Developing a New Taxonomy for Comets Based on Updated Molecular Abundances

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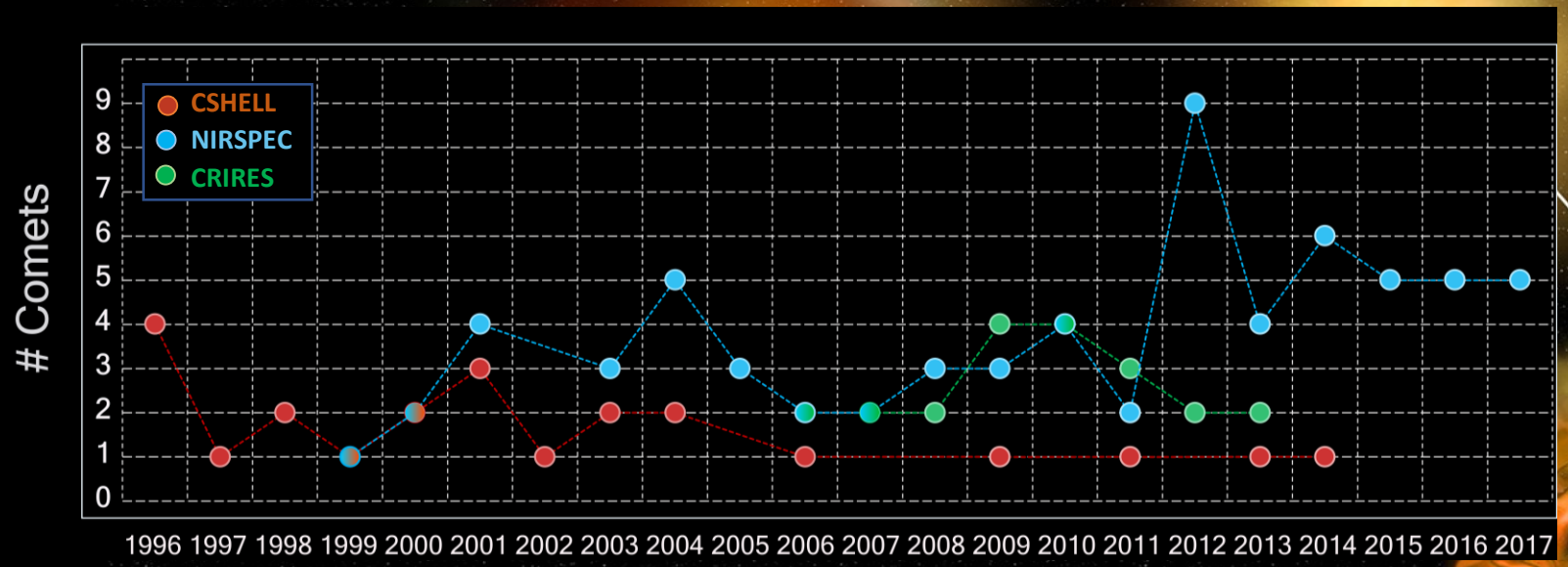
IR Spectra database



More than 60 comets observed from 1996 to 2017 with CSHELL, NIRSPEC and CRIRES

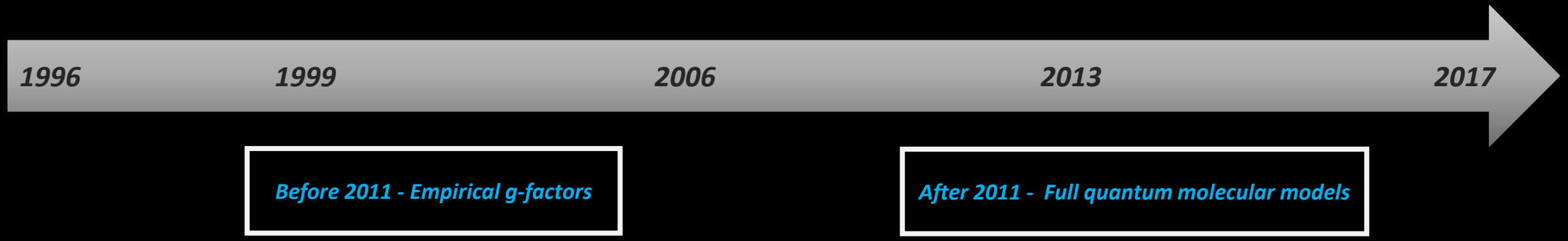
How does the composition vary among different comets?

How comets are related to the chemical composition of the protoplanetary disk?

What was/is the role of comets in the transportation of organics and water within our Solar System?

IR observations of comets from 1996 to 2017

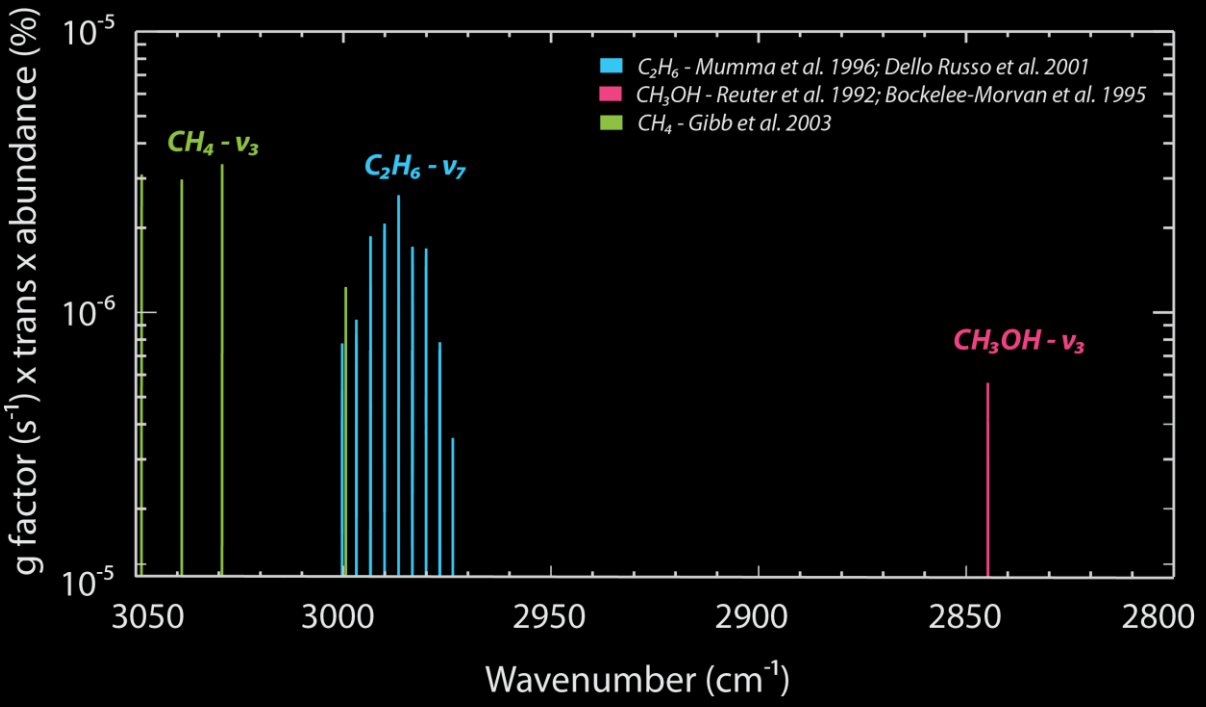
Data in the literature may contain systematic errors introduced by the evolving ability to observe and analyze high-resolution spectra of comets at infrared wavelengths



