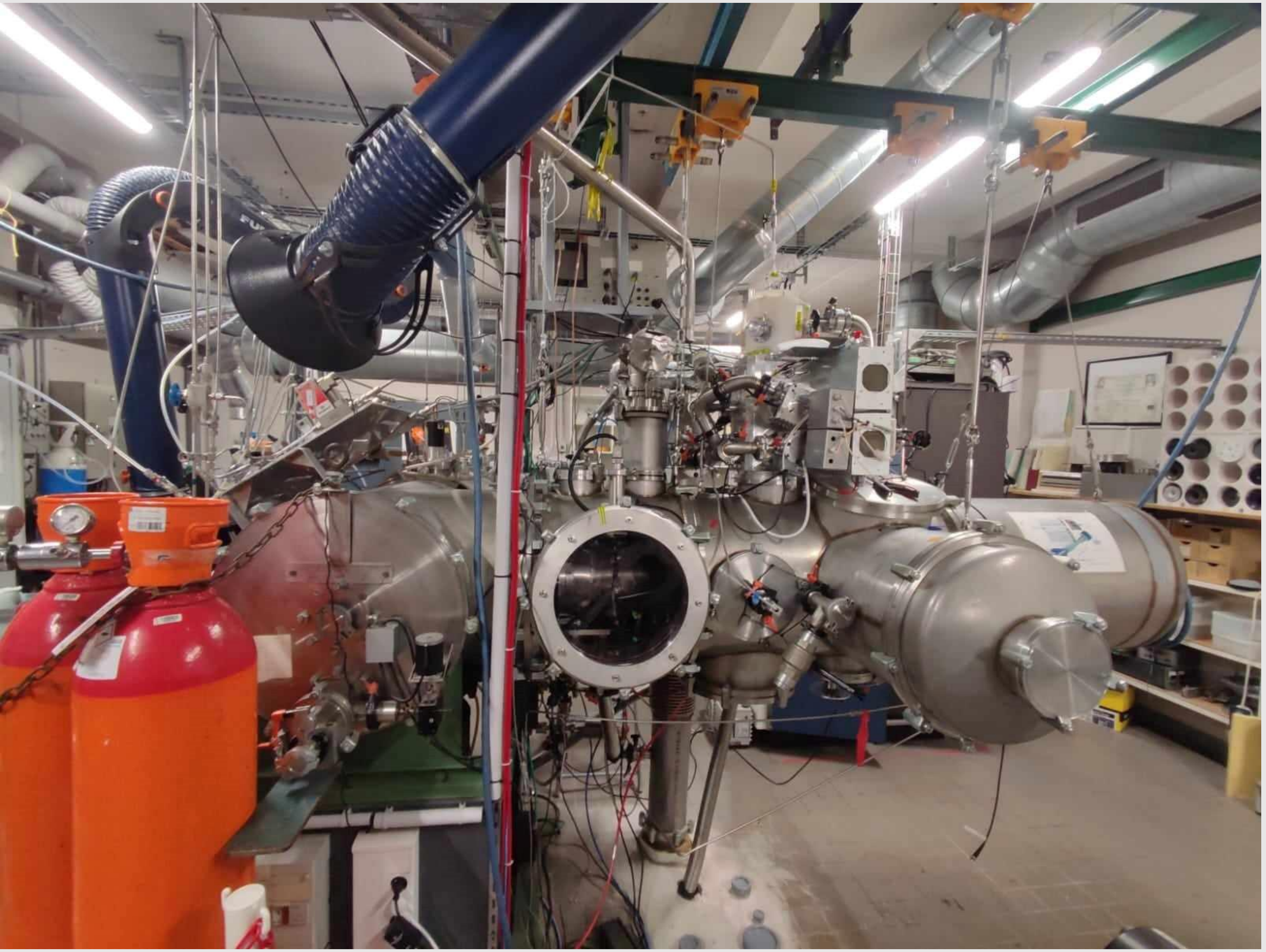


Rapid molecular growth induced by low-temperature ion-molecule reactions of CH_3^+ with a selection of hydrocarbons : insights into the interstellar carbon chemistry

PCMI Bordeaux 30/10/2024

E. Ogden, S. Carles, A. Benidar, F. Lique, R. Jara-Toro, A. Taillard, J.-C. Loison, F. Tonolo, L. Biennier

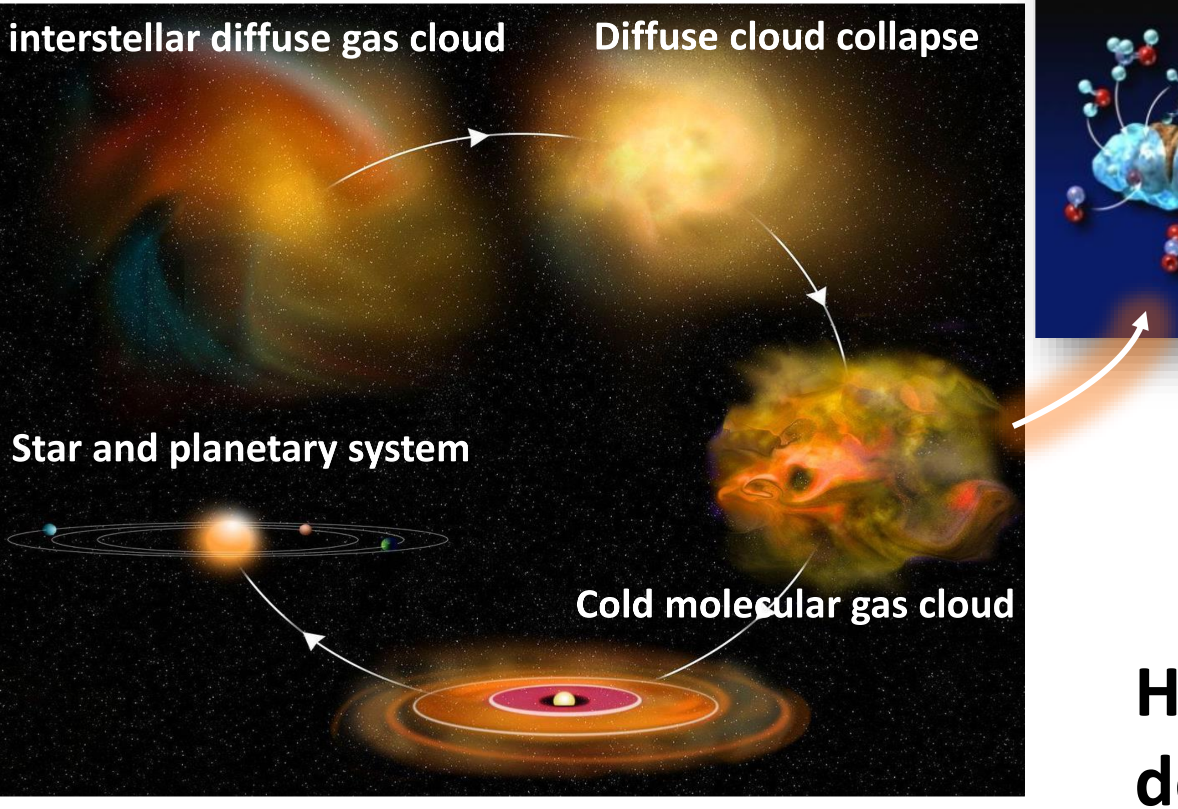
Department of Molecular Physics, Institut de Physique de Rennes,

Centro de Astrobiología, Madrid

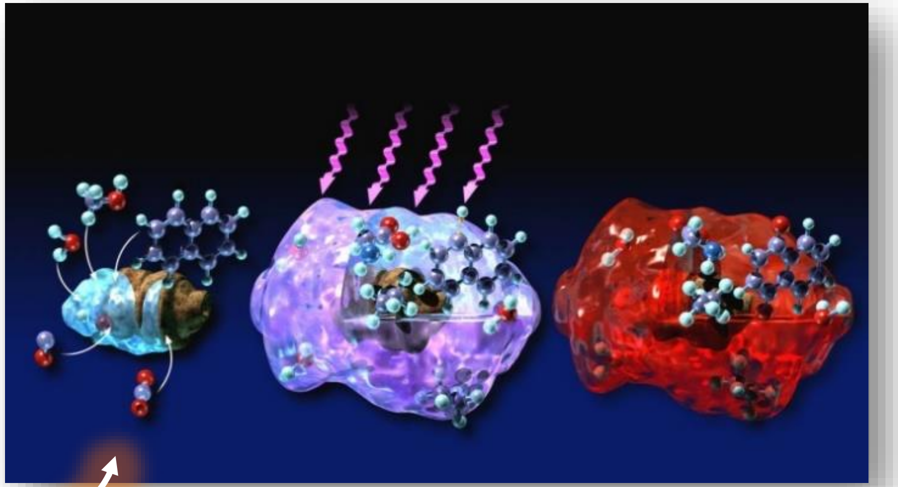
Institut des Sciences Moléculaires, Bordeaux

Malo Briend

Intertwined solid and gas phase interstellar chemistry



Protoplanetary disc

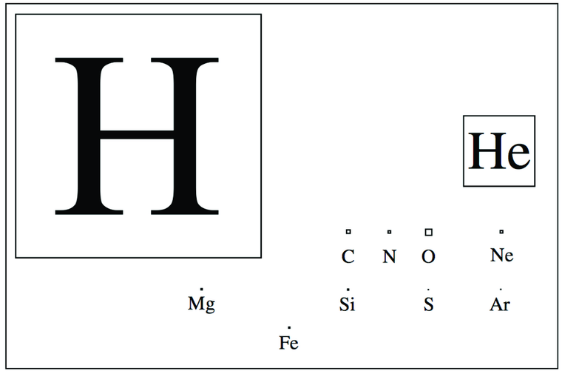


- Grains are an established chemical catalyst in the ISM
- They play a key role in the production of complex molecules
- Yet, the vast majority of detections are performed in the gas phase through radio emission

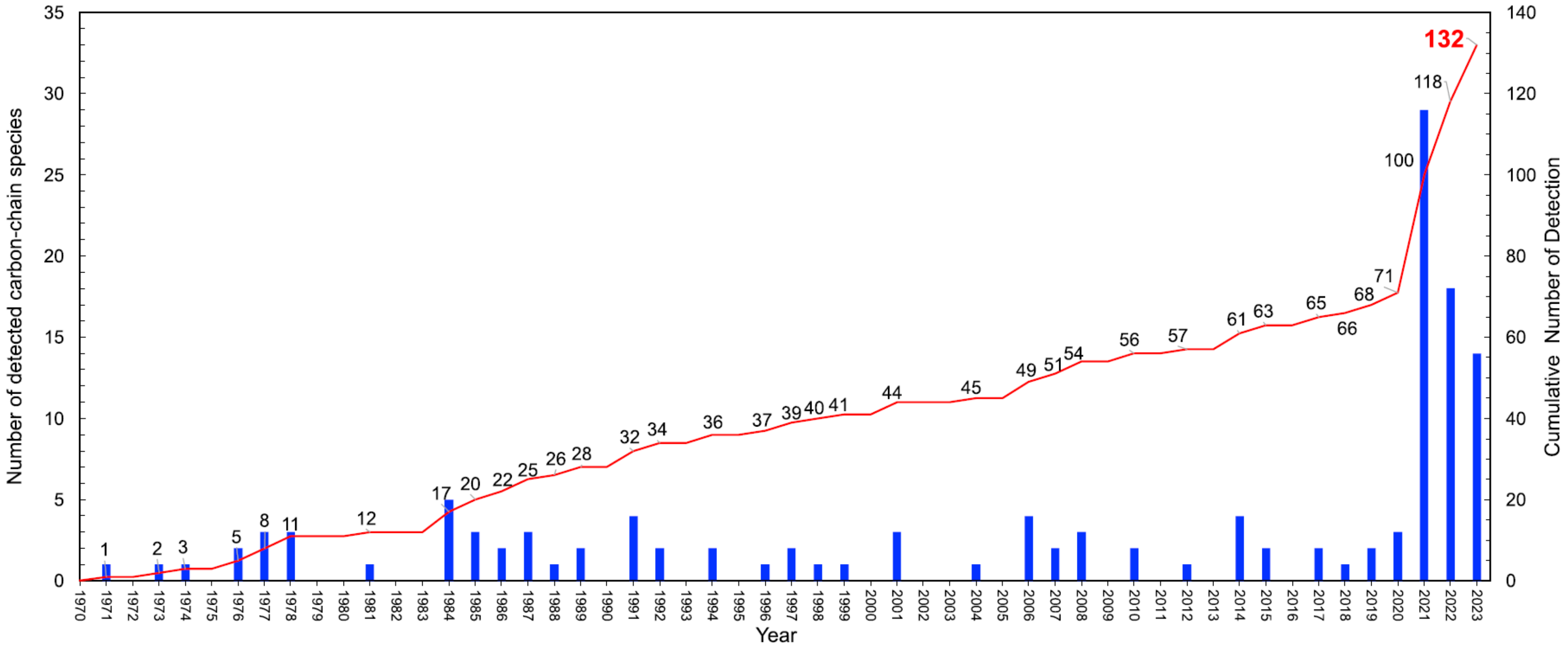
How does gas-phase chemistry impact desorbed COMs and hydrocarbons?

