

PAPER • OPEN ACCESS

## Non-adiabatic transitions in the near-UV photodissociation of $\text{H}_3^+$

To cite this article: X Urbain *et al* 2020 *J. Phys.: Conf. Ser.* **1412** 102007

View the [article online](#) for updates and enhancements.



**IOP | ebooks™**

Bringing together innovative digital publishing with leading authors from the global scientific community.

Start exploring the collection—download the first chapter of every title for free.

## Non-adiabatic transitions in the near-UV photodissociation of $\text{H}_3^+$

X Urbain<sup>1\*</sup>, A Dochain<sup>1</sup>, R Marion<sup>1</sup>, T Launoy<sup>1,2</sup> and J Loreau<sup>1,2</sup>

<sup>1</sup>Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, chemin du cyclotron 2, B-1348 Louvain-la-Neuve, Belgium

<sup>2</sup>Laboratoire de Chimie Quantique et Photophysique, Université libre de Bruxelles, Av. F. Roosevelt 50, B-1050 Brussels, Belgium

**Synopsis** The near-UV photodissociation of  $\text{H}_3^+$  has been studied in a fast beam experiment. The kinetic energy release and branching ratio among the fragmentation channels were obtained by three-dimensional imaging of the dissociation products. It is found that the photodissociation of vibrationally excited  $\text{H}_3^+$  mostly produces vibrationally cold  $\text{H}_2^+$  and hot  $\text{H}_2$ . The non-adiabatic repopulation of the ground potential energy surface after excitation is accounted for by modelling the wavepacket dynamics on the intersecting potential energy surfaces.

The molecular ion  $\text{H}_3^+$  is observed in many astrophysical environments [1], playing a central role in the interstellar medium for the formation of hydrides and as a tracer of particle precipitation in the upper atmosphere of giant planets.  $\text{H}_3^+$  is also a key species to understand deuterium fractionation.

The ground and first excited  $^1A'$  potential energy surfaces of  $\text{H}_3^+$  exhibit an avoided crossing seam at large  $\text{H}_2 - \text{H}^+$  separation [2]. While the charge transfer reactions  $\text{H}_2 + \text{H}^+ \rightleftharpoons \text{H}_2^+ + \text{H}$  probe this crossing seam in a full collision, the photodissociation of  $\text{H}_3^+$  is actually probing it from within, as fragments depart from the classical turning point accessed via a vertical transition from the ground state potential well.

In this work, we consider the electronic excitation of the  $\text{H}_3^+$  ground state to the first excited  $^1A'$  state by UV photons of 3 to 5 eV, that triggers rapid dissociation into  $\text{H}_2 + \text{H}^+$  and  $\text{H}_2^+ + \text{H}$  products at wavelengths from 266 nm to 410 nm. Such wavelengths mainly probe the photodissociation from highly excited vibrational states of  $\text{H}_3^+$  that are populated following its formation in the ion source plasma. This observation is corroborated by the storage ring experiments of Petrigani et al [3] that displayed a rapid decay of the photodissociation signal vs. storage time.

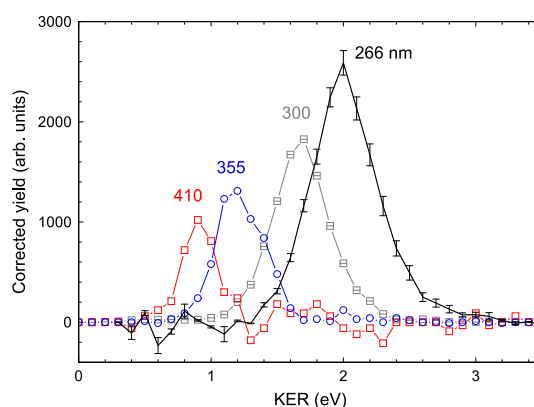
An analysis of the kinetic energy release of both channels was performed, showing a dominant contribution from the  $\text{H}_2^+ + \text{H}$  channel with  $\text{H}_2^+$  in the ground vibrational state. On the other hand, a strong vibrational excitation was observed for the  $\text{H}_2$  fragments.

These findings were rationalised by perform-

\*E-mail: [xavier.urbain@uclouvain.be](mailto:xavier.urbain@uclouvain.be)

ing time-dependent wavepacket simulations of the photodissociation process, demonstrating the impact of the non-adiabatic seam on the dynamics [4].

This work was supported by the Fonds de la Recherche Scientifique-FNRS through IISN grant No. 4.4504.10.



**Figure 1.** Measured kinetic energy release distributions for the  $\text{H}_2^+ + \text{H}$  channel at various wavelengths. Integrated counts are corrected for the geometrical acceptance of the detection system and the contribution of rest gas collisions.

### References

- [1] Oka T 2013 *Chem. Rev.* **113** 8738-8761
- [2] Preston R K and Tully J C 1971 *J. Chem. Phys.* **54** 4297
- [3] Petrigani A *et al* 2010 *J. Phys. Chem. A* **114** 4864
- [4] Urbain X *et al* 2019 submitted for publication in *Phil. Trans. R. Soc. A*