Updated molecular models

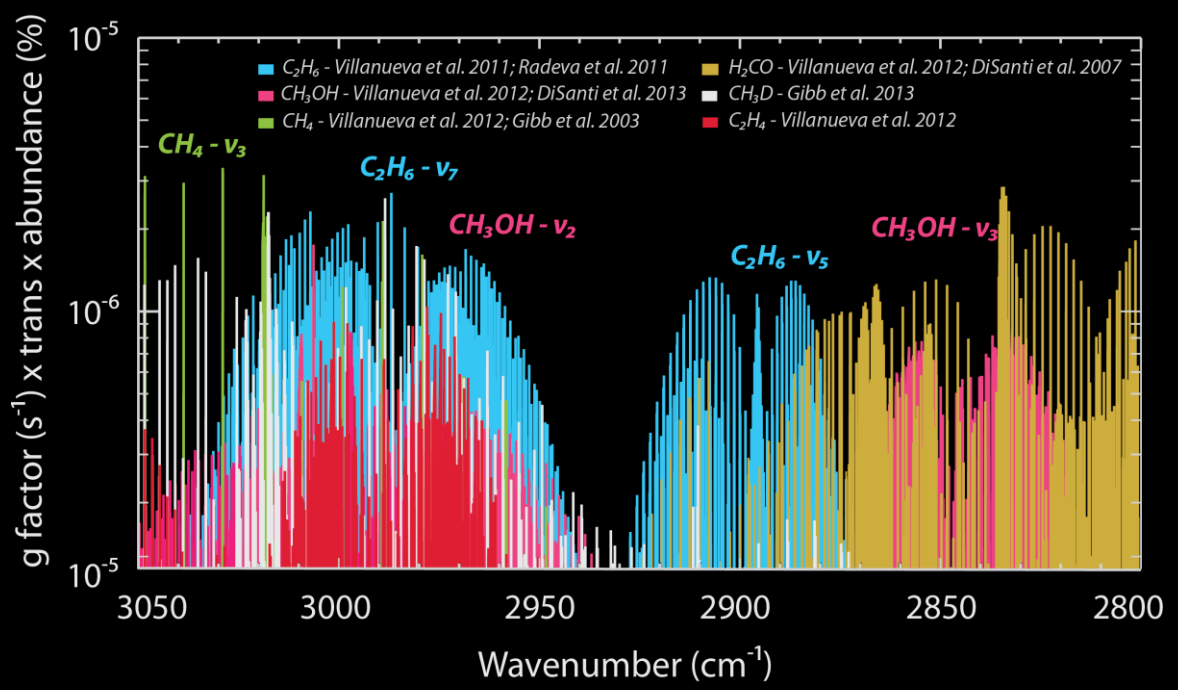
Before 2011

Empirical g-factors



After 2011

Quantum molecular models



Updated atmospheric models

SSP
Spectrum Synthesis Program (Kunde and Maguire 1974) accessing the **HITRAN 1992** (Rothman 1992)

LBLRTM
line-by-line radiative transfer model *(Clough et al 2005)* Accessing **HITRAN 1992** and **HITRAN 2008**

PUMAS
Planetary and Universal Model of Atmospheric Scattering that make use of **MERRA-2** (NASA Modern-Era Retrospective Analysis for Research and Applications) *(Villanueva et al. 2018, Gelaro et al., 2018)*

GENLN2
General Line-by-line Atmospheric Transmittance and Radiance Model *(Edwards 1992)*

2012: Incorporation of complete, and comprehensive databases for H_2O, C_2H_6, and CO *(Villanueva et al. 2012b, Villanueva et al. 2011b, Villanueva et al. 2008a)*

IR observations of comets from 1996 to 2017

Possible instrumental/observational and analysis biases.

Using a robust and common set of analytical tools we can now correct for data reduction related systematic errors and apply a reliable statistic to the results to build a new cometary taxonomy

Improving observations, reduction and analysis and interpretation of the cometary data

