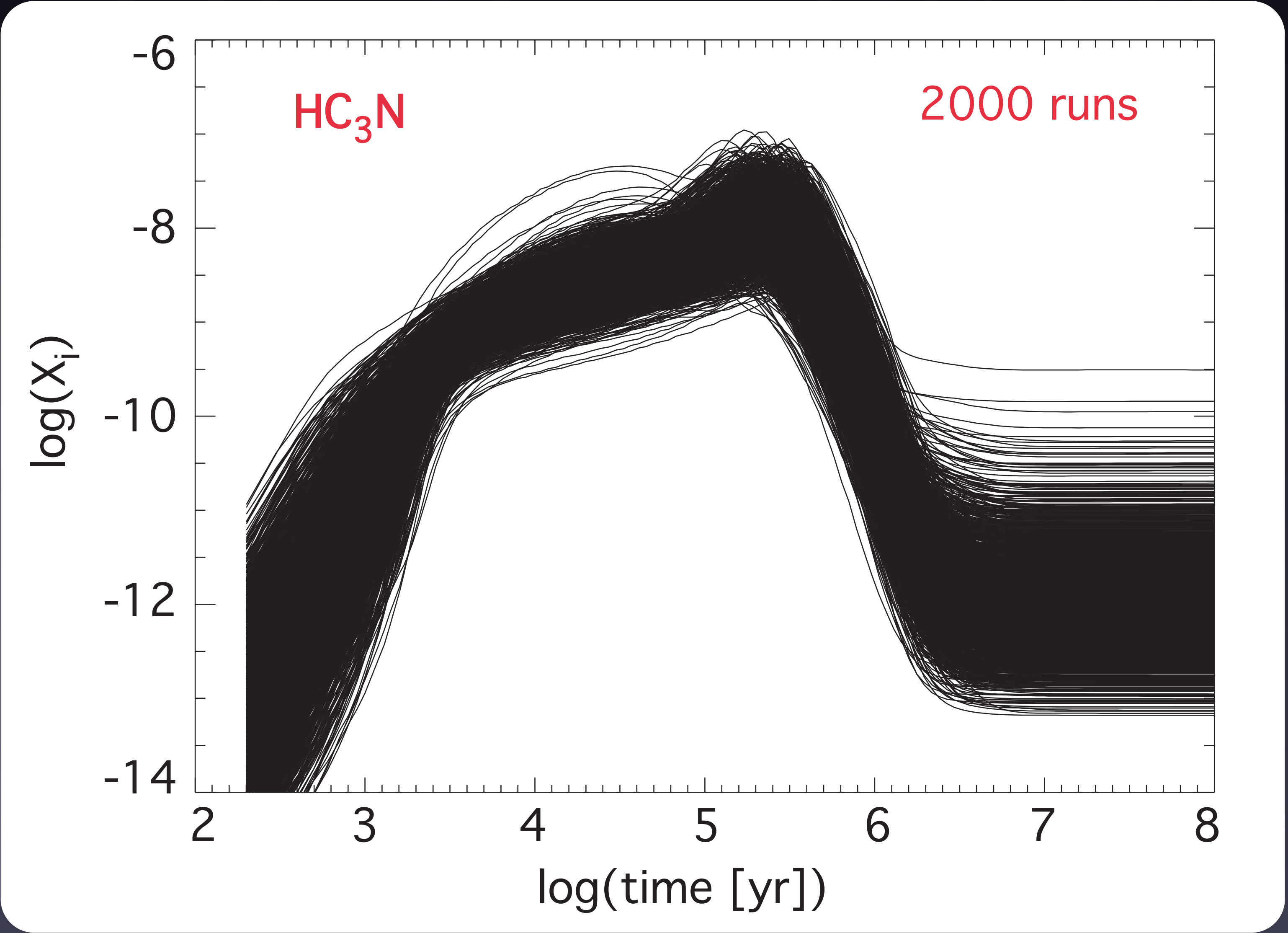
Needs to define :
- the chemical network
- the astronomical object
- the time

Identification of "key" reactions

- Monte-Carlo simulations

- Variations of the rate coefficients within a certain range

- Computation of the Pearson correlation coefficients $P^i_j(t)$ (larger P -> stronger correlation)



$$P^i_j(t) = \frac{\sum^l (\log(X^l_j(t)) - \overline{\log(X_j(t))})(\log(k^l_i) - \overline{\log(k_i)})}{\sqrt{(\sum^l (\log(X^l_j(t)) - \overline{\log(X_j(t))})^2 \sum^l (\log(k^l_i) - \overline{\log(k_i)})^2}},$$

The International Space Science Institute Team

Identification of key reactions

↓

Review on the existing data

↓

New values proposed with uncertainties

↓

Impact on the model predictions

INTERNATIONAL SPACE SCIENCE INSTITUTE

International Team of the
International Space Science Institute 2008
http://www.issibern.ch/teams/HSOALMA/

Review paper in Space Science Reviews (2010, 156, 13): Wakelam, Smith, Herbst, Troe, Geppert, Linnartz, Öberg, Roueff, Agùndez, Pernot, Cuppen, Loison, Talbi

Key reactions for dark cloud conditions

Table 3 List of key reactions by number of species influenced.