Bill Saxton, NRAO/AUI/NSF

Carbonaceous species in the interstellar medium



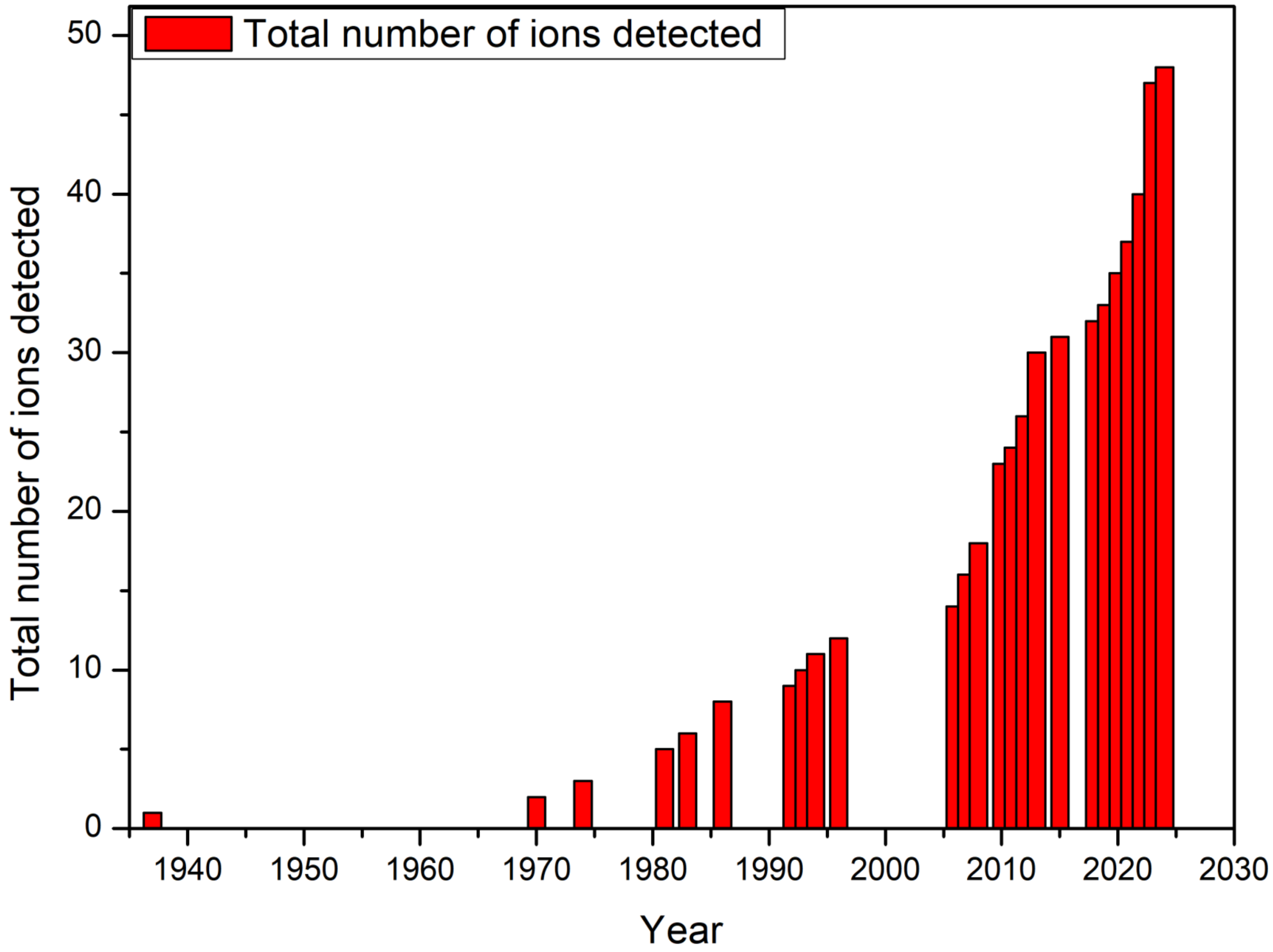
McCall 2001, the astronomer periodic table.



Taniguchi, K., Gorai, P., & Tan, J. C. (2024). Carbon-chain chemistry in the interstellar medium. *Astrophysics and Space Science*, *369*(4), 34.

- 40% of interstellar molecules discovered contain carbon, this atom is a cornerstone of organic chemistry

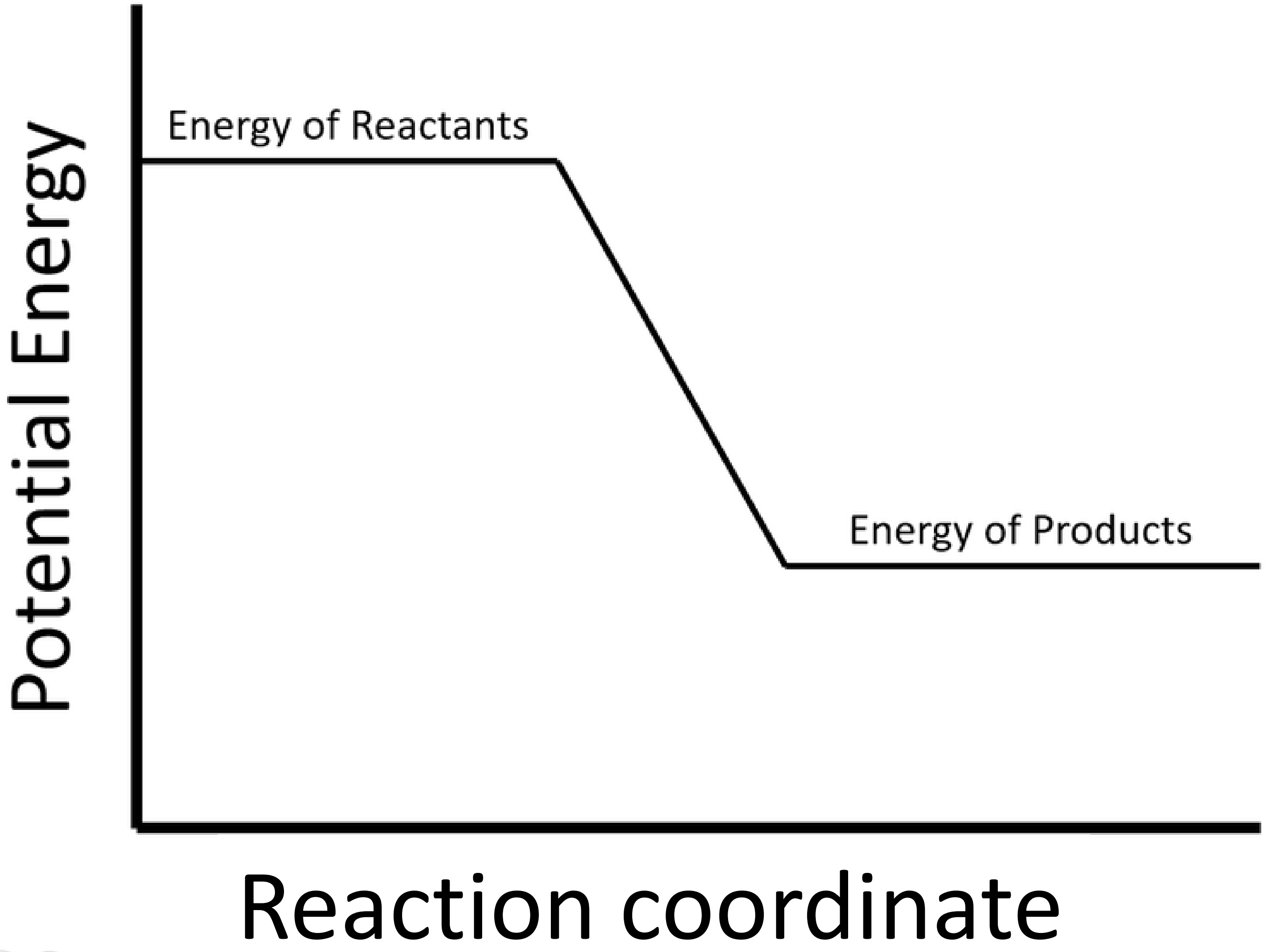
Ionic species in the interstellar medium



http://astrochymist.org/astrochymist_ism.html

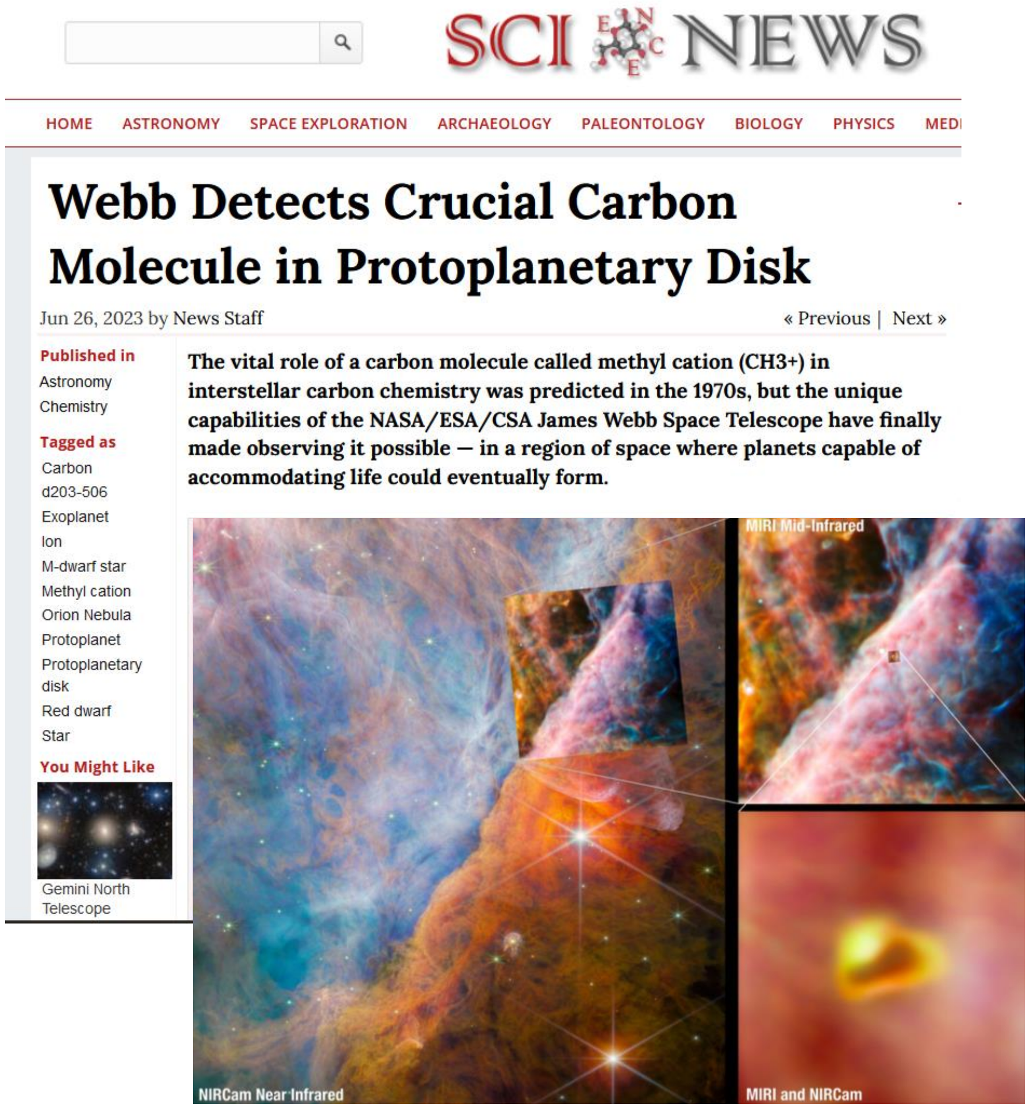
Physico-chemical processes in a gas phase medium