Before 2011 - Empirical g-factors

After 2011 - Full quantum molecular models

SSP + HITRAN 1992 GENLINE

2005: LBRTM + HITRAN 1992

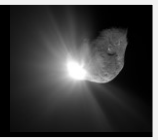
2008: LBRTM + HITRAN 2008

Incorporation of updated molecular databases

PUMAS + MERRA-2

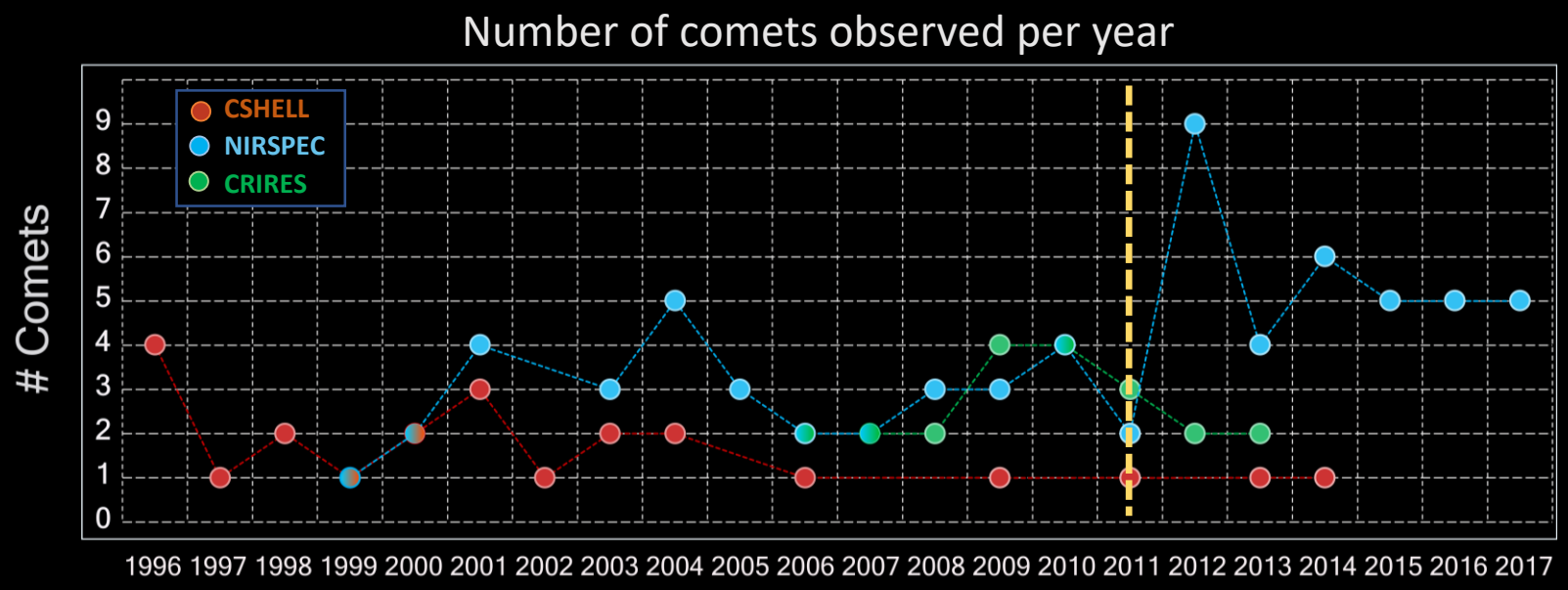
2004 - 2011 – Stardust

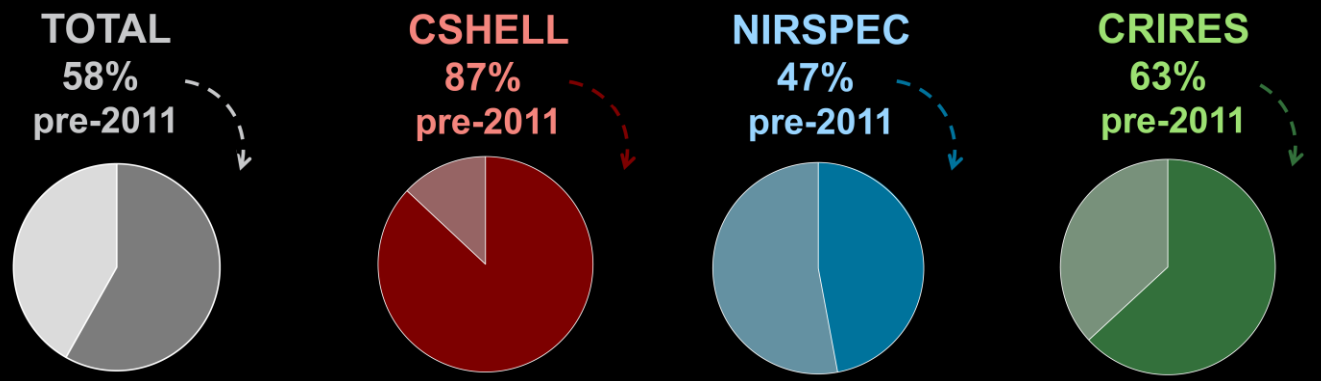
2005 – 2010 Deep impact



2014 - 2016 – Rosetta

Comet Database



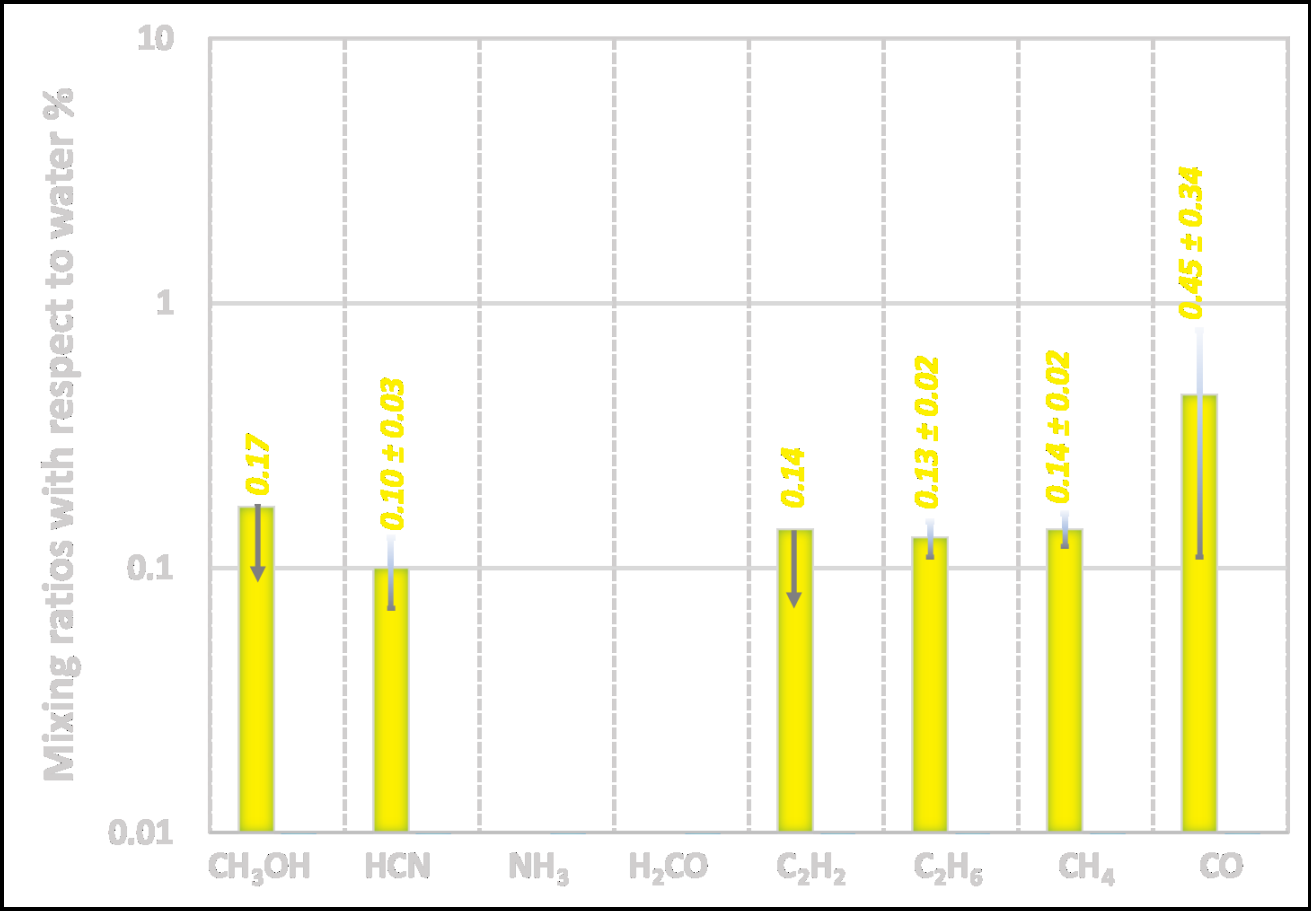


More than 60 comets observed from 1996 to 2017 with CSHELL, NIRSPEC and CRIRES

Considering 2011 as representative of the transition from empirical g-factors to quantum molecular models, at least 58% of the results need to be revised

