DESTRUCTION OF INTERSTELLAR DIMETHYL ETHER IN COLLISIONS WITH $\text{He}^+$

SUPERVISORS: D. ASCENZI, P. TOSI
ATOMIC AND MOLECULAR PHYSICS LAB
### List of interstellar molecules (NASA Goddard, July 2014)

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### AROUND 200 MOLECULES

- **SEEDS OF LIFE**
- **ASTROCHEMICAL CLOCKS**
Precursors of biopolymers
THE PHYSICAL CONDITIONS

TEMPERATURE & DENSITY (H)

Interstellar clouds are very cold environments, with low probabilities of collisions

From 100 K and 1-100 cm$^{-3}$ in diffuse clouds

To 10 K and $10^4$-$10^6$ cm$^{-3}$ in dense clouds

CHEMISTRY IS POSSIBLE IN THE ISM VIA BARRIERLESS REACTIONS

▸ GAS-SURFACE PROCESSES
▸ GAS-PHASE PROCESSES

GENERAL CATEGORIES

DESTRUCTION PROCESSES

- UV PHOTONS

- COSMIC RAYS (keV-MeV)

- IONS (H\(^+\) - H\(_3\)\(^+\) - He\(^+\) - C\(^+\) - HCO\(^+\))

The dissociative charge transfer

\[ \text{He}^+ + \text{DME} \rightarrow \text{He} + (\text{DME}^+)^* \rightarrow \text{He} + \text{FRAGMENTS} \]

\[ \text{He}^+ + \text{MF} \rightarrow \text{He} + (\text{MF}^+)^* \rightarrow \text{He} + \text{FRAGMENTS} \]

One of the most important destruction mechanisms in interstellar space
THE GUIDED ION BEAM–MASS SPECTROMETER
IN LAB

OBSERVABLES

BRANCHING RATIOS

\[ A^+ + B \rightarrow P_1 + P_2 + \ldots + P_N \]

\[ \text{BR} = 100 \times \frac{P_i}{\sum P_i} \]

ABSOLUTE REACTIVE CROSS SECTIONS

\[ I = I_0 (1 - e^{-\sigma \rho}) \]

Lambert-Beer Law
IN LAB

OBSERVABLES

BRANCHING RATIOS

\[ A^+ + B \rightarrow P_1 + P_2 + \ldots + P_N \]

\[ \text{BR} = 100 \times \frac{P_i}{\sum P_i} \]

- \( l \) = product intensity
- \( l_0 \) = reagent intensity
- \( l \) = effective length of the scattering cell
- \( \rho \) = density
- \( \sigma \) = cross section

ABSOLUTE REACTIVE CROSS SECTIONS

\[ l = l_0(1 - e^{-l \sigma \rho}) \]

Lambert-Beer Law
THE RESULTS

He$^+$ + DME →

A. Cernuto et al., PCCP, 2017, 19, 554-565
From the diabatic curves it’s possible to obtain the transition probability $P$.

The total cross section in semiclassical approximation is given by

$$
\sigma(E) = \frac{\pi}{k^2} \sum_l P(l)(2l + 1)
$$

THE LANDAU-ZENER-STÜCKELBERG MODEL

As the nuclei pass twice through the crossing region,

\[ P = 2p(1 - p) \]

The non adiabatic single-passage probability \( p \) is expressed by the formula of L-Z-S:

\[ p(E, l) = \exp \left( - \frac{2\pi H^2}{\hbar n_r \Delta} \right) \]

THE PES

THE INTERACTION POTENTIAL IN [He−DME]+
1. Electrostatic contribution ($V_{\text{Elec}}$)

$$V(R, \theta, \varphi) = \frac{e^2}{4\pi \varepsilon_0} \left( -\frac{\delta^O}{R_{\text{He}^+ - O}} + \frac{\delta^{+C_1}}{R_{\text{He}^+ - C_1}} + \frac{\delta^{+C_2}}{R_{\text{He}^+ - C_2}} \right)$$
THE ENTRANCE CHANNEL

THE $\text{He}^+ + \text{DME}$ INTERACTION

1. Electrostatic contribution ($V_{\text{Elec}}$)

2. Non Electrostatic contribution ($V_{\text{NElec}}$):
   Improved Lennard Jones Potential ($V_{\text{ILJ}}$)

$$V_{\text{NElec}}(R, \theta, \varphi) = V_{\text{ILJ}}(R_0) + V_{\text{ILJ}}(R_{C1}) + V_{\text{ILJ}}(R_{C2})$$

$$V_{\text{ILJ}}(r) = \varepsilon \left[ \frac{m}{n(r) - 4 \left( \frac{r_m}{r} \right)^n(r)} - \frac{n(r)}{n(r) - m \left( \frac{r_m}{r} \right)^m} \right]$$

F. Pirani et al., *PCCP*, 2008, 10, 5489-5503
THE EXIT CHANNEL

THE \( \text{He} + \text{DME••}^+ \) INTERACTION

1. Induction contribution (\( V_{\text{Ind}} \))

\[
V_{\text{Ind}}(R) = -\frac{e^2}{4\pi \varepsilon_0} \frac{\alpha_{\text{He}}}{R^4}
\]

THE **HE + DME**\textsuperscript{+} INTERACTION

1. Induction contribution ($V_{\text{Ind}}$)

2. Van der Waals contribution ($V_{\text{vdW}}$)

\[V_{\text{vdW}}(R, \theta, \varphi) = V'_{ILJ}(R_0) + V'_{ILJ}(R_{C1}) + V'_{ILJ}(R_{C2})\]

\[V_{ILJ}(r) = \varepsilon \left[ \frac{m}{n(r) - 4 \left( \frac{r_m}{r} \right)^n} - \frac{n(r)}{n(r) - m \left( \frac{r_m}{r} \right)^m} \right]\]

F. Pirani et al., PCCP, 2008, 10, 5489-5503
THE PES

THE CROSSINGS

A. Cernuto et al., PCCP, 2017, 19, 554-565
The realistic representation of the He$^+$-DME interaction allows to estimate the stereochemistry of the process at low $E_{\text{coll}}$ with strong orientation of the colliding system.
THE COMPLEX SYSTEM

THE PARADOX

THE STRONGEST ATTRACTIVE DIRECTION SHOULD BE ALSO THE LESS REACTIVE

CORRECTION OF COUPLING TERM (H)
FINALLY

THE RESULT: TOTAL CROSS SECTION

AGREEMENT WITH THE EXPERIMENTAL RESULTS AT LOW $E_{\text{coll}}$

A. Cernuto et al., PCCP, 2017, 19, 554-565
CONCLUSIONS

- Experimental results necessary to improve astrochemical models
- The anisotropy of the interaction and the electron densities of the involved orbitals are crucial to understand and to model the charge transfer processes of complex colliding systems
WHAT ARE WE PLANNING?

FUTURE PROSPECTS

- Use the new $k(T)$ in the astrochemical models (C. Ceccarelli - IPAG Grenoble)
- Reactions with other COMs such as methanol, ethanol, acetic acid, glycolaldehyde, acetaldehyde, acetone, ...
D. ASCENZI, P. TOSI AND THE FAM GROUP

F. PIRANI (PERUGIA)

N. BALUCANI (PERUGIA)

C. CECCARELLI (GRENOBLE)
ACKNOWLEDGEMENT

THANK YOU FOR YOUR ATTENTION