Ion-molecule reactions		
Charge transfer	$A^+ + B$	$\rightarrow A + B^+$
Radiative association	$A^+ + B$	$\rightarrow AB^+ + h\nu$
Atom transfer	$AB^+ + C$	$\rightarrow A^+ + BC$
Anion - neutral	$A^- + BC$	$\rightarrow AB^- + C$
Associative detachment	$A^- + B$	$\rightarrow AB + e^-$
Electronic recombination		
Radiative	$A^+ + e^-$	$\rightarrow A + h\nu$
Dissociative	$AB^+ + e^-$	$\rightarrow A + B$
Neutral-neutral reactions		
Atom transfer	$A + BC$	$\rightarrow AB + C$
Radiative association	$A + B$	$\rightarrow AB + h\nu$
Photochemical reactions		
Photo-dissociation	$AB + h\nu$	$\rightarrow A + B$
Photo-detachement	$A^- + h\nu$	$\rightarrow A + e^-$
Neutralization		
Cation-anion reaction	$A^+ + B^-$	$\rightarrow AB$
Ionisation		
Electron impact	$A + e^-$	$\rightarrow A^+ + e^- + e^-$
Photo-ionisation	$A + h\nu$	$\rightarrow A^+ + e^-$
Electronic attachment		
Dissociative	$AB + e^-$	$\rightarrow A^- + B$
Radiative	$A + e^-$	$\rightarrow A^- + h\nu$
Three-body reactions		
Termolecular association	$A + B + M$	$\rightarrow AB + M$



https://keystagewiki.com/index.php/Exothermic

Detection of CH_3^+ in a protoplanetary disk, by the JWST


SCI NEWS

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Webb Detects Crucial Carbon Molecule in Protoplanetary Disk

Jun 26, 2023 by News Staff « Previous | Next »

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Methyl cation
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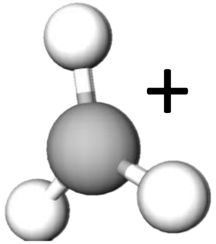
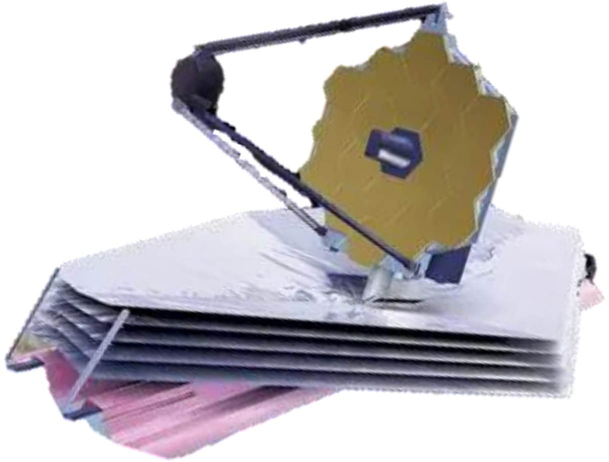
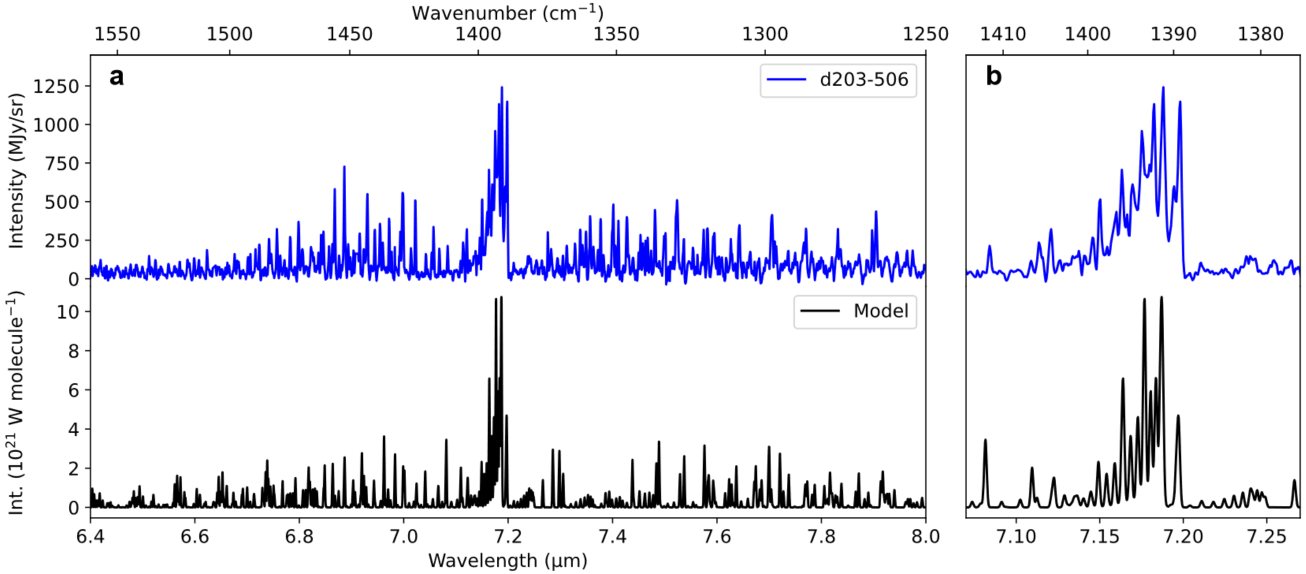
Gemini North Telescope

The vital role of a carbon molecule called methyl cation (CH3+) in interstellar carbon chemistry was predicted in the 1970s, but the unique capabilities of the NASA/ESA/CSA James Webb Space Telescope have finally made observing it possible — in a region of space where planets capable of accommodating life could eventually form.

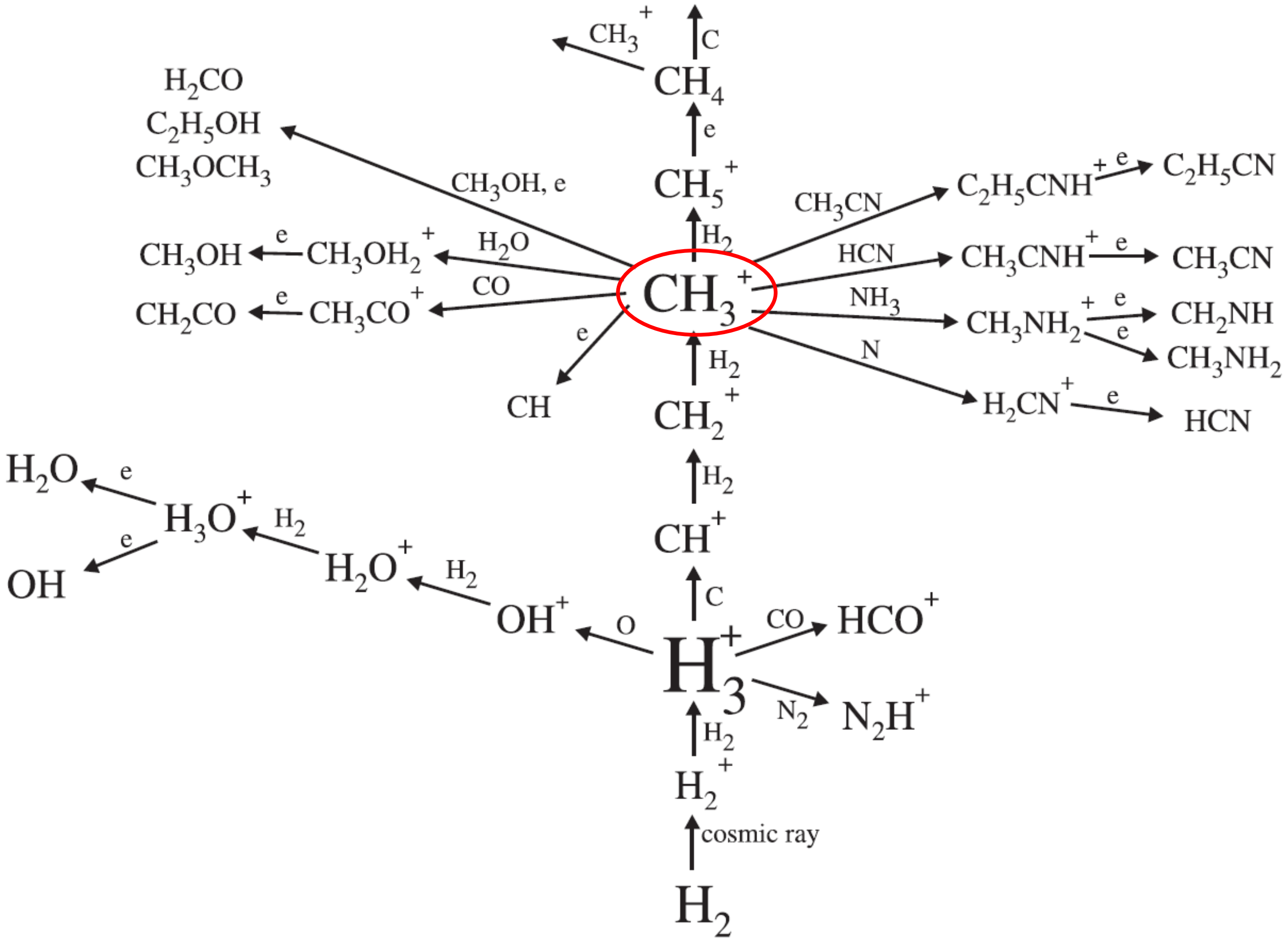


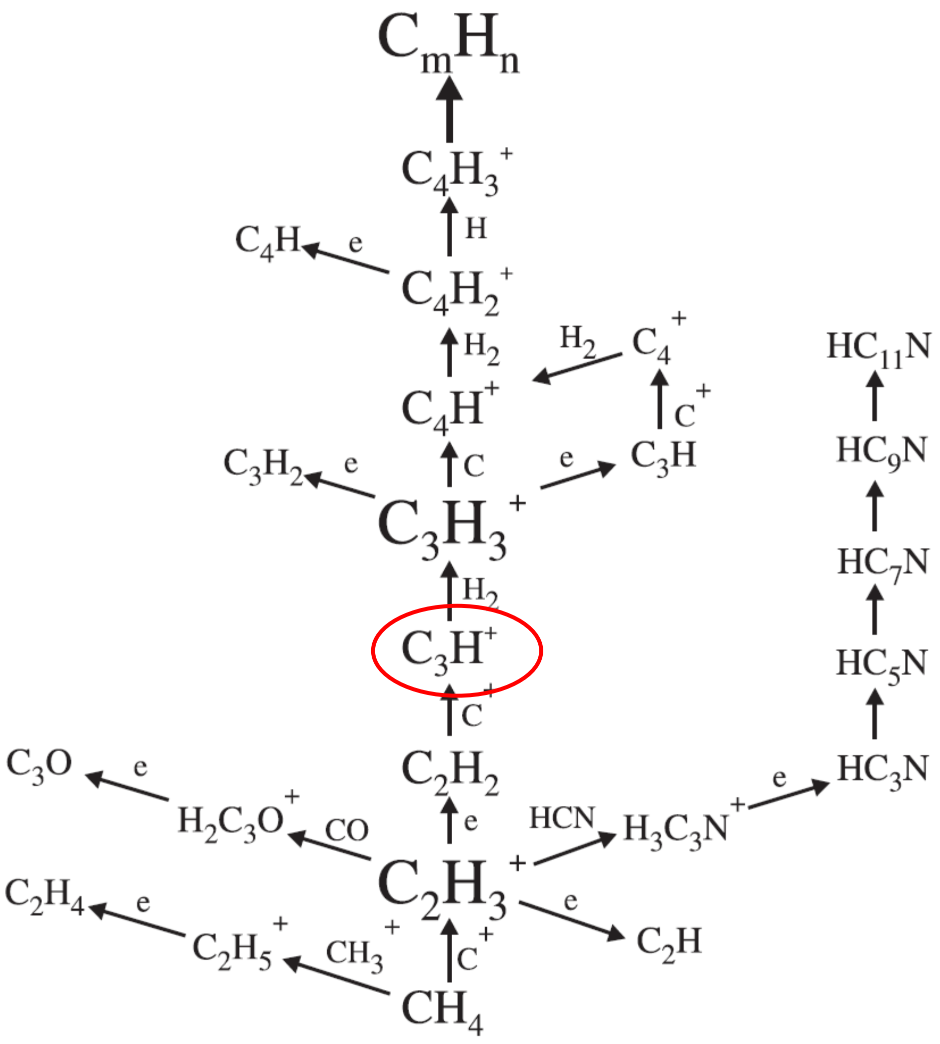




Berné, O., Martin-Drumel, M. A., Schroetter, I., Goicoechea, J. R., Jacovella, U., Gans, B., ... & Wolfire, M. G. (2023). Formation of the methyl cation by photochemistry in a protoplanetary disk. *Nature*, *621*(7977), 56-59.