C/1999 S4: a case study

Observing date: 13 July 2000



Rotational temperatures (K)			
Molecule	Mumma et al. 2001		
H_2O	50 (assumed)		

Water production rate (10^{26} mol/s)			
Setting	Mumma et al. 2001		
KL1			
KL2			
MW	446 ± 72		

KL1 ~3370 cm^{-1}; KL1 ~3440 cm^{-1}; MW ~2150 cm^{-1}

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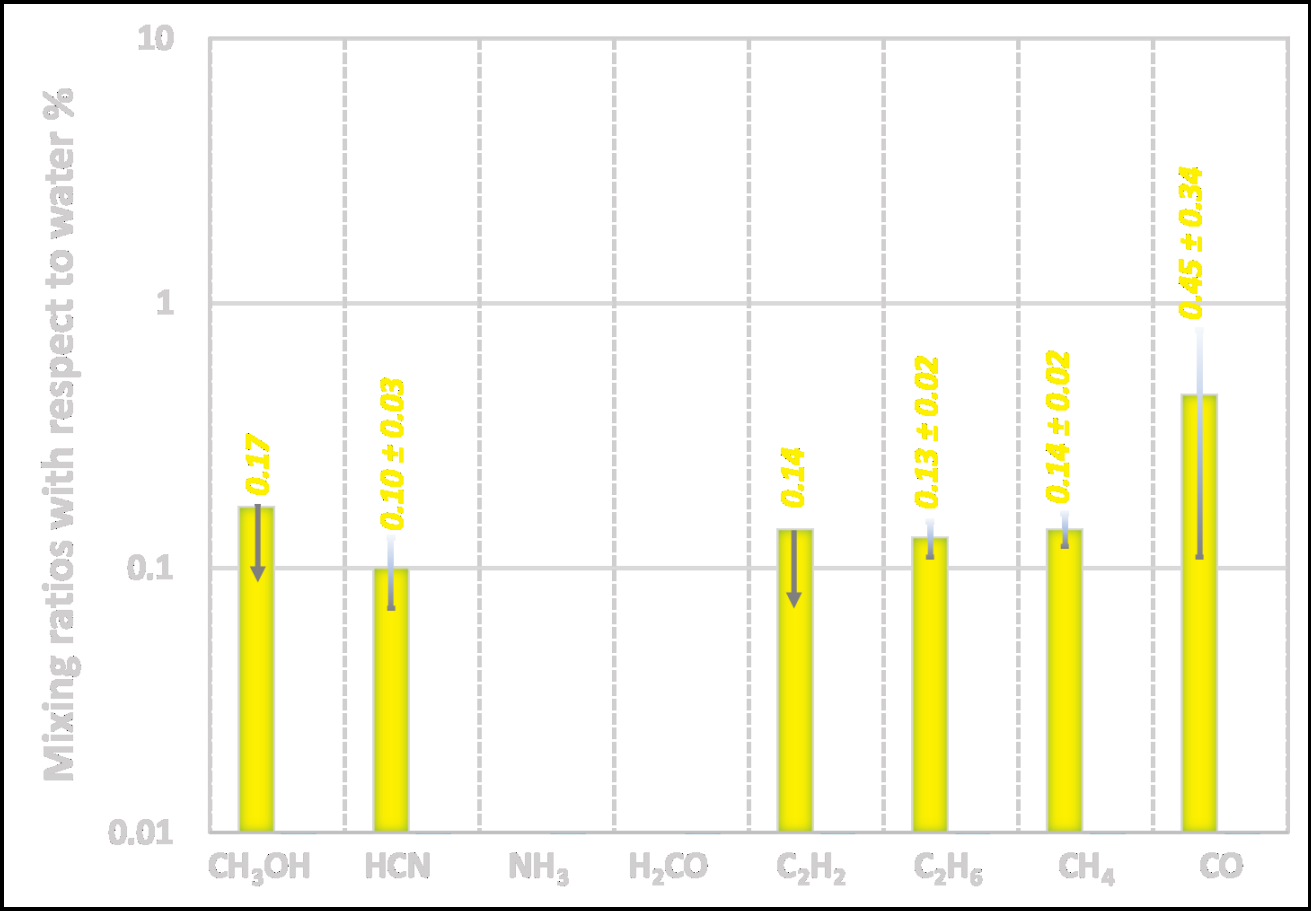

Rotational temperatures (K)			
Molecule	Mumma et al. 2001	Dello Russo et al. 2005	
H_2O	50 (assumed)	$73\ ^{+8}_{-6}$	

Water production rate (10^{26} mol/s)			
Setting	Mumma et al. 2001	Dello Russo et al. 2005	
KL1		673 ± 56	
KL2		673 ± 119	
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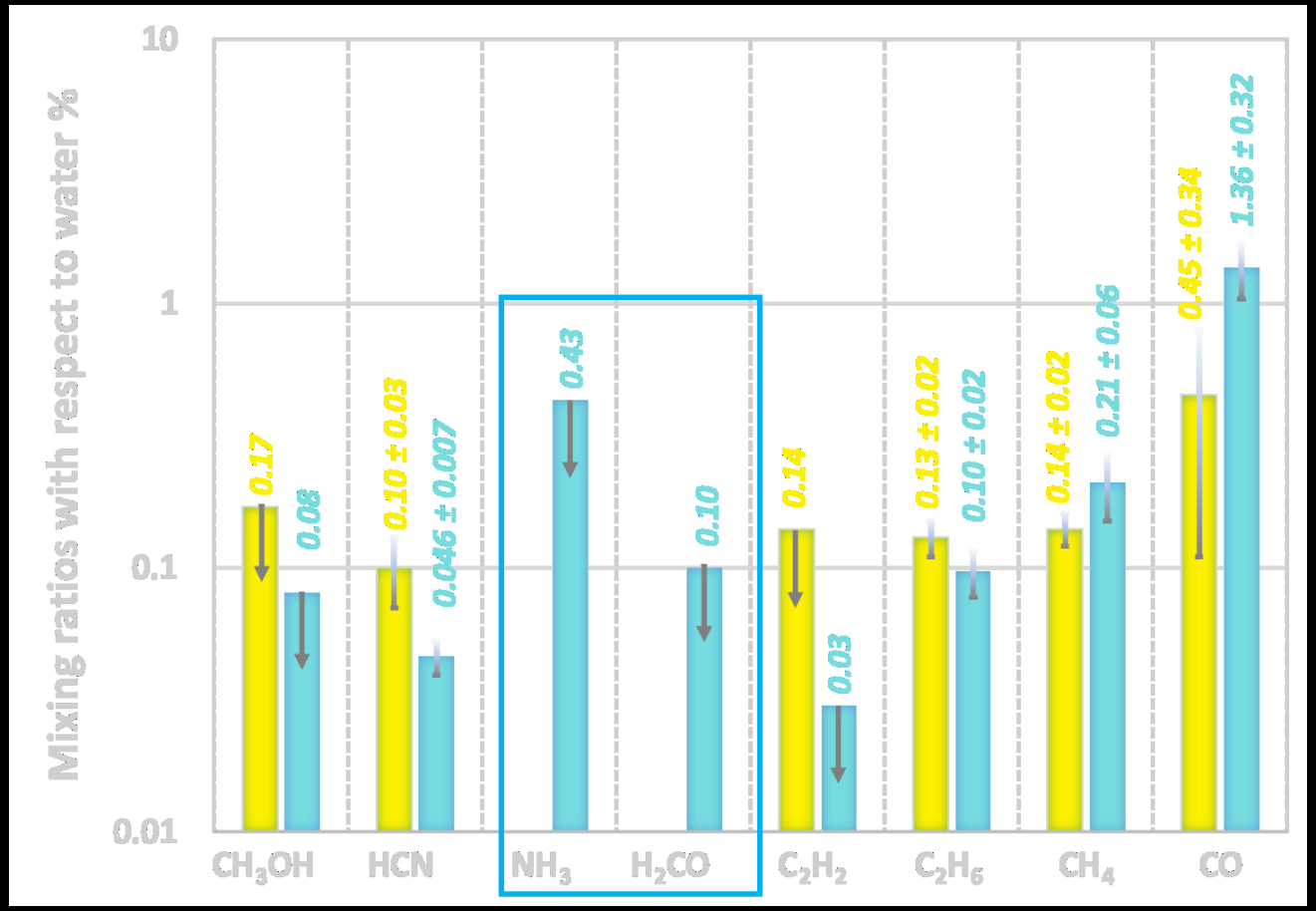