Reaction	Strongly affected species[1]
$C + H_2 \rightarrow CH_2 + h\nu$	73
$CH_3^+ + H_2 \rightarrow CH_5^+ + h\nu$	18
$C_2H_2^+ + H_2 \rightarrow C_2H_4^+ + h\nu$	C_2H_2O, C_2H_3, $C_2H_2^+$, C_2HO^+, $C_2H_2N^+$, $C_2H_4^+$
$CH_3^+ + CO \rightarrow C_2H_3O^+ + h\nu$	C_2H_2O, $C_2H_3O^+$
$C_2H_4^+ + e^- \rightarrow C_2H_3 + H$	C_2H_2O, C_2H_3
$HSiO^+ + e^- \rightarrow SiO + H$	Si, SiO
$HSiO^+ + e^- \rightarrow Si + OH$	Si, SiO
$C_3H^+ + H_2 \rightarrow C_3H_3^+ + h\nu$	C_3H_2, H_2C_3, C_3H^+, $C_3H_2^+$, $C_3H_3^+$, $H_3C_3^+$
$C_3H^+ + H_2 \rightarrow H_3C_3^+ + h\nu$	C_3H_2, H_2C_3, C_3H^+, $C_3H_2^+$, $C_3H_3^+$, $H_3C_3^+$
$CH_3^+ + HCN \rightarrow C_2H_4N^+ + h\nu$	C_2H_2N, HC_3N, C_2H_3N, $C_2H_4N^+$
$C_4H_2^+ + H \rightarrow C_4H_3^+ + h\nu$	C_4H_2, C_5H, C_6H_6, $C_4H_3^+$
$CH_3^+ + NH_3 \rightarrow CH_6N^+ + h\nu$	CH_3N, CH_5N
$C_4H_2^+ + O \rightarrow HC_4O^+ + H$	C_3O, HC_4O^+

Table 4 List of key reactions for specific species

Neutral-Neutral reactions	Affected species
$C + C_3O \rightarrow C_3 + CO$	C_3O
$C + OCN \rightarrow CO + CN$	OCN
$H + CH_2 \rightarrow CH + H_2$	CH
$O + CN \rightarrow CO + H$	CN
$N + CN \rightarrow C + N_2$	CN
$O + NH \rightarrow NO + H$	NH
$O + C_2 \rightarrow CO + C$	C_2
$O + C_2H \rightarrow CO + CH$	C_2H
$O + C_3H \rightarrow C_2H + CO$	C_3H
$N + C_3 \rightarrow CN + C_2$	C_3
$N + NO \rightarrow N_2 + O$	NO
$O + NH_2 \rightarrow HNO + H$	NH_2
$O + HNO \rightarrow NO_2 + H$	N_2O
$O + HNO \rightarrow N_2O + H$	N_2O
$CN + NH_3 \rightarrow NH_2CN + H$	NH_2CN
$O + C_3N \rightarrow CO + C_2N$	C_3N
$N + C_4N \rightarrow CN + C_3N$	C_4N
$N + C_4H \rightarrow C_4N + H$	C_4N
$N + C_2N \rightarrow CN + CN$	C_2N
$CN + HC_5N \rightarrow NC_6N + H$	NC_6N
$CN + HC_3N \rightarrow NC_4N + H$	NC_4N
Association reactions	**Affected species**
$C_4H_2^+ + HC_3N \rightarrow C_7H_3N^+ + h\nu$	HC_7N
$HS^+ + H_2 \rightarrow H_3S^+ + h\nu$	H_2S
$HCO^+ + H_2O \rightarrow CH_3O_2^+ + h\nu$	CH_2O_2
$C^+ + H_2 \rightarrow CH_2^+ + h\nu$	C_3
$S + CO \rightarrow OCS + h\nu$	OCS
$CH_3^+ + HC_3N \rightarrow C_4H_4N^+ + h\nu$	CH_3C_3N
$CH_3^+ + HC_5N \rightarrow C_6H_4N^+ + h\nu$	CH_3C_5N
$Si^+ + H_2 \rightarrow SiH_2^+ + h\nu$	HNSi
Ion-neutral reactions	**Affected species**
$C_2H_3^+ + O \rightarrow C_2H_2O^+ + H$	$C_2H_2O^+$
$C^+ + S \rightarrow S^+ + C$	H_2CS
$C_5H^+ + N \rightarrow C_5N^+ + H$	$C_5H_2N^+$, HC_5N
$C_2H_4^+ + N \rightarrow C_2H_2N^+ + H_2$	$C_2H_2N^+$
$C_4H_2^+ + S \rightarrow HC_4S^+ + H$	C_4S
$H_3^+ + C \rightarrow CH^+ + H_2$	C_3H_3
$H_3^+ + O \rightarrow OH^+ + H_2$	H_3O^+
$C_2H_3^+ + N \rightarrow C_2NH^+ + H_2$	C_2NH^+
Dissociative recombination	**Affected species**
$HC_4O^+ + e^- \rightarrow C_3O + CH$	C_3O
$H_2NC^+ + e^- \rightarrow HNC + H$	HNC, H_2NC^+
$C_5H_2N^+ + e^- \rightarrow C_5N + H_2$	$C_5H_2N^+$
$HC_4S^+ + e^- \rightarrow C_4S + H$	C_4S
$H_2CO^+ + e^- \rightarrow CO + H + H$	H_2CO^+
$CNC^+ + e^- \rightarrow CN + C$	CNC^+
$HC_4S^+ + e^- \rightarrow C_4S + H$	C_4S
$HC_3S^+ + e^- \rightarrow C_3S + H$	C_3S
$HC_3S^+ + e^- \rightarrow C_2S + CH$	C_3S

Key reactions for dark cloud conditions

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$CH_3^+ + CO \rightarrow C_2H_3O^+ + h\nu$	C_2H_2O, $C_2H_3O^+$
$C_2H_4^+ + e^- \rightarrow C_2H_3 + H$	C_2H_2O, C_2H_3
$HSiO^+ + e^- \rightarrow SiO + H$	Si, SiO
$HSiO^+ + e^- \rightarrow Si + OH$	Si, SiO
$C_3H^+ + H_2 \rightarrow C_3H_3^+ + h\nu$	C_3H_2, H_2C_3, C_3H^+, $C_3H_2^+$, $C_3H_3^+$, $H_3C_3^+$
$C_3H^+ + H_2 \rightarrow H_3C_3^+ + h\nu$	C_3H_2, H_2C_3, C_3H^+, $C_3H_2^+$, $C_3H_3^+$, $H_3C_3^+$
$CH_3^+ + HCN \rightarrow C_2H_4N^+ + h\nu$	C_2H_2N, HC_3N, C_2H_3N, $C_2H_4N^+$
$C_4H_2^+ + H \rightarrow C_4H_3^+ + h\nu$	C_4H_2, C_5H, C_6H_6, $C_4H_3^+$
$CH_3^+ + NH_3 \rightarrow CH_6N^+ + h\nu$	CH_3N, CH_5N
$C_4H_2^+ + O \rightarrow HC_4O^+ + H$	C_3O, HC_4O^+