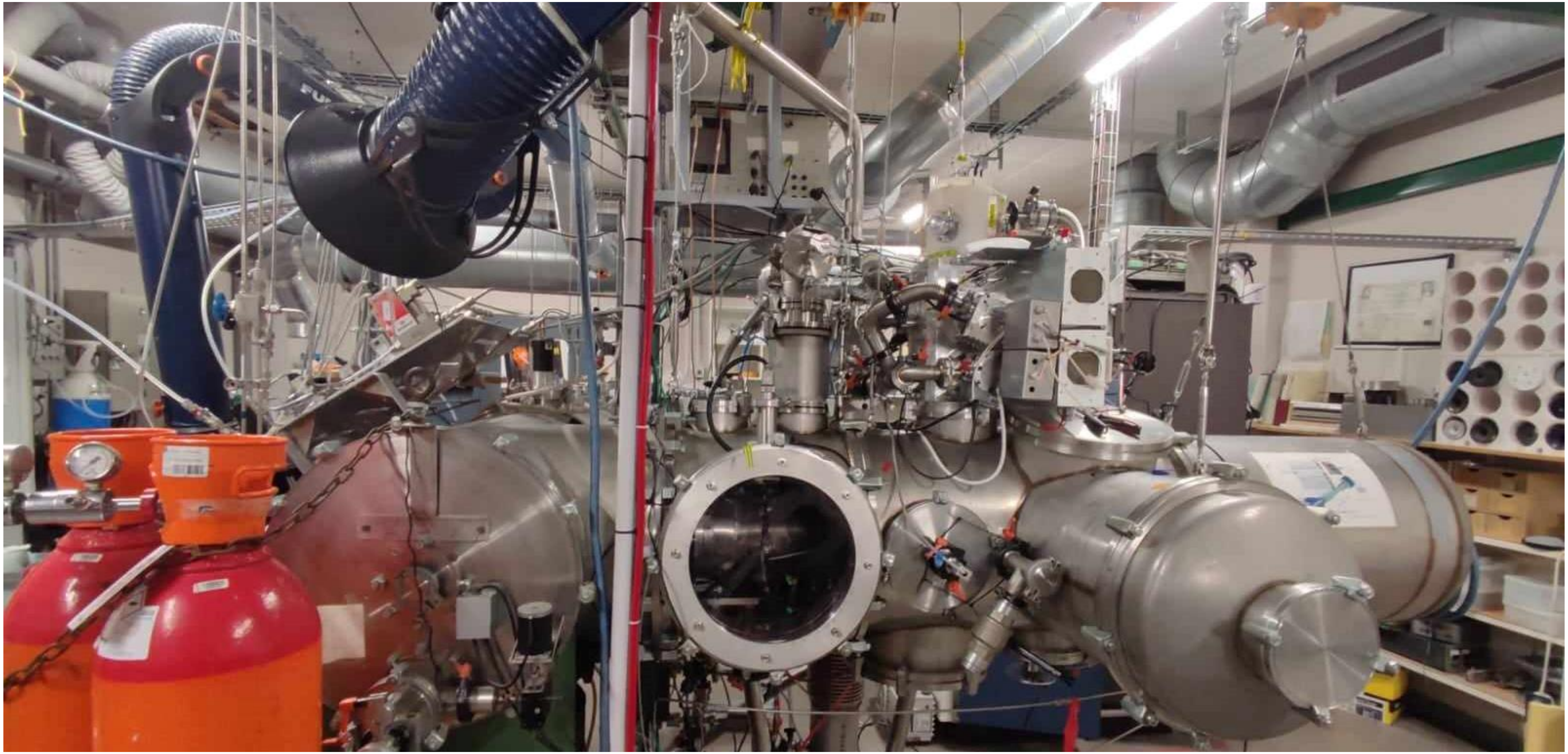
Zooming in on a key organic ion



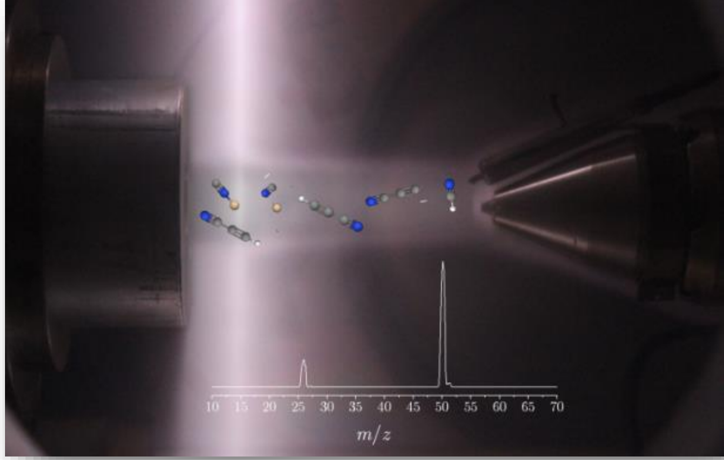


Geppert, W. D., & Larsson, M. (2008).. *Molecular Physics*, *106*(16-18), 2199-2226.

Investigating ion reactivity at low temperatures



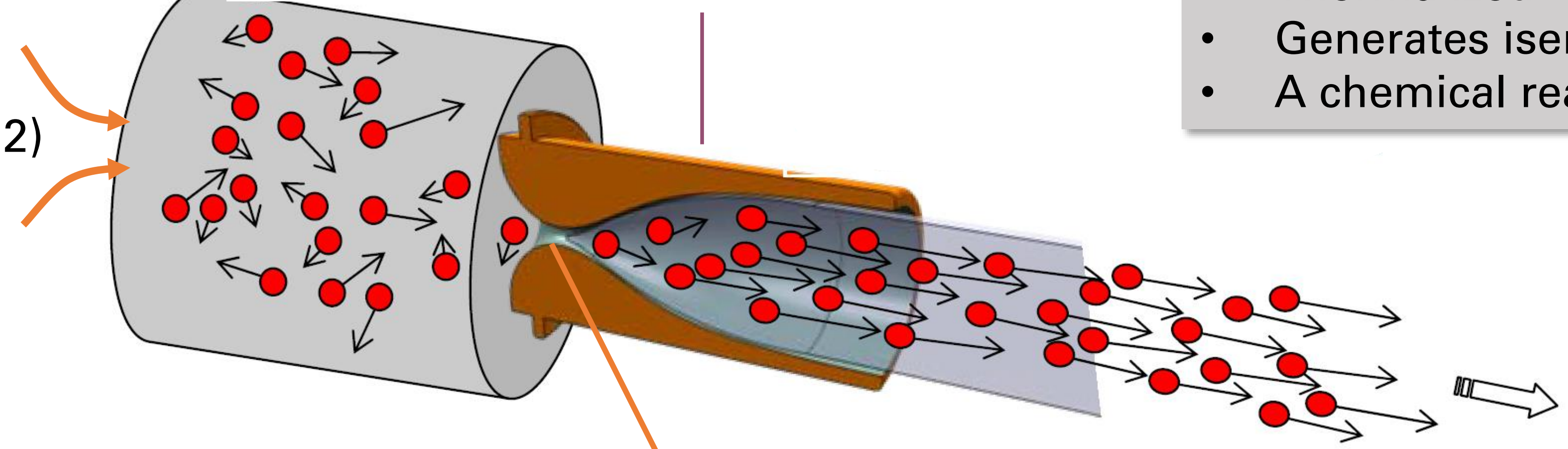
The CRESU method



Kinetics of Reactions in Uniform Supersonic Flows (CRESU) :
Invented in Meudon in the 1980s (Rowe & Marquette) and transferred shortly afterwards to Rennes.

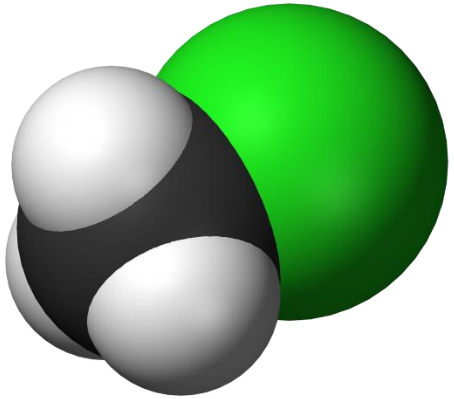
Highlights of the method :

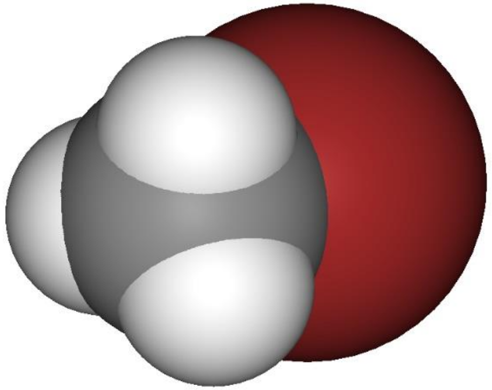
- Temperature range: 10 - 220 K
- Thermalized
- Generates isentropic flow
- A chemical reactor without walls



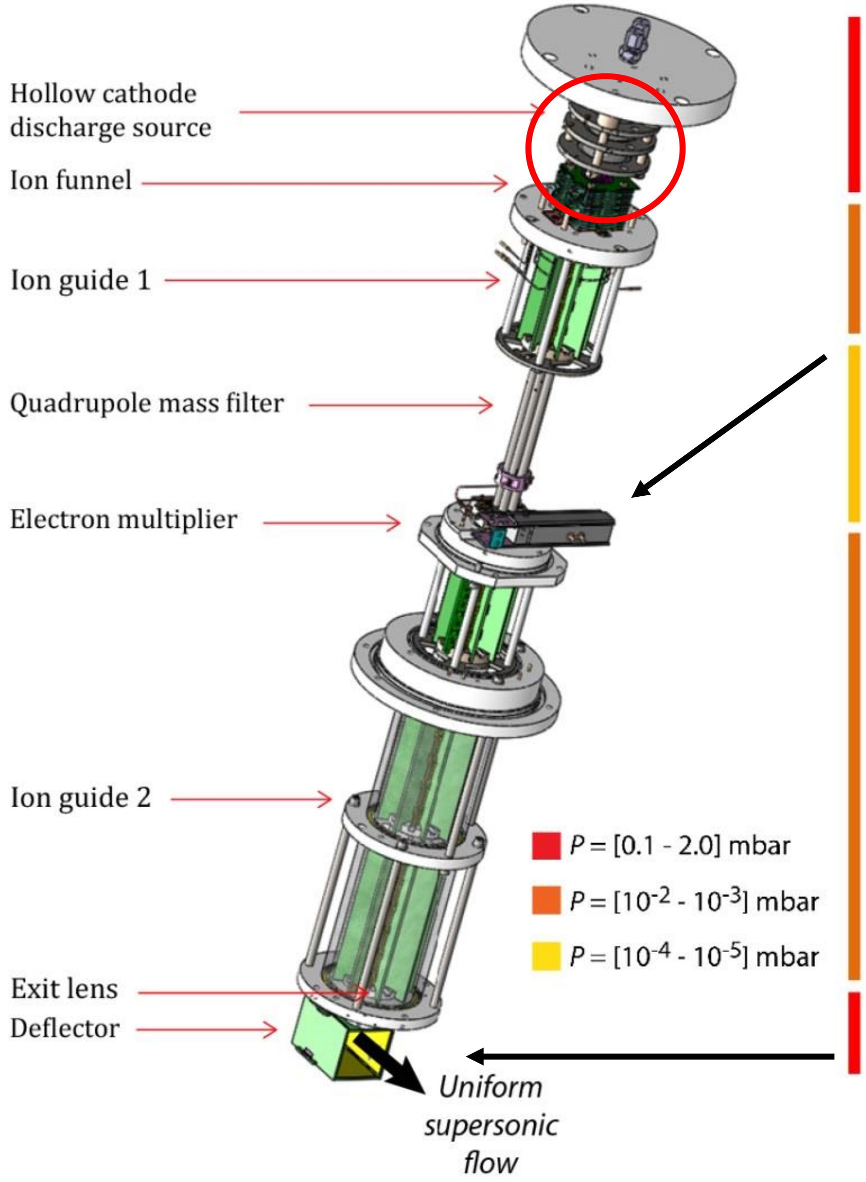
The “perfect” precursor for CH_3^+

- Acetone CH_3COCH_3
- Acetonitrile CH_3CN
- Bromomethane CH_3Br
- Chloromethane CH_3Cl