Rotational temperatures (K)			
Molecule	Mumma et al. 2001	Dello Russo et al. 2005	Lippi et al. 2020 (in press)
H_2O	50 (assumed)	$73\ ^{+8}_{-6}$	75 ± 5

Water production rate (10^{26} mol/s)			
Setting	Mumma et al. 2001	Dello Russo et al. 2005	Lippi et al. 2020 (in press)
KL1		673 ± 56	704 ± 100
KL2		673 ± 119	478 ± 34
MW	446 ± 72		303 ± 29

KL1 ~3370 cm^{-1}; KL2 ~3440 cm^{-1}; MW ~2150 cm^{-1}

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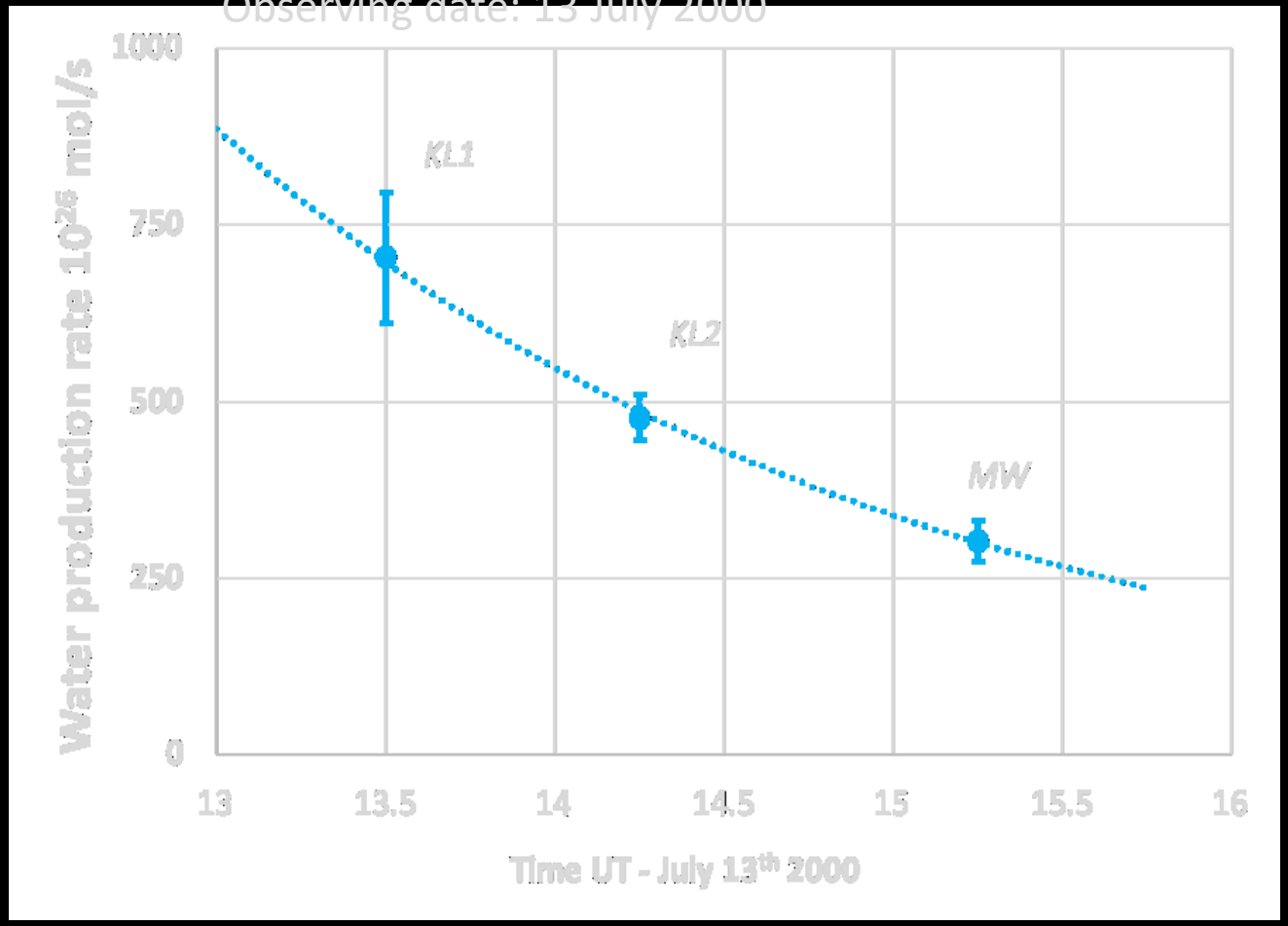