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$O + CN \rightarrow CO + H$	CN
$N + CN \rightarrow C + N_2$	CN
$O + NH \rightarrow NO + H$	NH
$O + C_2 \rightarrow CO + C$	C_2
$O + C_2H \rightarrow CO + CH$	C_2H
$O + C_3H \rightarrow C_2H + CO$	C_3H
$N + C_3 \rightarrow CN + C_2$	C_3
$N + NO \rightarrow N_2 + O$	NO
$O + NH_2 \rightarrow HNO + H$	NH_2
$O + HNO \rightarrow NO_2 + H$	N_2O
$O + HNO \rightarrow N_2O + H$	N_2O
$CN + NH_3 \rightarrow NH_2CN + H$	NH_2CN
$O + C_3N \rightarrow CO + C_2N$	C_3N
$N + C_4N \rightarrow CN + C_3N$	C_4N
$N + C_4H \rightarrow C_4N + H$	C_4N
$N + C_2N \rightarrow CN + CN$	C_2N
$CN + HC_5N \rightarrow NC_6N + H$	NC_6N
$CN + HC_3N \rightarrow NC_4N + H$	NC_4N
Association reactions	**Affected species**
$C_4H_2^+ + HC_3N \rightarrow C_7H_3N^+ + h\nu$	HC_7N
$HS^+ + H_2 \rightarrow H_3S^+ + h\nu$	H_2S
$HCO^+ + H_2O \rightarrow CH_3O_2^+ + h\nu$	CH_2O_2
$C^+ + H_2 \rightarrow CH_2^+ + h\nu$	C_3
$S + CO \rightarrow OCS + h\nu$	OCS
$CH_3^+ + HC_3N \rightarrow C_4H_4N^+ + h\nu$	CH_3C_3N
$CH_3^+ + HC_5N \rightarrow C_6H_4N^+ + h\nu$	CH_3C_5N
$Si^+ + H_2 \rightarrow SiH_2^+ + h\nu$	HNSi
Ion-neutral reactions	**Affected species**
$C_2H_3^+ + O \rightarrow C_2H_2O^+ + H$	$C_2H_2O^+$
$C^+ + S \rightarrow S^+ + C$	H_2CS
$C_5H^+ + N \rightarrow C_5N^+ + H$	$C_5H_2N^+$, HC_5N
$C_2H_4^+ + N \rightarrow C_2H_2N^+ + H_2$	$C_2H_2N^+$
$C_4H_2^+ + S \rightarrow HC_4S^+ + H$	C_4S
$H_3^+ + C \rightarrow CH^+ + H_2$	C_3H_3
$H_3^+ + O \rightarrow OH^+ + H_2$	H_3O^+
$C_2H_3^+ + N \rightarrow C_2NH^+ + H_2$	C_2NH^+
Dissociative recombination	**Affected species**
$HC_4O^+ + e^- \rightarrow C_3O + CH$	C_3O
$H_2NC^+ + e^- \rightarrow HNC + H$	HNC, H_2NC^+
$C_5H_2N^+ + e^- \rightarrow C_5N + H_2$	$C_5H_2N^+$
$HC_4S^+ + e^- \rightarrow C_4S + H$	C_4S
$H_2CO^+ + e^- \rightarrow CO + H + H$	H_2CO^+
$CNC^+ + e^- \rightarrow CN + C$	CNC^+
$HC_4S^+ + e^- \rightarrow C_4S + H$	C_4S
$HC_3S^+ + e^- \rightarrow C_3S + H$	C_3S
$HC_3S^+ + e^- \rightarrow C_2S + CH$	C_3S

34 reactions studied in total

Proposed changes:

11/18 neutral-neutral

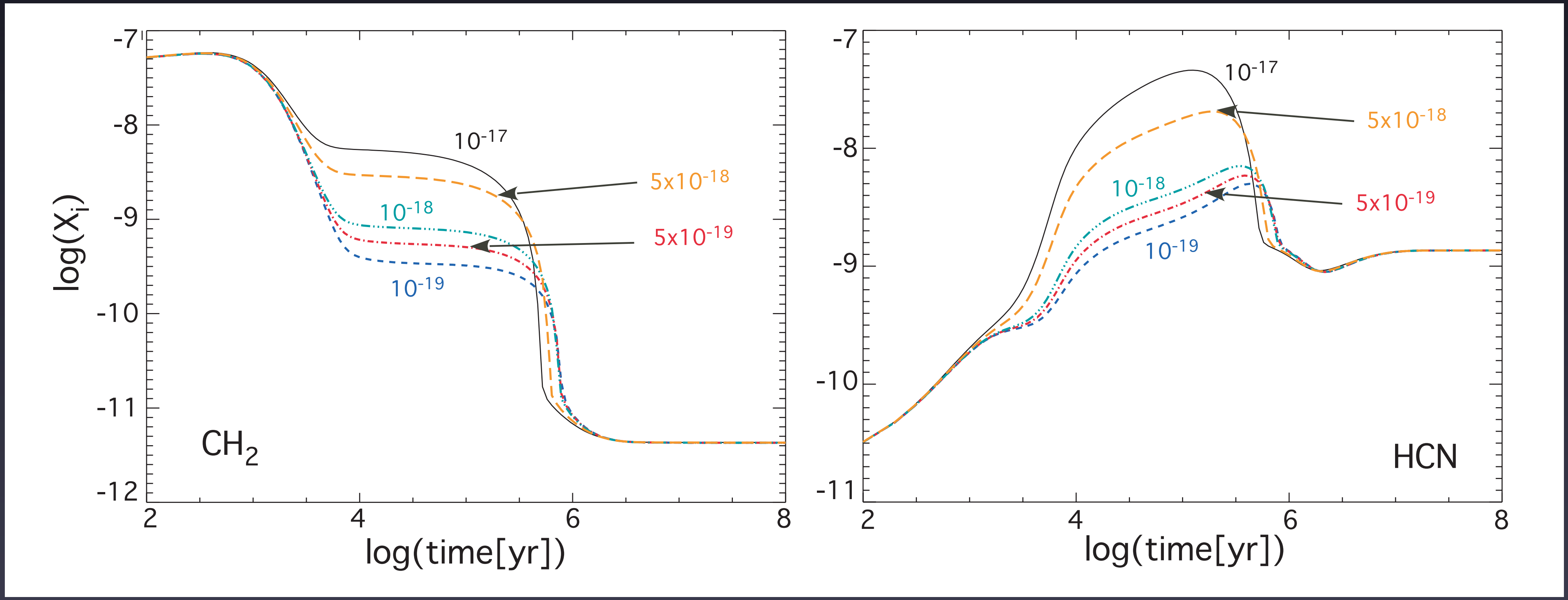
2/2 ion-neutral

5/5 association reactions

4/9 dissociative recombination

Identification of important reactions

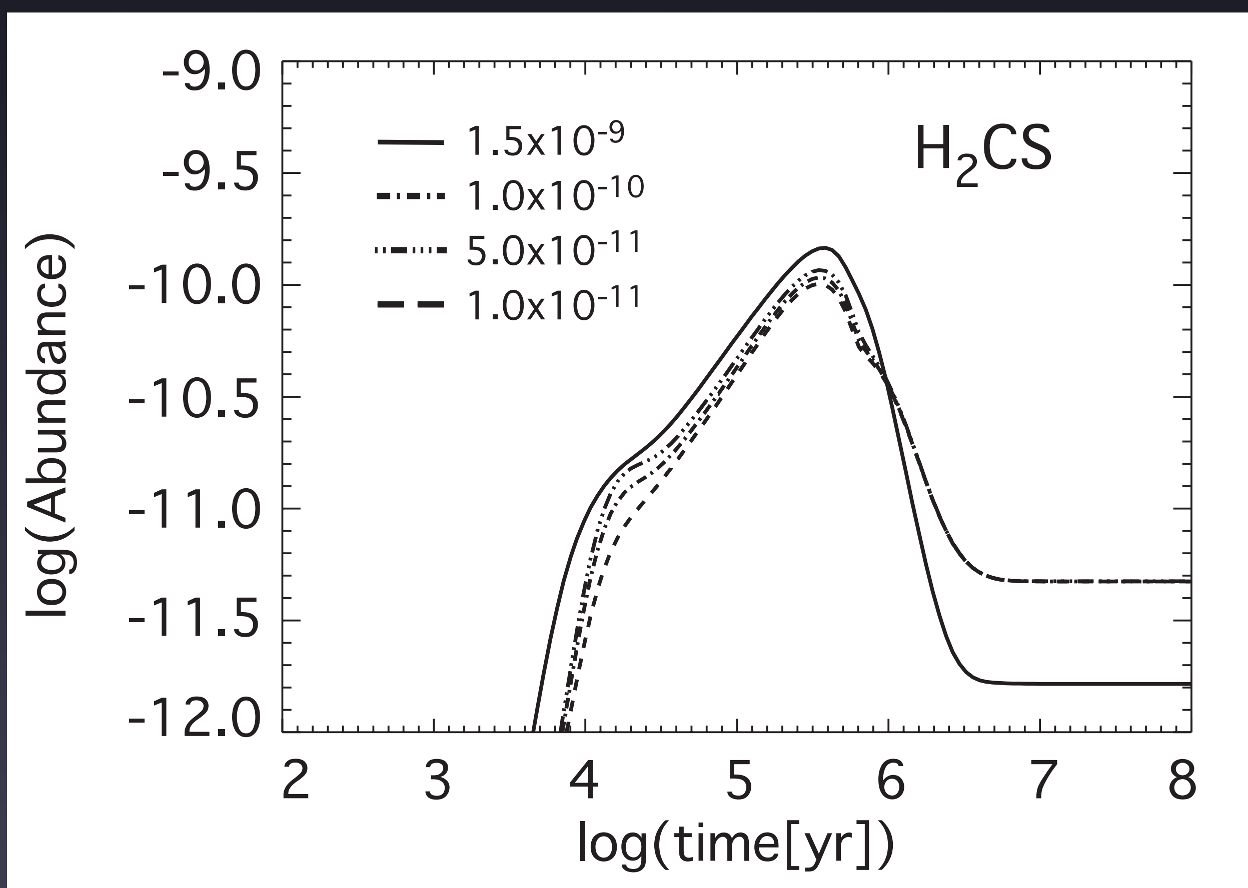
For dark cloud chemistry: $C + H_2 \rightarrow CH_2 + h\nu$ identified by Wakelam et al. (2010)



→ Detailed calculations are needed for this system (ongoing work)