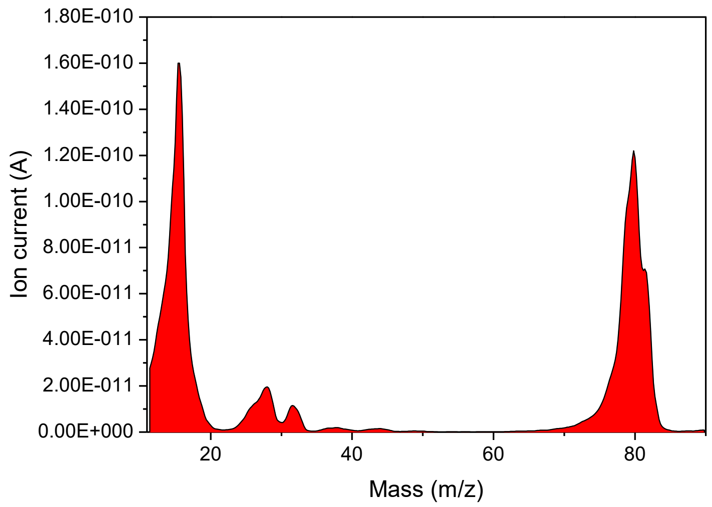


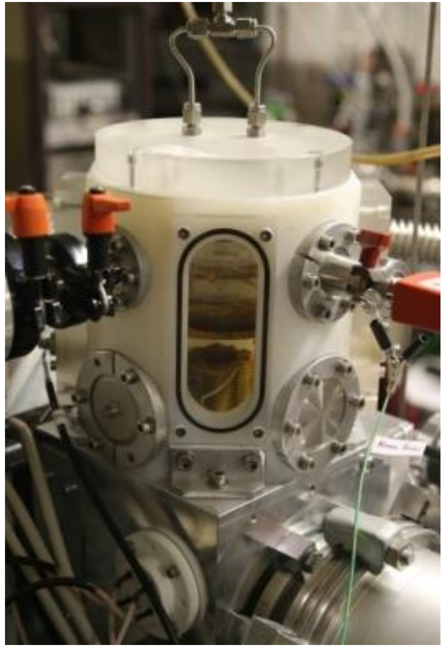


The ion source

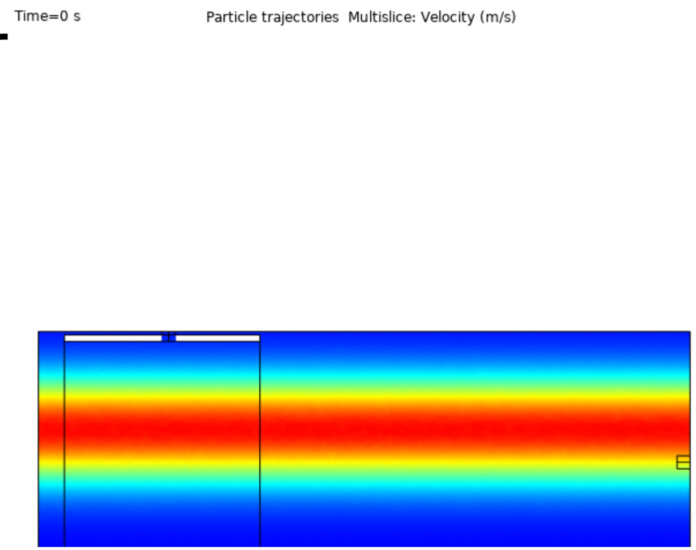


Ion production in a hollow cathode discharge source





Mass selection in the filter; ion transfer; injection

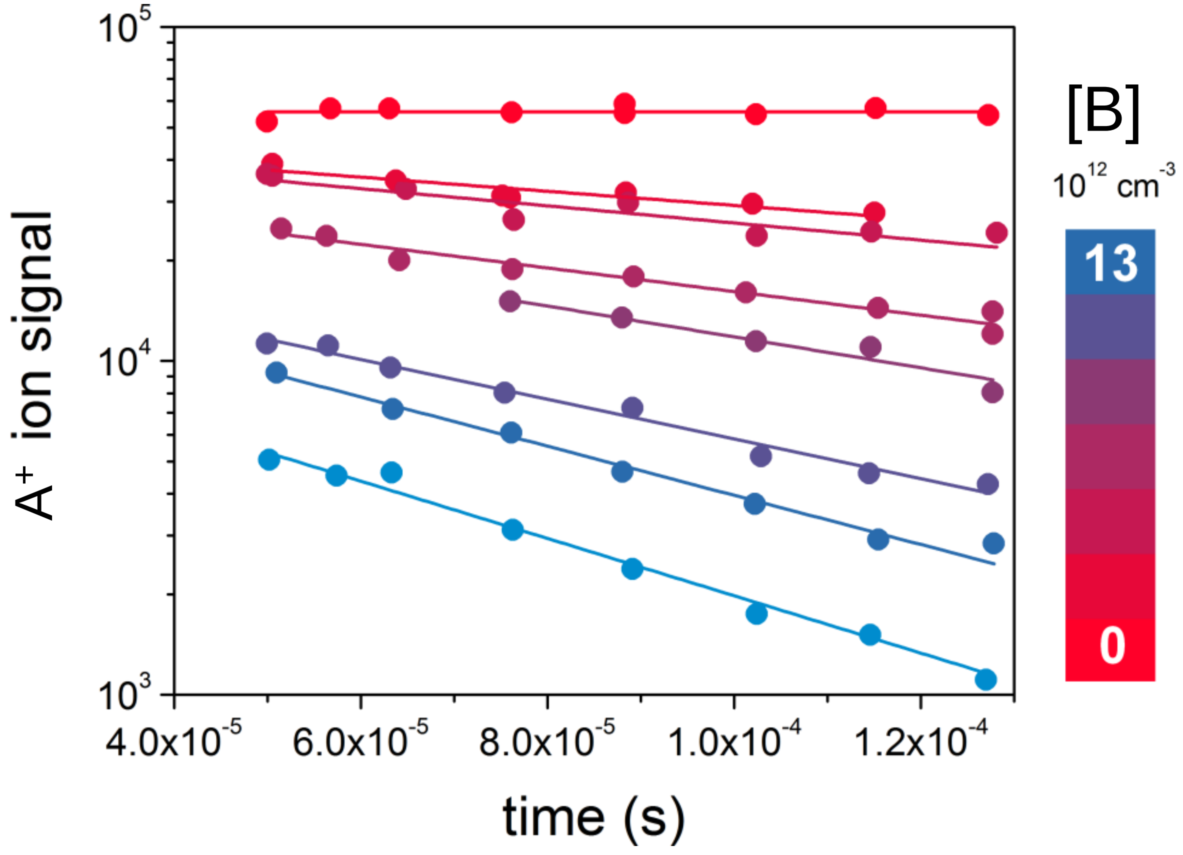


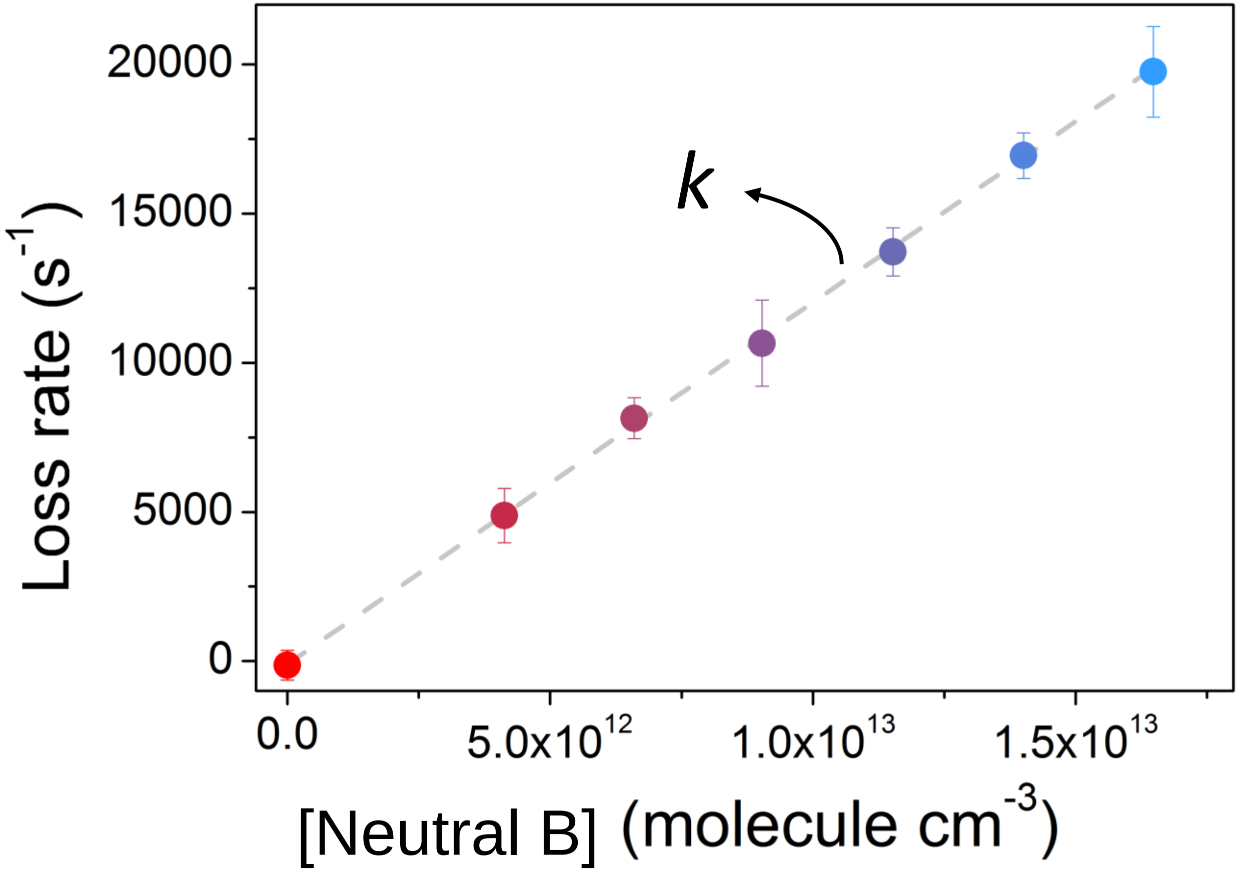
CFD simulations of the velocity + ion trajectory calculations