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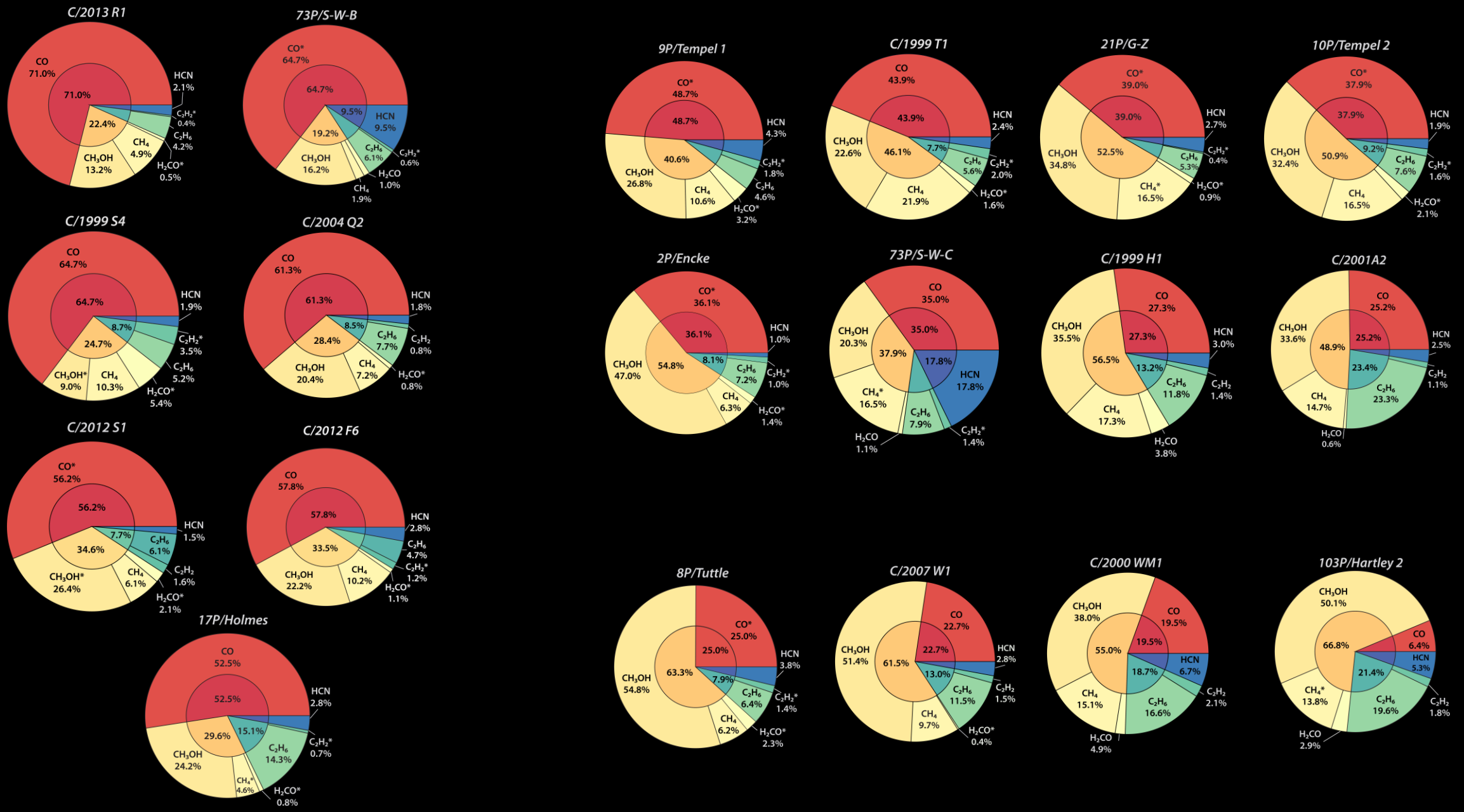
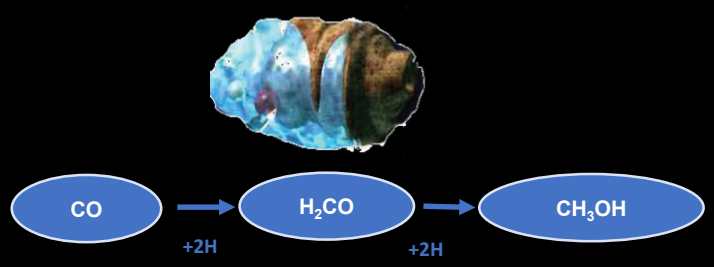
Comet recipes

- **CO** – interstellar origin
- **CH_3OH, CH_4, H_2CO** – Hydrogenation of CO can produce H_2CO and CH_3OH; hydrogenation of C on grain surfaces can produce CH_4
- **C_2H_2, C_2H_6** – Hydrogenation of C_2H_2 can produce C_2H_6
- **HCN** – N-bearing molecules(in our database) - (**NH_3** challenging)