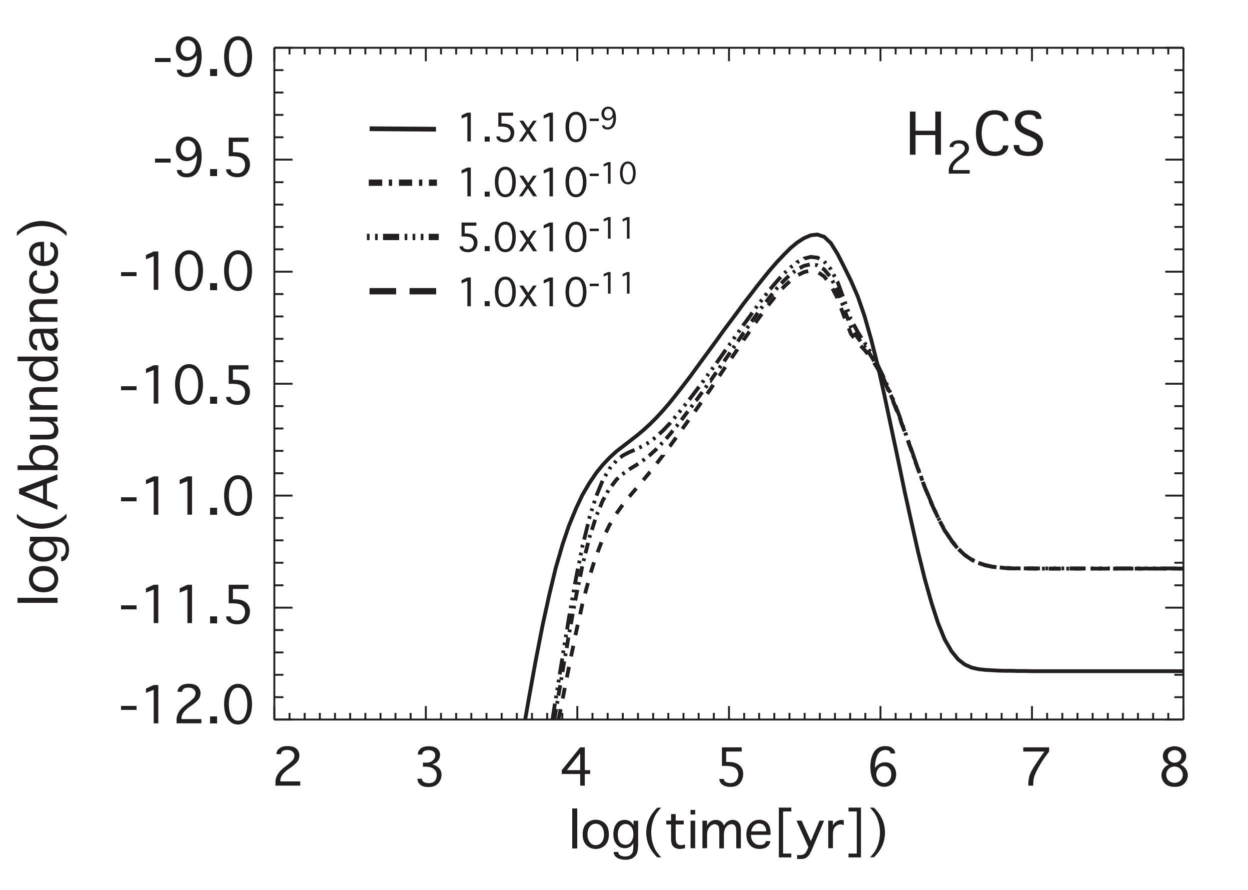
Combined effects:
$C + H_2 \rightarrow CH_2 + h\nu$ and $C^+ + S \rightarrow S^+ + C$

Different values for the rate coefficient of $C^+ + S \rightarrow S^+ + C$ ($C + H_2$: 10^{-17} s^{-1} cm^{-3})