A. Benidar

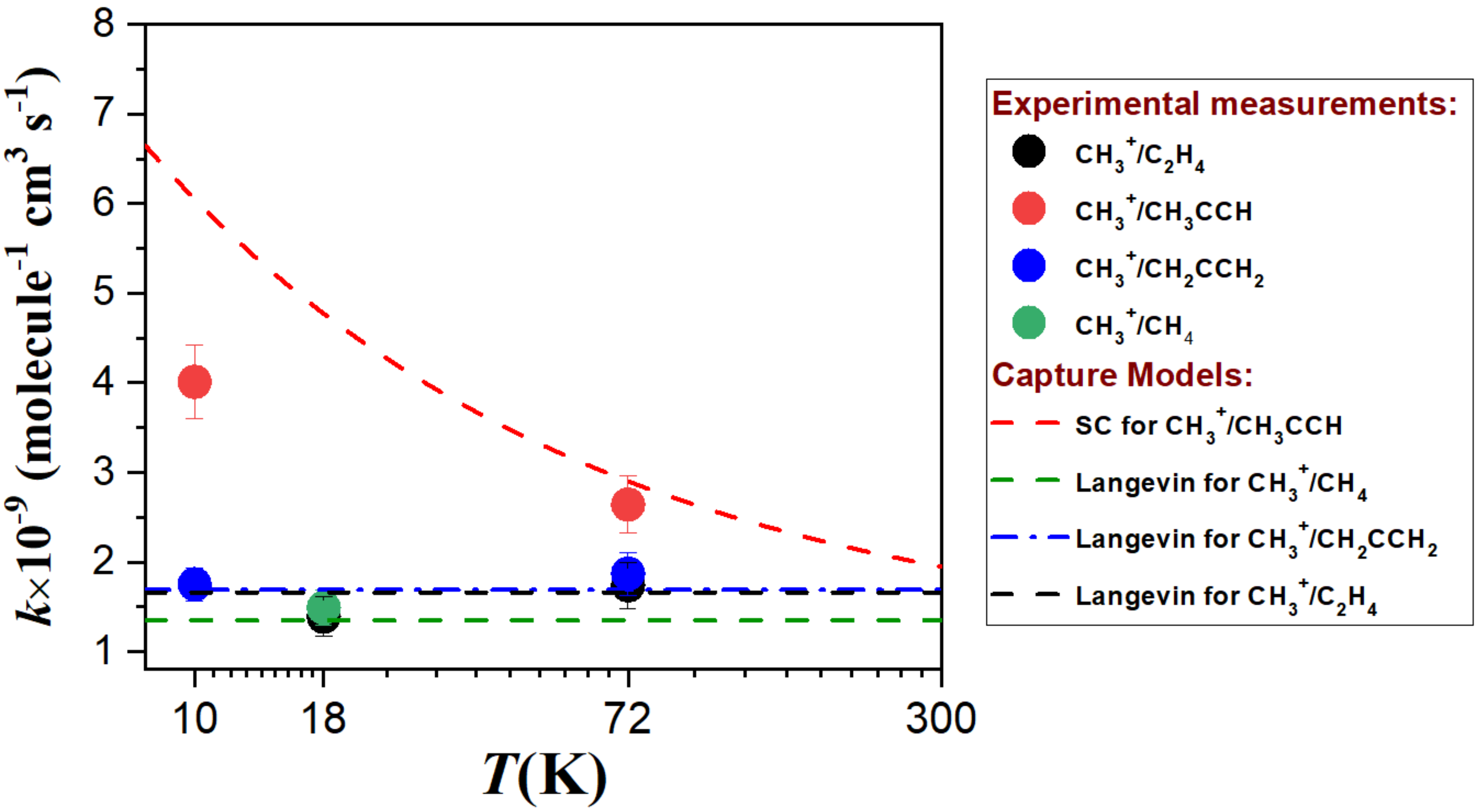
Kinetic Measurements

$$A^+ + B \xrightarrow{k} \text{products}$$



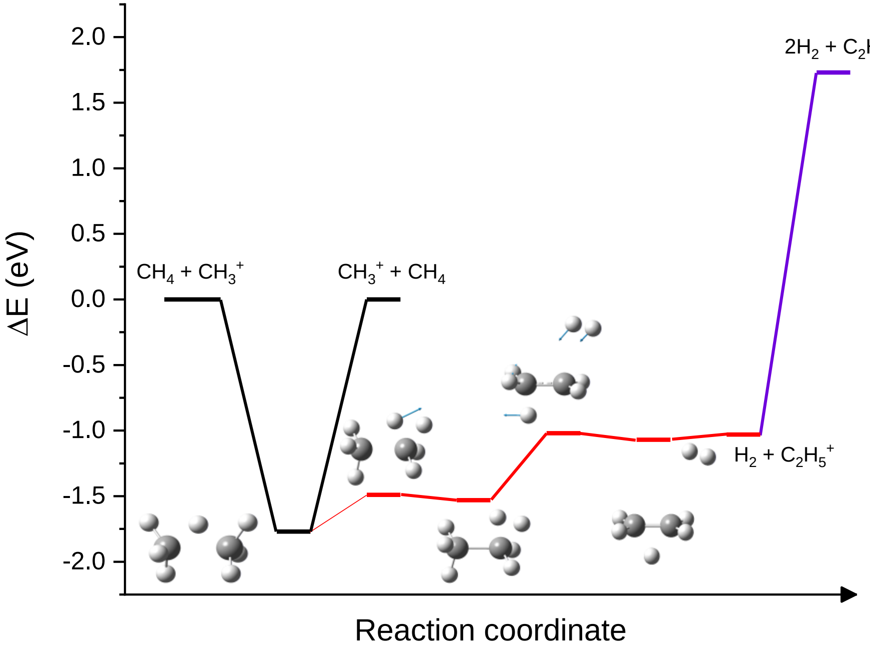


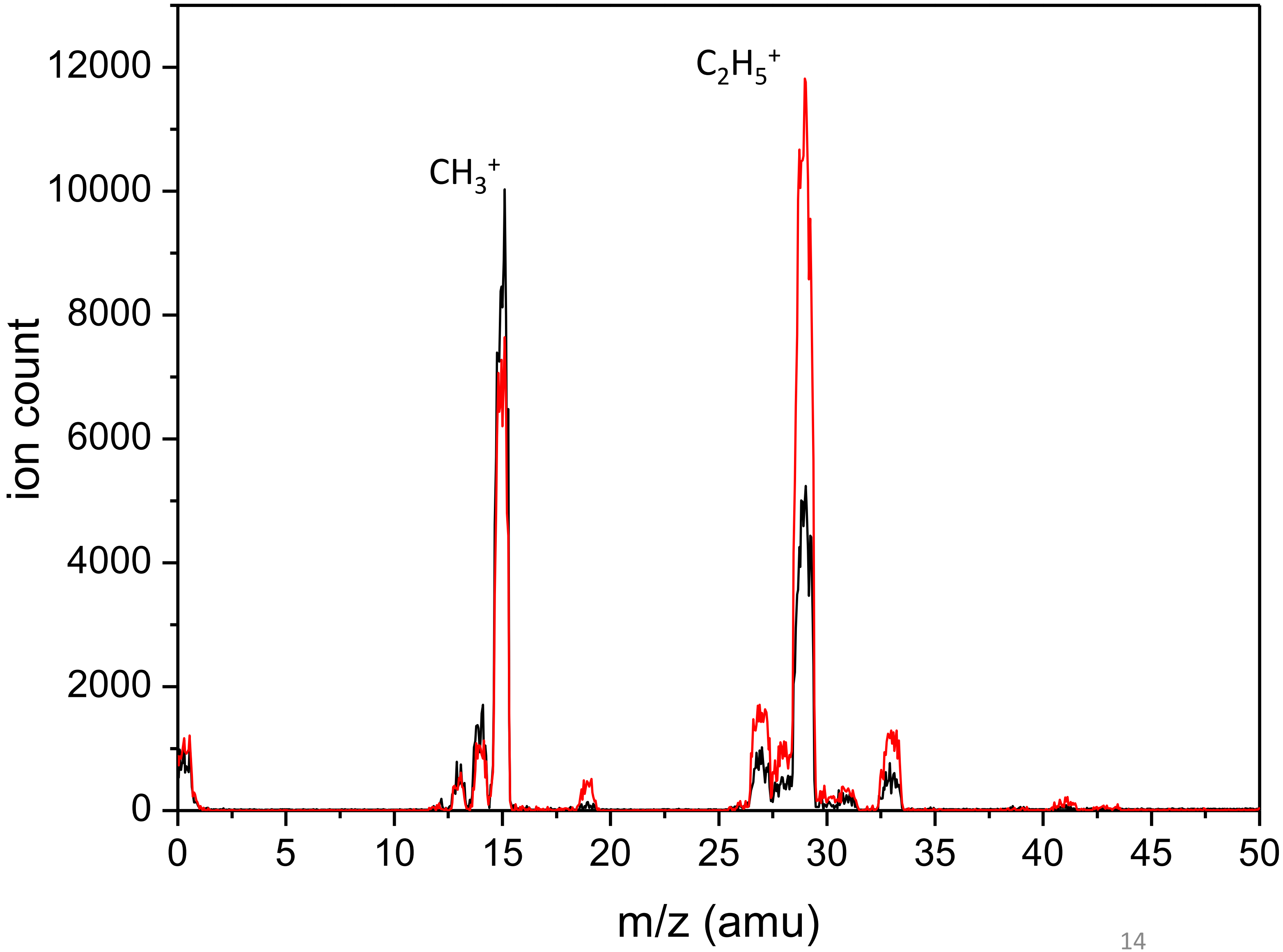
Preliminary kinetic results on CH_3^+ with a selection of hydrocarbons



Reaction $CH_3^+ + CH_4$: branching ratios at 24.1K

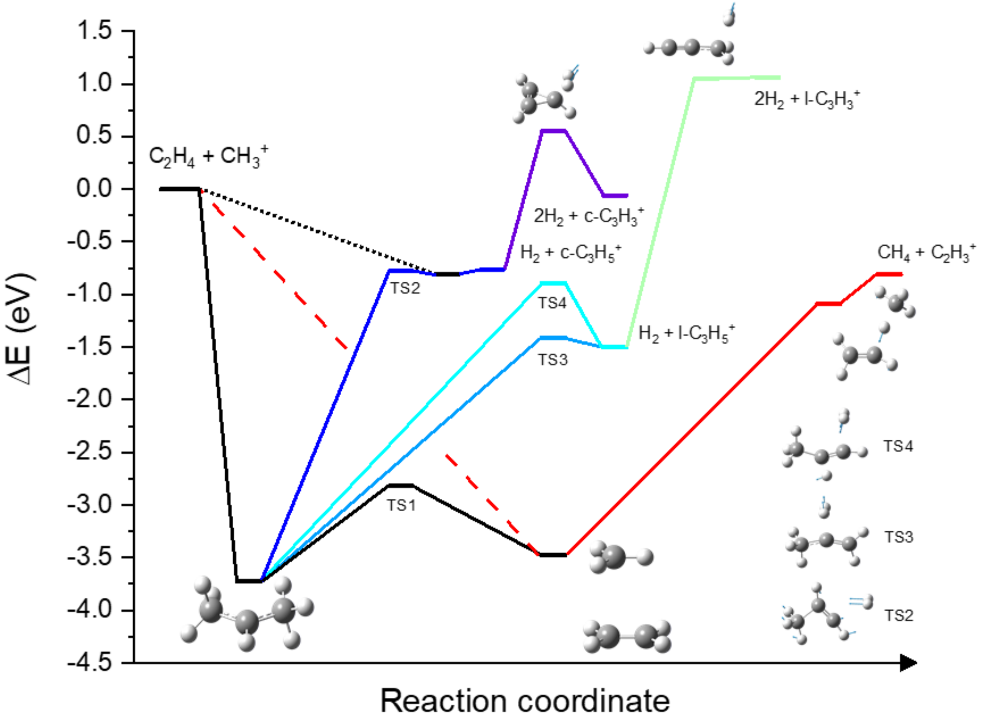
$CH_3^+ + CH_4 \rightarrow C_2H_5^+ + H_2$