CO --- CH_3OH, H_2CO, CH_4 --- C_2H_2, C_2H_6 --- HCN

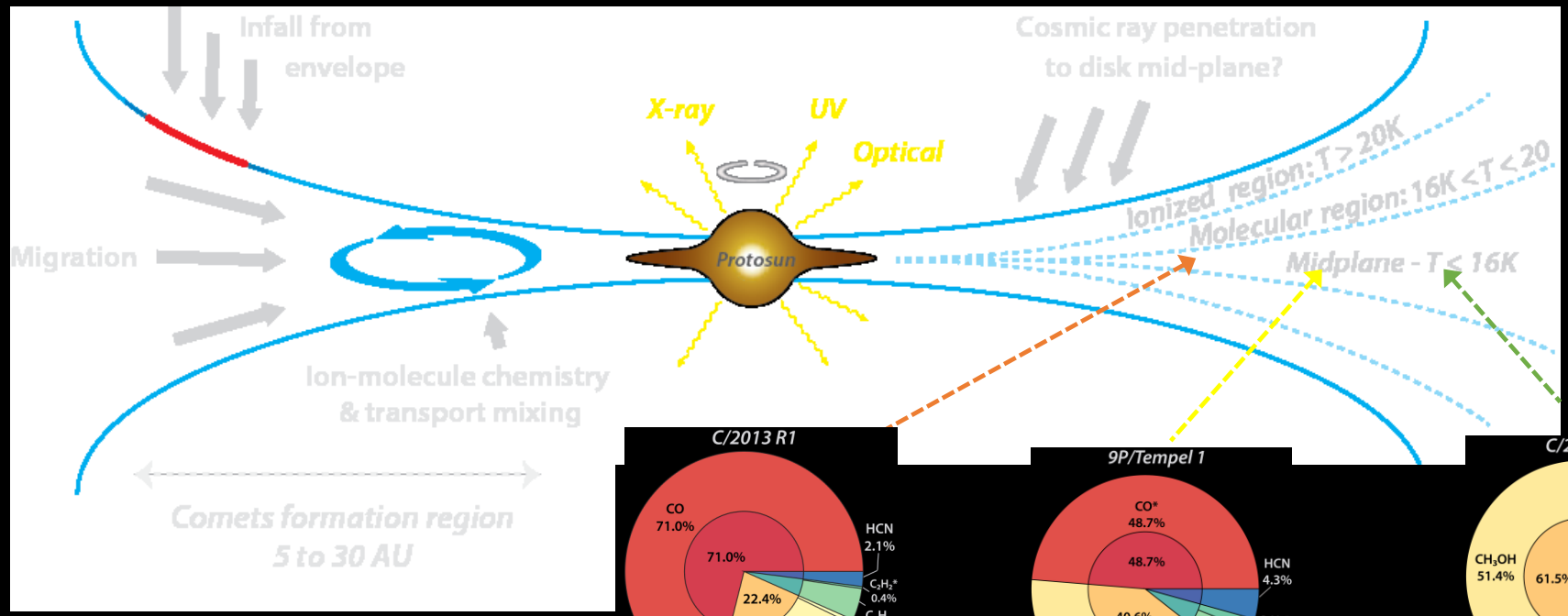


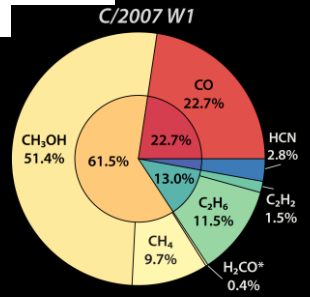
Where did comets form?



Low efficiency in CO Hydrogenation
=> Higher formation temperature

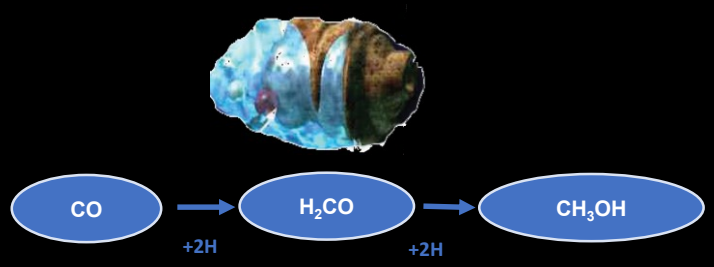
High efficiency in CO Hydrogenation
=> Lower formation temperature

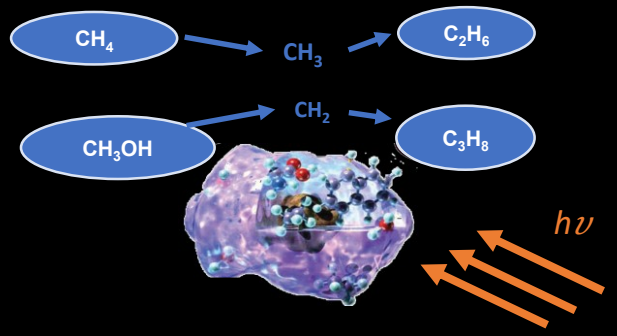


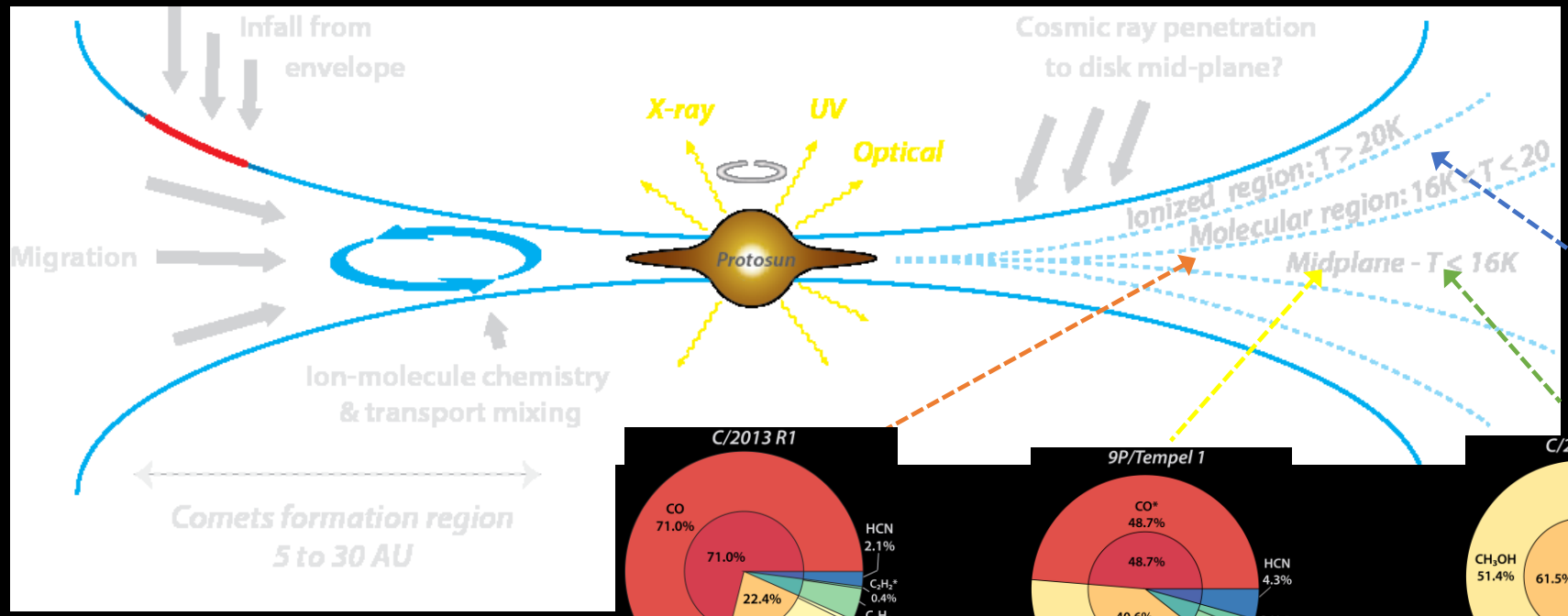


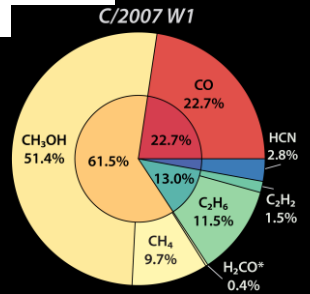
Adapted from: Mumma & Charnley 2011

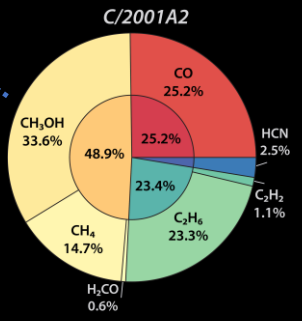
Where did comets form?