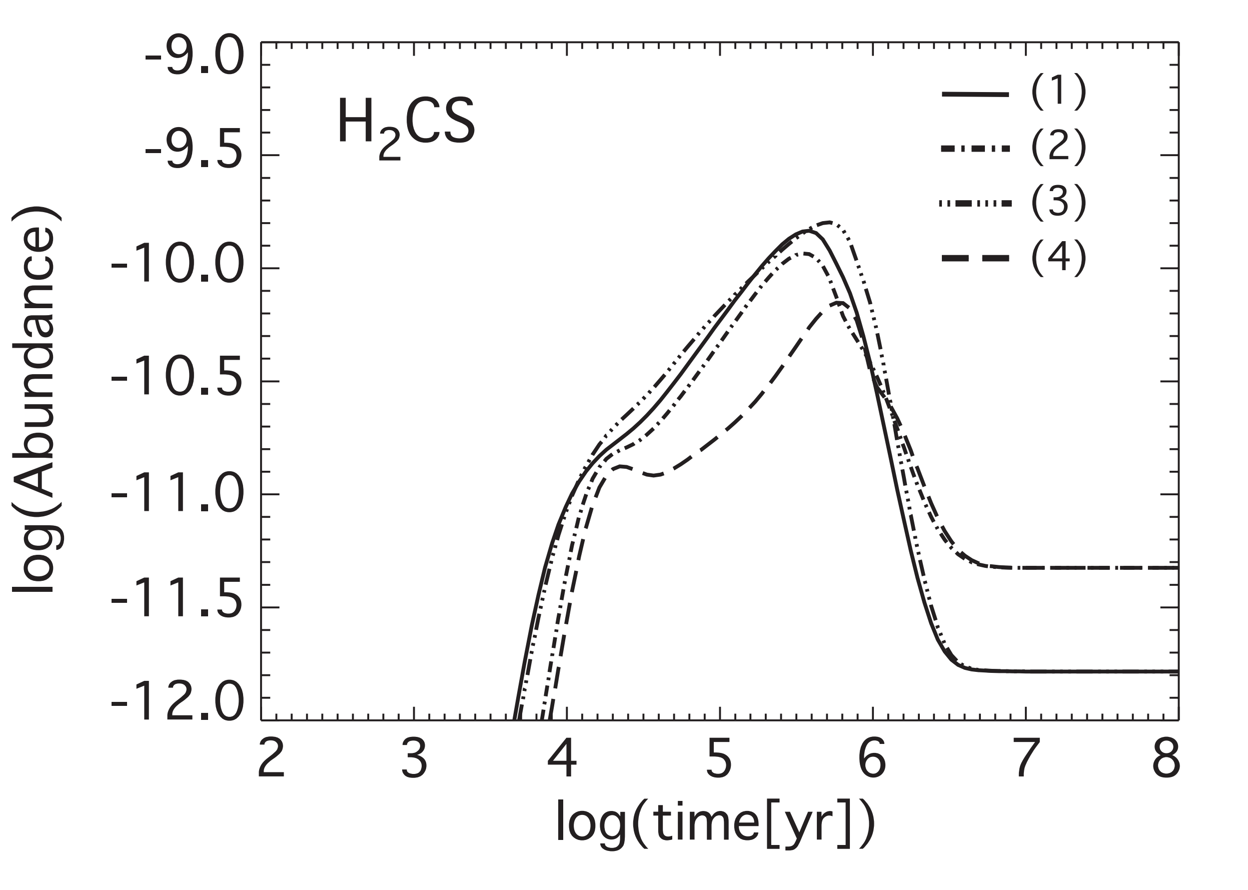


Combined effects:
$C + H_2 \rightarrow CH_2 + h\nu$ and $C^+ + S \rightarrow S^+ + C$

Different values for the rate coefficient of $C^+ + S \rightarrow S^+ + C$ ($C + H_2$: 10^{-17} s^{-1} cm^{-3})



Different values for both rate coefficients



(1) $C + H_2$: 10^{-17} $C^+ + S$: 1.5×10^{-9}

(2) $C + H_2$: 10^{-17} $C^+ + S$: 10^{-10}

(3) $C + H_2$: 10^{-18} $C^+ + S$: 1.5×10^{-9}

(4) $C + H_2$: 10^{-18} $C^+ + S$: 10^{-10}

Key reactions in different types of sources

Diffuse clouds :
Vasyunin et al., 2004 Astronomy Letters, 30, 566-576

Dense clouds:
Vasyunin et al., 2004 Astronomy Letters, 30, 566-576
Wakelam et al., 2009 A&A, 495, 513-521
Wakelam et al., accepted to Space Science Reviews

Hot cores:
Wakelam et al., 2005 A&A, 444, 883-891

Protoplanetary disks:
Vasyunin et al., 2008 ApJ, 672, 629-641

Titan atmopshere:
Dobrijévic et al., 2010 Advances and Space Research, 45, 77-91

Neptune atmosphere:
Dobrijévic et al., 2010 Planetary and Space Science, 58, 1555-1566

KInetic Database for Astrochemistry: KIDA

Existing databases

Interstellar medium :

UMIST/UDFA (http://www.udfa.net/), OSU (http://www.physics.ohio-state.edu/~eric/research.html)
Meudon databases (PdR, Shock ...)

Planetary atmospheres :

NASA-JPL Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies http://jpldataeval.jpl.nasa.gov/
Critical reviews from Journal of Physical and Chemical Reference Data (Atkinson et al., Baulch et al., Herron et al., Tsang et al.,...) http://www.nist.gov/srd/reprints.htm

General databases :

NIST http://kinetics.nist.gov/kinetics/index.jsp, Anicich (ion-neutral) - word or pdf documents

Photo-dissociations :

* Database from LISA http://w3.lisa.univ-paris12.fr/GPCOS/SCOOPweb/SCOOP.html
* Harvard-Smithsonian Center for Astrophysics Molecular Data http://www.cfa.harvard.edu/amp/tools.html
* MPI-Mainz-UV-VIS Spectral Atlas of Gaseous Molecules http://www.atmosphere.mpg.de/enid/2295
* science-softCon UV/Vis+ Spectra Data Base (UV/Vis+Photochemistry Database) http://www.uv-spectra.de/
* SWRI Photo cross sections and rate coefficients http://amop.space.swri.edu/

KInetic Database for Astrochemistry: KIDA

Motivations for a new database

☹ Updates of existing databases : nonexistant, partial or delayed

☹ Comprehensivity : Databases dedicated to a type of reactions, temperature domains or even astrophysical objects

☹ Format : online consultation only, word/pdf document

☹ Quality aspects : compilation of all existing data without quality information or unique data chosen by the administrator (not necessary an expert in the field)

KIDA

KInetic Database for Astrochemistry

http://kida.obs.u-bordeaux1.fr/

A kinetic database of gas-phase reactions for the chemistry in the interstellar medium and planetary atmospheres.

Online since May 2010 - about 130 unique visitor per month
Rate coefficients included little by little

KInetic Database for Astrochemistry: KIDA

KIDA
KInetic Database for Astrochemistry
Centralisation tool

Chemical models
(dense clouds, disk, Titan...)

Sensitivity Methods

Important reactions
(depends on the system and the chemical network)

Group of experts in chemistry

Review and propositions
for reference values

KIDA

Kinetic Database for Astrochemistry

KIDA is a database of kinetic data of interest for astrochemical (interstellar medium and planetary atmospheres) studies. In addition to the available referenced data, KIDA provides recommendations over a number of important reactions.

Chemists and physicists can add their data to the database through several paths listed here.
Astrophysicists can download the database through the download form. You need to log in to add or download data. Forms below allows to consult and download the data.

The website will be improved little by little so the database may not be accessible time to time. Data will also be implemented later in the database especially data for planetary atmospheres.