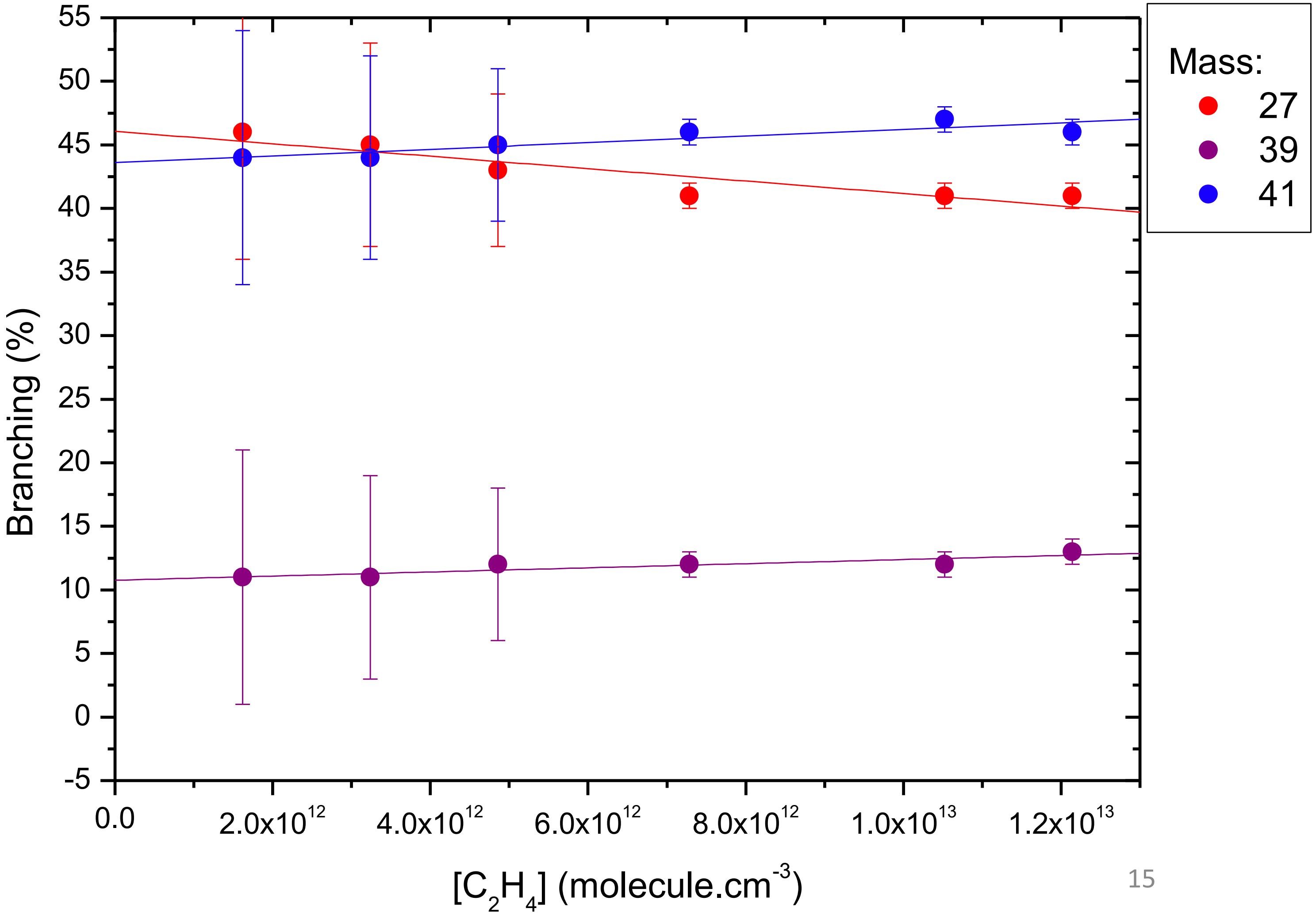




Reaction $CH_3^+ + C_2H_4$: branching ratios at 24.1K

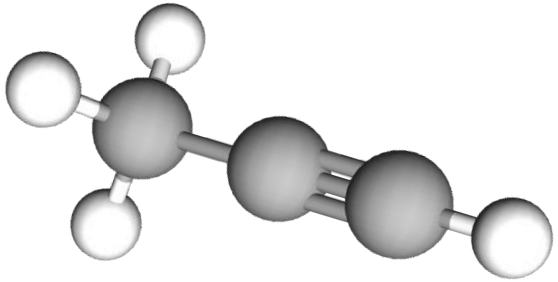
		Branching ratio (%)
$CH_3^+ + C_2H_4$	$\rightarrow C_2H_3^+ + CH_4$	46
	$c\text{-}C_3H_3^+ + 2H_2$	11
	$c\text{-}C_3H_5^+ + H_2$	43

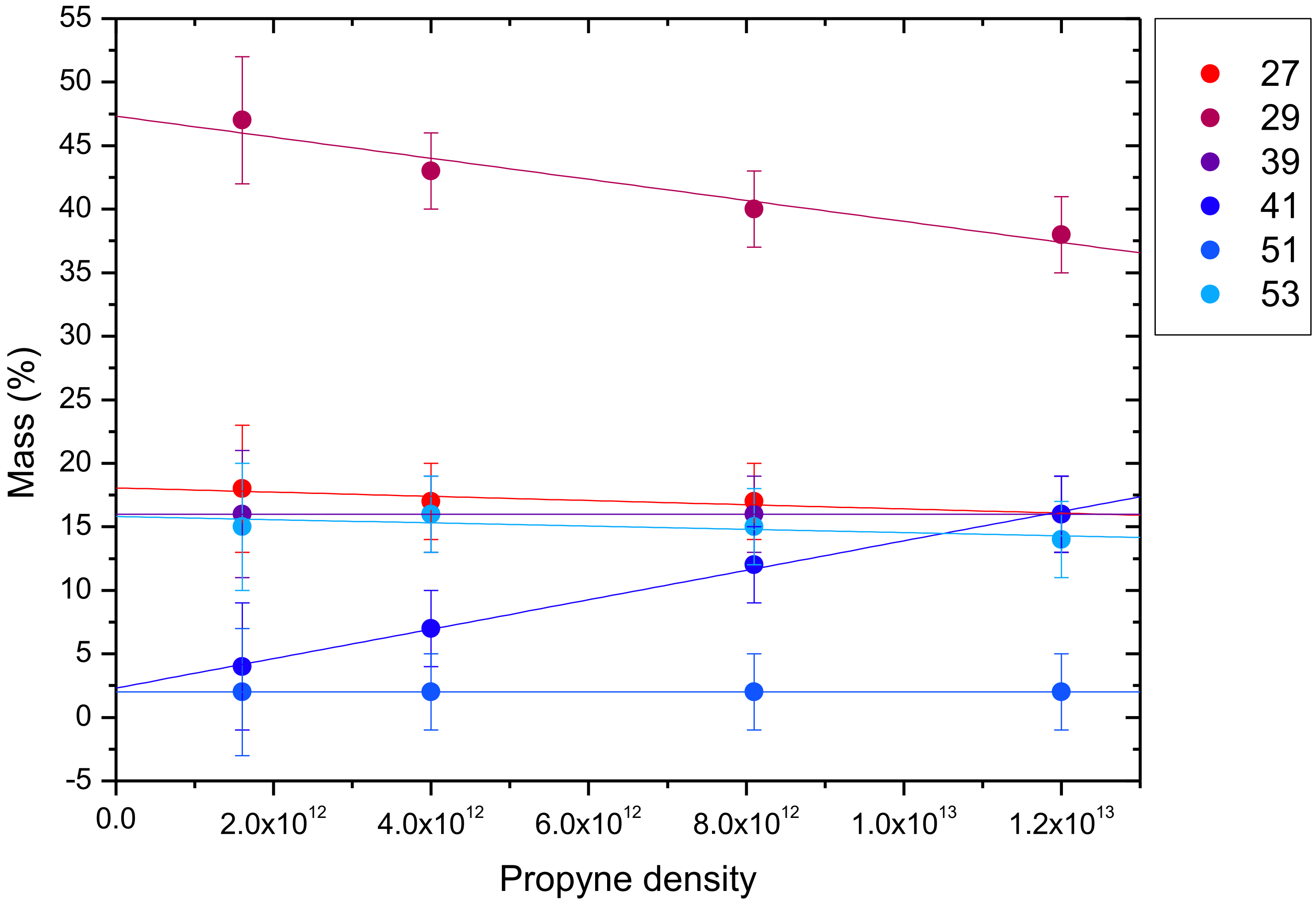




Reaction $CH_3^+ + C_3H_4$: branching ratios at 24.1K

		Branching ratio (%)
$CH_3^+ + C_3H_4$	$\rightarrow C_2H_3^+ + CH_4$	18
	$C_2H_5^+ + CH_3$	47
	$C_3H_3^+ + 2H_2$	16
	$C_3H_5^+ + H_2$	2
	$C_4H_3^+ + 2H_2$	2
	$C_4H_5^+ + H_2$	15



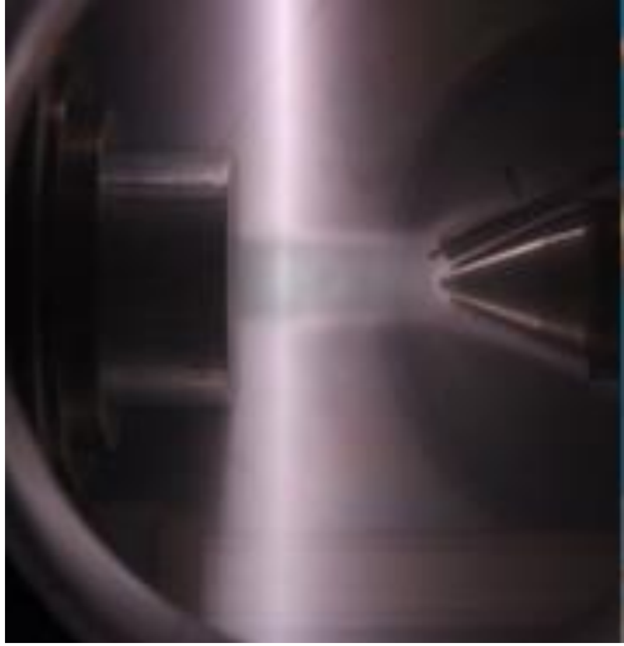


Reaction CH_3^+: experimental branching ratios

				Branching ratios			
				This work 24.1K		*Measurements 298K	
Reactive		Products	mass of the ionic product (amu)	Value (%)	Error (%)	Value (%)	
CH_3^+ +CH_4	→	**$C_2H_5^+$ + H_2**	**29**	**100**		100	**Always promotes growth**
CH_3^+ +C_2H_4	→	$C_2H_3^+$ + CH_4	27	46	9	46	**Promotes growth in 57% of cases**
		$C_3H_3^+$ + 2H_2	**39**	**11**	7	4	
		$C_3H_5^+$ +H_2	**41**	**43**	12	51	
CH_3^+ +C_3H_4	→	$C_2H_3^+$ + C_2H_4	27	18	4	**No previous measurements**	**Promotes growth in 17% of cases**
		$C_2H_5^+$ +C_2H_2	29	47	11		
		$C_3H_3^+$ + CH_4	39	16	1		
		$C_3H_5^+$ +CH_3	41	2	3		
		$C_4H_3^+$ + 2 H_2	**51**	**2**	1		
		$C_4H_5^+$ + H_2	**53**	**15**	7		

Anicich, V. G. (2003). *An index of the literature for bimolecular gas phase cation-molecule reaction kinetics* (No. JPL-Publ-03-19).

Conclusions



The CRESU Method:

- Unique tool to study ion reactions with large neutrals at low temperatures down to 10 K.

Reactivity of CH_3^+ ion :

- The methenium ion CH_3^+ seems to equally promote growth at both high and low temperatures.
- Another example of the synergy between theory and experimental works.

Next step :

- Branching ratios for the CH_3^+ ion with abundant interstellar co-reactants: Acetylene C_2H_2, Methanol CH_3OH, Cyano-acetylene HC_3N, Acetonitrile CH_3CN and Ammonia NH_3.
- Method to study termolecular reactions ($A^+ + B + M \rightarrow AB^+ + M$), and derive an upper limit of radiative association rates ($A^+ + B \rightarrow AB^+ + \text{Photon}$).