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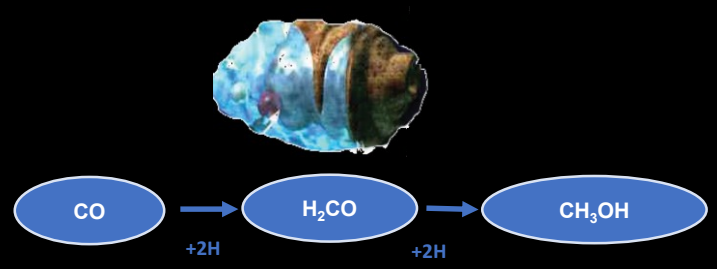

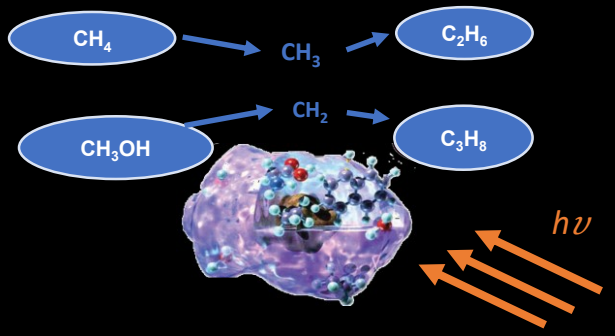

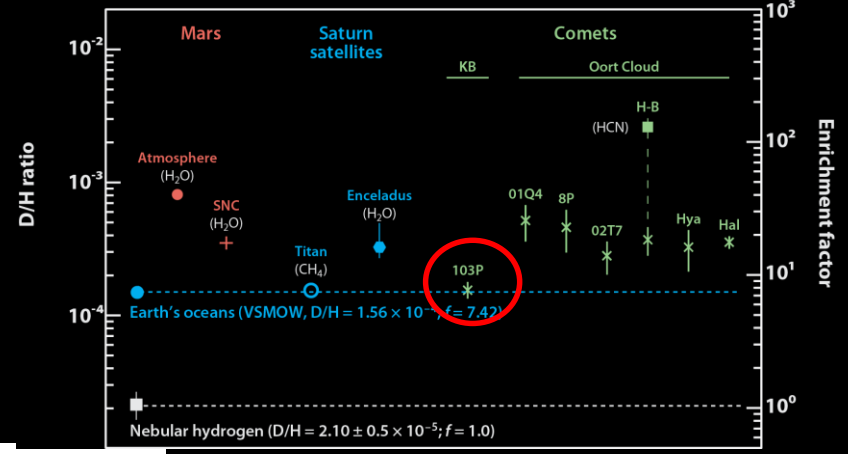

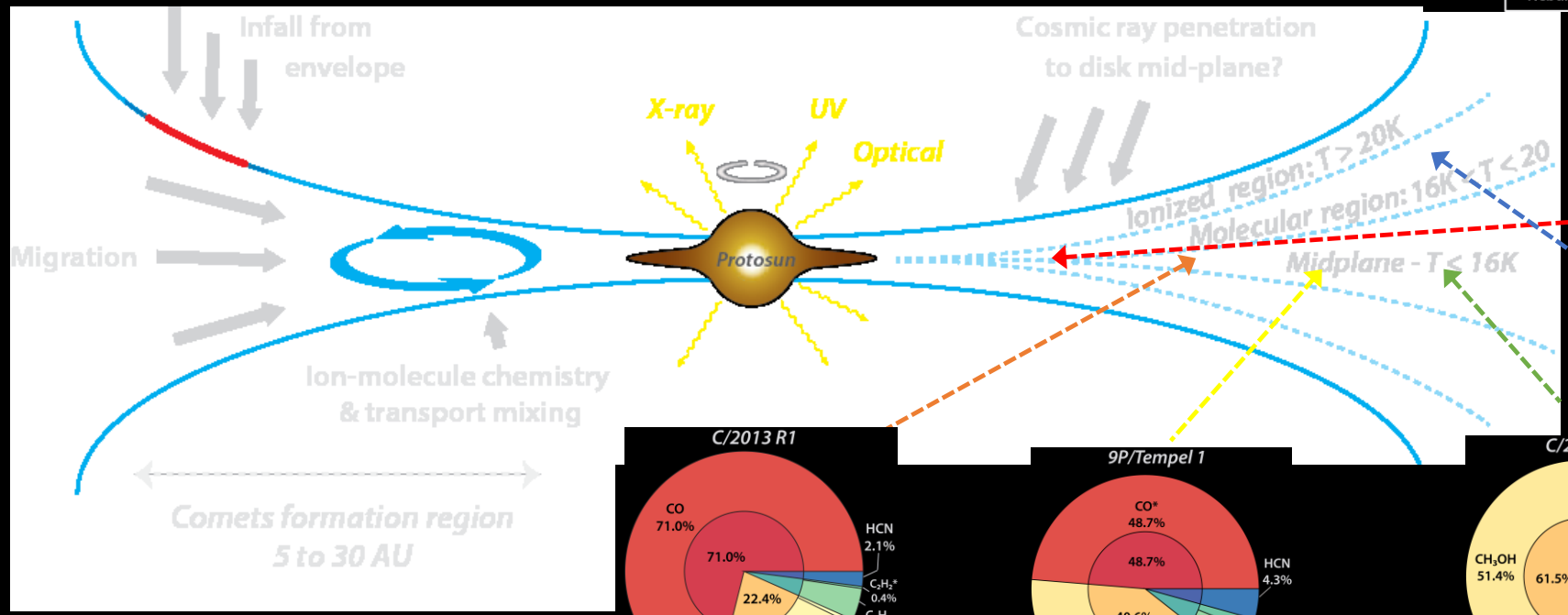

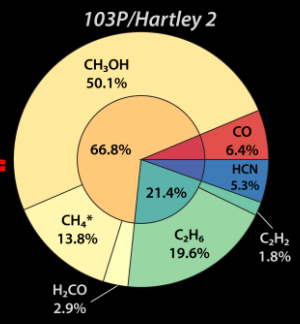

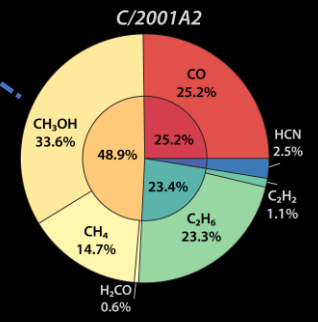

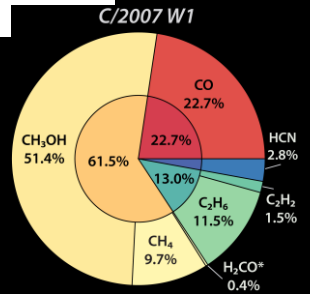

Next steps and conclusions

- Complete the revision of the data in the database.
- Include other cosmogonic indicators and cross check for their consistency
- Analyze the results using data mining techniques to find hidden trends if any

- Cometary data relative to IR spectroscopy in the literature may be affected by systematic errors introduced by different analysis approaches.
- Using the latest tools we can correct for these unevenness and apply a more reliable statistic to the results
- This will help us to understand the early phases of our Solar System and Earth formation.

Thank you!