New data

New recommendations for the association reaction C2H2+ + H2

Previous news

Search for species data

Search by species name

Species name *

Formula   Inchi code   Exact

Search

Ex : H2O, NaOH, C+ , InChI=1S/OS/c1-2
Warning : Second letter of 2-letters elements have to be lowercase, eg Na

Search by element

Species contains the element *

positive ion   negative ion   neutral

Search

Ex : C will search for all species with C atoms
Ex : O H will search for all species with O or H atoms
Ex : OH will search for all species with O and H atoms
Warning : Second letter of 2-letters elements have to be lowercase, eg Na

Search for reactions

Indicate a species (ex: CH, H3O+) or a couple of species (ex: C + H2)

Species name*

Search in

Isomers   Exact formula

Reactant   Product   Both

Ion + neutral   Neutral

Compute rate coefficient at 10 K

Type of reaction

All

search

Download list of reactions

Download

KInetic Database for Astrochemistry

VAMDC | Europlanet | EARTHS

Home | Models | Detected Molecules | Help | Publications | Contact | Jobs | Credit | Sign In

Your search may contain lot of results. Try some of these tips to filter results :

Species name: O2

- (•) Isomers
- ( ) Exact formula

Isomers found :

- O2 : O2 ?

Specify reactant or product

- (•) Reactant
- ( ) Product
- ( ) Both

Specify ion or neutral

- (•) Ion + neutral
- ( ) Neutral

Specify a type of reaction: All

search

Search for reactions > Results of the search "O2"

If available, only recommended reaction rate coefficients are listed below. Click on details to see other values

Click on the blue icon to get details on the type of reaction and on the formula.

Help

Results for the search of reactions containing "O2"

52 result(s). (1 to 15).

First | Previous | 1 - 2 - 3 - 4 | Next | Last (4)

Type	Details	Reactants	Products	α	β	γ	F_0	g	Formula	k(10) * $cm^3 s^{-1}$	T (K) / UV Field *	Evaluation
AD		$O_2 + S^-$	$SO_2 + e^-$	3e-11	0e0	0e0	2	0	Kooij	3.00e-11	10 - 280	?
AD		$O_2 + C^-$	$CO_2 + e^-$	5e-11	0e0	0e0	2	0	Kooij	5.00e-11	10 - 280	?
CE		$O_2 + NH^+$	$NH + O_2^+$	4.5e-10	0e0	0e0	1.25	0	Kooij	4.50e-10	10 - 280	?
CE		$O_2 + N^+$	$N + O_2^+$	4e-10	0e0	0e0	1.25	0	Kooij	4.00e-10	10 - 280	?
CE		$O_2 + He^+$	$He + O_2^+$	3.3e-11	0e0	0e0	1.25	0	Kooij	3.30e-11	10 - 280	?
CE		$O_2 + H_2^+$	$H_2 + O_2^+$	8e-10	0e0	0e0	1.25	0	Kooij	8.00e-10	10 - 280	?
CE		$O_2 + CN^+$	$CN + O_2^+$	7.8e-10	0e0	0e0	1.25	0	Kooij	7.80e-10	10 - 280	?
CE		$O_2 + SO_2^+$	$SO_2 + O_2^+$	2.5e-10	0e0	0e0	1.25	0	Kooij	2.50e-10	10 - 280	?

$O + OH \rightarrow H + O_2$

Type of reaction:	Bimolecular reactions
Enthalpy of the channel	N/A
Status:	Reviewed between 150 - 500 and 10 - 50
Number of values:	7 (2 recommended , 4 waiting for approval)

Value's number	α	β	γ	F_0	g	Type of uncertainty	T Range (K)	Evaluation	Comments	Added By	Added On
1	4e-11	0e0	0e0	3	0	logn	10 - 50		0	J. LOISON	2010-12-09 23:33:44
2	3.5e-11	0e0	0e0	1.29	0	logn	39 - 142		0	V. WAKELAM	2009-03-27 09:19:20
3	2.4e-11	0e0	-110e0	1.2	50	logn	150 - 500		0	J. LOISON	2010-11-30 14:33:50
All									0		

See Waiting for approval values

Rate Coefficient | Recommendation | References | Comments

All values | Not recommended values | Not rated values | Recommended Values

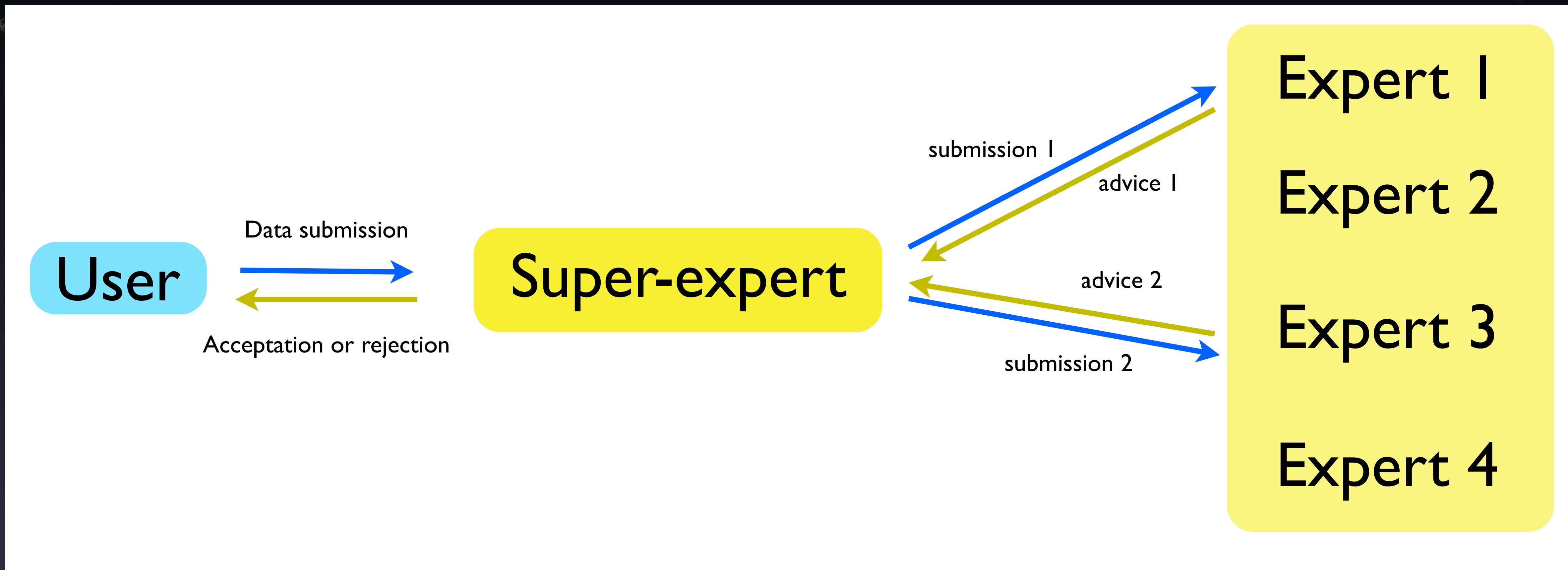
Value's number	Formula	k(10) cm^3s^{-1}	Method	Description	Origin	Evaluation	Authors
1	Kooij	4.00e-11	Reviews and Evaluations	KIDA experts recommendation ,see datasheet	Datasheet		
2	Kooij	3.50e-11	Measurements		Other database		Carty, D. et al
3	Kooij	1.44e-6	Reviews and Evaluations		Bibliography		Atkinson, R. et al