Acknowledgments

IPR RESEARCH

- Elliot OGDEN
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- Francesca TONOLO

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- Jonathan THIÉVIN
- Jonathan COURBE

COLLABORATIONS

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- Jean Christophe Loison

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Université de Rennes

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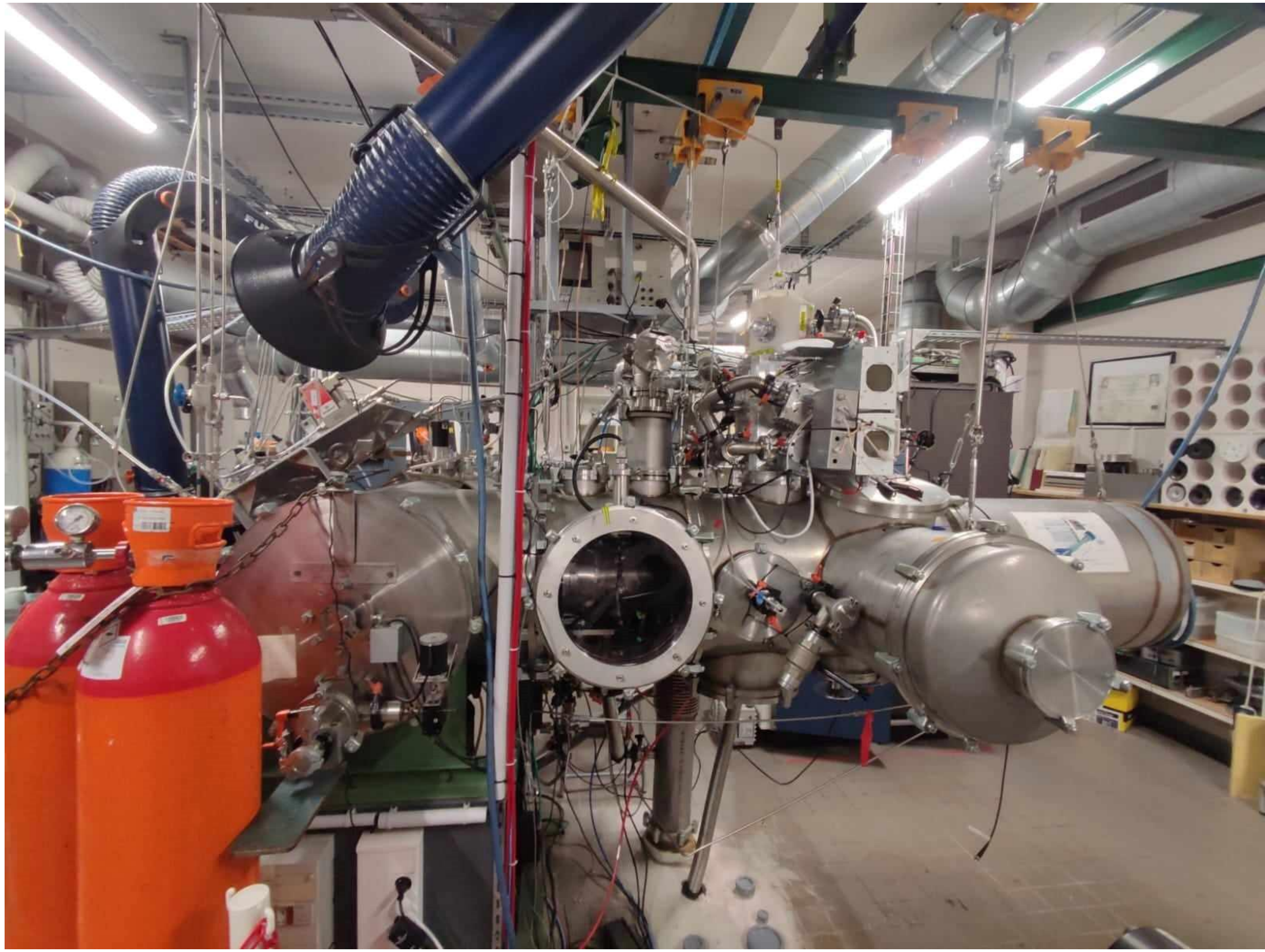

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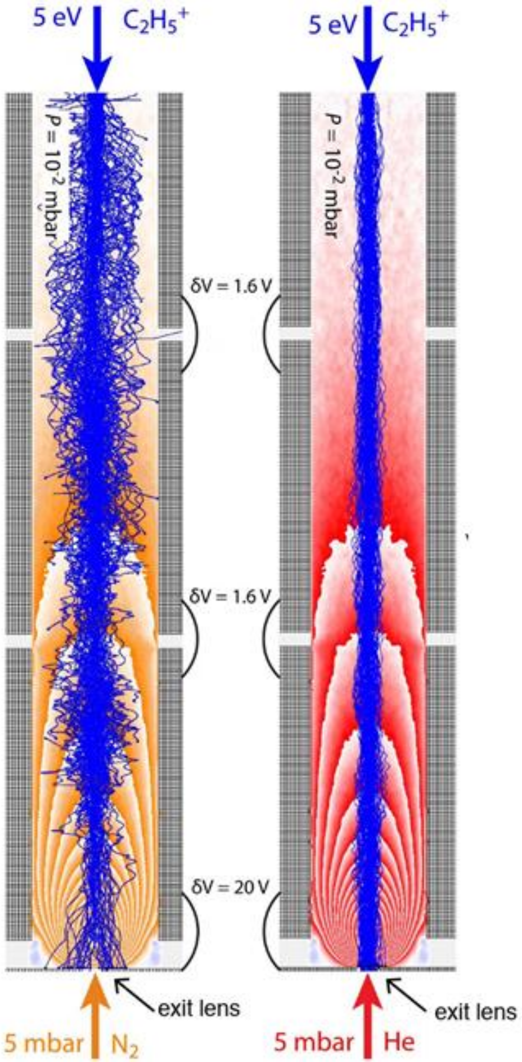
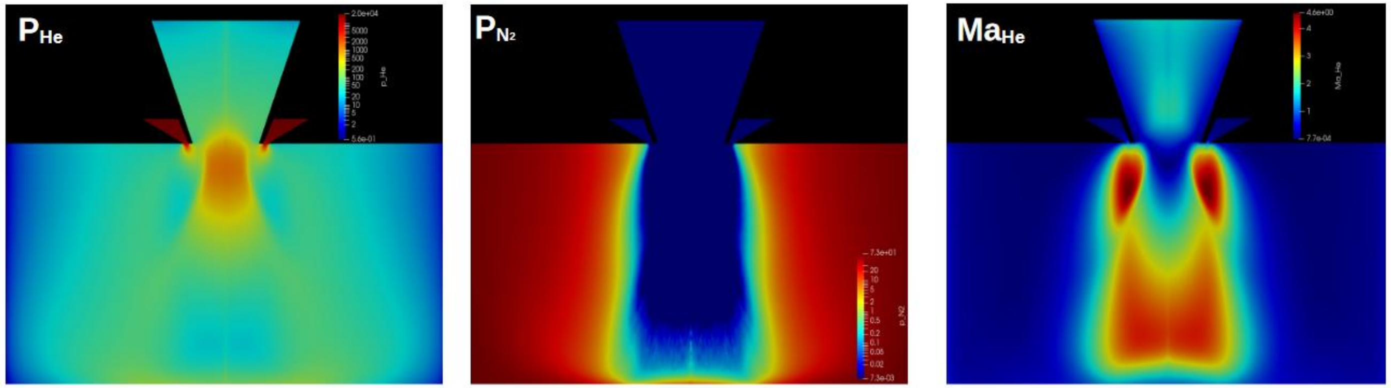
- Ahmad MORTADA, Ion-molecule reactions at low temperature with uniform supersonic flows and insights into the chemistry of astrophysical environments
- Ahmad Mortada, Sophie Carles, Sándor Demes, Baptiste Joalland, François Lique, Abdessamad Benidar, Panayotis Lavvas, and Ludovic Biennier

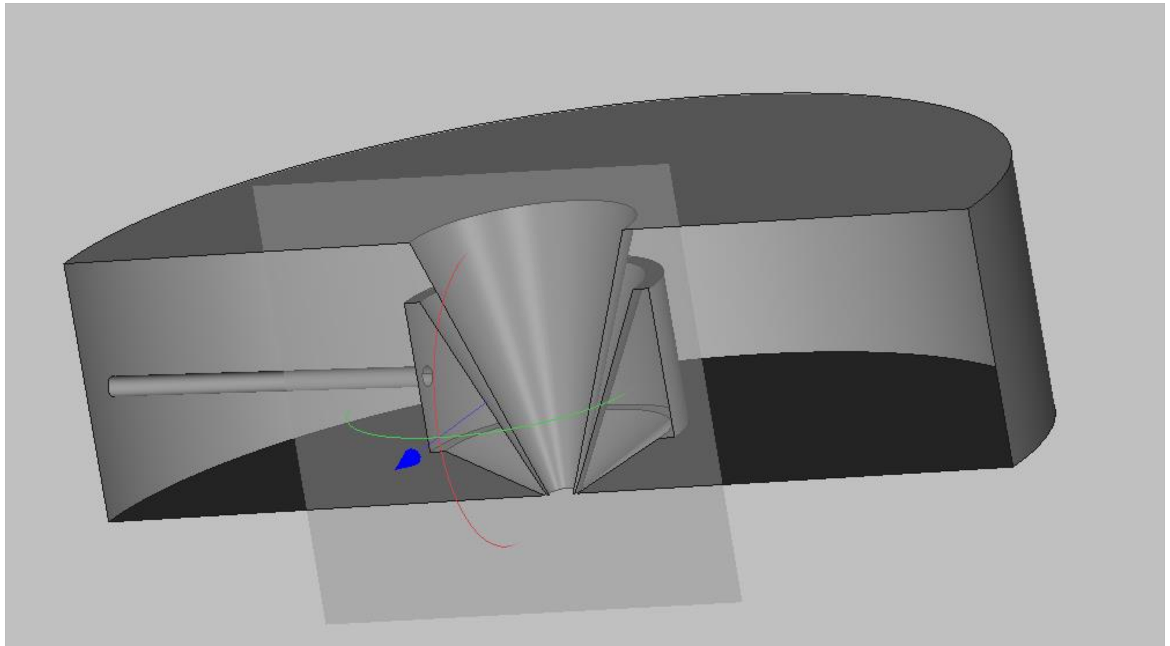
CRESU-SIS_Venturi-100um_He_nplus_Remesh

$P_{flush,He}$ = 20000 Pa
$Q_{v,std}$ = 10 slm

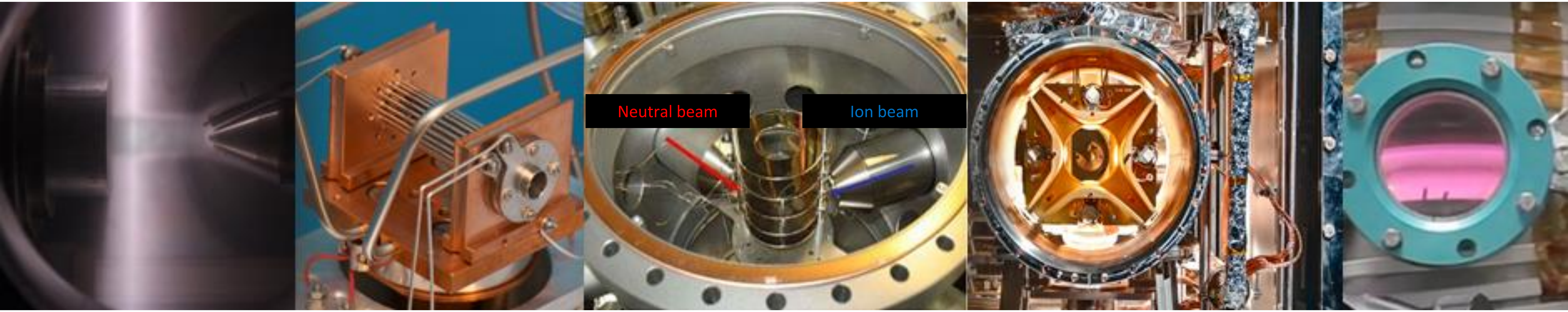




Direct Simulation
Monte Carlo,
N. Suas-David



Design: Jan Zabka,
J.Heyrovsky Institute
of physical Chemestry



flows ❶	Traps ❷	Crossed beams ❸	Storage rings ❹	Simulation chamber ❺
$k(T)$	$k(T)$	$\sigma(E)$, Dynamics	$\sigma(E)$	mécanismes
6—1800 K	A few K	Typ. 0.1– 5 eV	> meV	Variable T