What can you do with KIDA?

- Consult existing data
- Comment on existing data
- Include your own data
- Propose recommendations
- Store your list of reactions as an ascii file for published models
- Download a list of reactions

Needs to be registered

KIDA Experts



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Dahbia Talbi
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Jürgen Troe
Roland Wester
Laurent Wiesenfeld

Datasheets

IUPAC format

Currently about 50 datasheets in KIDA

Authors:

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$O(^3P) + OH(X^2\Pi) \rightarrow H(^2S) + O_2(X^3\Sigma^-_g)$

Thermodynamic Data

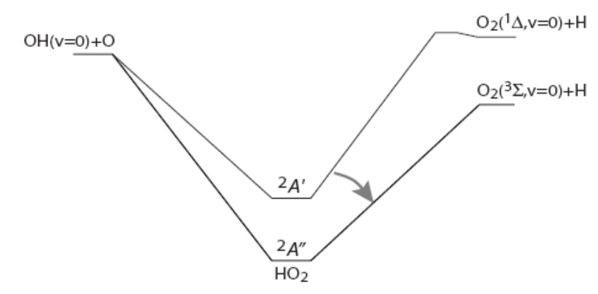
$\Delta H^o_{298} = -68.4$ kJ mol^{-1} (1)

Rate Coefficient Data *k*

k / cm^3 molecule^{-1} s^{-1}	T / K	Reference	Ref
Rate Coefficient Measurements			
k = $(3.85\pm0.13)\times10^{-11}\times(T/298)^{-(0.50\pm0.12)}$	250-515K	Howard and Smith, 1980-81	(2,3)
k = $(3.0\pm1.15)\times10^{-11}\times(T/298)^{-(0.36\pm0.07)}$	221-499	Lewis and Watson, 1980	(4)
$(3.1\pm0.5)\times10^{-11}$		Brune et al, 1983	(5)
k = $f_{el}\times3.7\times10^{-11}\times(T/298)^{-0.24}$	158-294K	Smith and Stewart, 1994	(6)
$f_{el}= 2/[\{5 + 3\exp(-228/T) + \exp(-326/T)\}\{2 + 2\exp(-205/T)]$			(7)
$(3.17\pm0.51)\times10^{-11}$	295	Robertson and Smith, 2002	(8)
k = $1.8\times10^{-11}\times(T/298)^{-0.32}\exp(177/T)$	136-377	Robertson and Smith, 2006	(9)
$(3.5\pm1.0)\times10^{-11}$	39-142K	Carty et al, 2006	(10)
Review			
k = $2.4\times10^{-11}\times\exp((110\pm50)/T)$	150-500K	Atkinson et al, 2004	(11)
Theory			
No expressions are given for theoretical calculations. The range of the calculations was in general quite wide (10-5000K).			
7×10^{-11}	10K	Harding *et al*, 2000	(12)
$0.026\times(T/1000)^{1.47} + 1.92\times(1000/T)^{0.46}$	300-5000K	Troe and Ushakov, 2001	(13)
5.4×10^{-13}	10K	Xu *et al*, 2007	(14)
7.8×10^{-12}	10K	Lin *et al*, 2008	(15)
4×10^{-11}	10K	Lique *et al*, 2009	(16)
4×10^{-11}	10K	Quéméner *et al*, 2009	(17)

Comments

The reaction $O + OH \rightarrow H + O_2$ is slightly exothermic (-68.4 kJ mol^{-1}). $O(^3P)$ + $OH(X^2\Pi)$ correlates with $3^2A'$ + $3^2A''$ + $3^4A'$ + $3^4A''$ surfaces. Only two surfaces ($^2A''$ + $^4A''$) correlate with the reaction products $H(^2S) + O_2(X^3\Sigma^-_g)$ but the $^4A''$ surface is purely repulsive. The $^2A'$ surface, populated without barrier from O + OH, correlates only with the excited $H + O_2$ $(a^1\Delta_g)$ product channel. So it is generally assumed that reaction only occurs over the lowest $^2A''$ surface which corresponds to the electronic ground state of the HO_2 intermediate. Nevertheless, temporary population of excited electronic states during the reaction may take place and influence the rate. (12,18,19)



The study of this reaction has attracted considerable experimental attention (2-6,8-10), and there have also been a large number

List of funding

The KIDA team acknowledges all the institues and countries participating in the development of this database.
List of agencies funding this project is available below.

European Research Council

Astronet

Seven Framework Program of the European Commission FP7

International Space Science Institute (Switzerland)

Agence Nationale de la Recherche (France)

Centre National de la Recherche Scientifique (France,PCMI and PNP)

University of Bordeaux (France)

Laboratoire d'Astrophysique de Bordeaux (France)

Observatoire Aquitain des Sciences de l'Univers

KInetic Database for Astrochemistry

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