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Vibrational spectroscopy of selectively prepared gas phase ions by coupling an FT-ICR-MS with a Free Electron Laser

Joël Lemaire,^{a,b} Luke MacAleese,^a Catherine Kapota,^c

Gilles Ohanessian,^c Pierre Boissel,^a Jean-Michel Ortega,^b Philippe Maître^a

^a Laboratoire de Chimie Physique, UMR 8000 du CNRS, Université de Paris-Sud, 91405 Orsay, France.

^b Laboratoire pour l'Utilisation du Rayonnement Electromagnétique, UMR 130 du CNRS, Université de Paris-Sud, CLIO-BP34, 91405 Orsay, France.

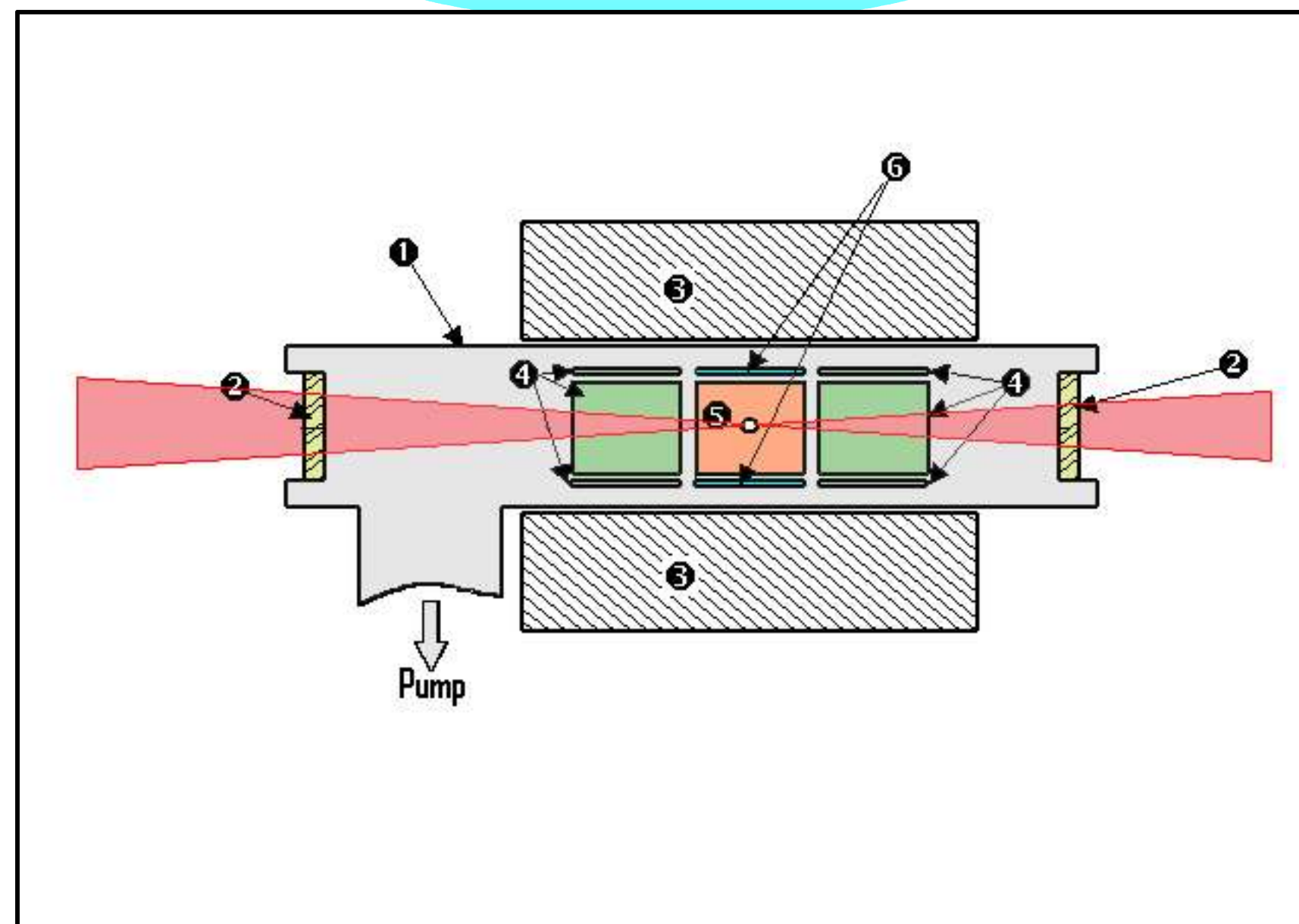
^c Laboratoire des Mécanismes Réactionnels, UMR 7651 du CNRS, Ecole Polytechnique, 91128 Palaiseau CEDEX, France.

Goals

The present studies aim at characterizing selectively prepared ions by infrared spectroscopy. The spectra are obtained by monitoring InfraRed MultiPhoton Dissociation (IRMPD) for which the use of an intense laser source is required. IR Free Electron Laser offering both high peak power and wide tunability are ideally suited for this particular spectroscopy.

Coupling with a Fourier Transform Ion Cyclotron Resonance Mass Spectrometer (FT-ICR-MS) gives access to a wide range of chemical species and allows for the study of reaction intermediates.

MICRA



The FTICR mass spectrometer MICRA (Mobile ICR Analyzer) is based on a 1.25 Tesla permanent magnet. The ions can be prepared by electron ionization, laser ablation or Matrix Assisted Laser Desorption.

Several ion reaction and mass selection steps can be performed before irradiation of the ions with the focussed IR beam.

CLIO

Characteristics of the CLIO free electron laser :

Tuning range : 3 – 120 μm

Average power : 1W peak power 40 MW

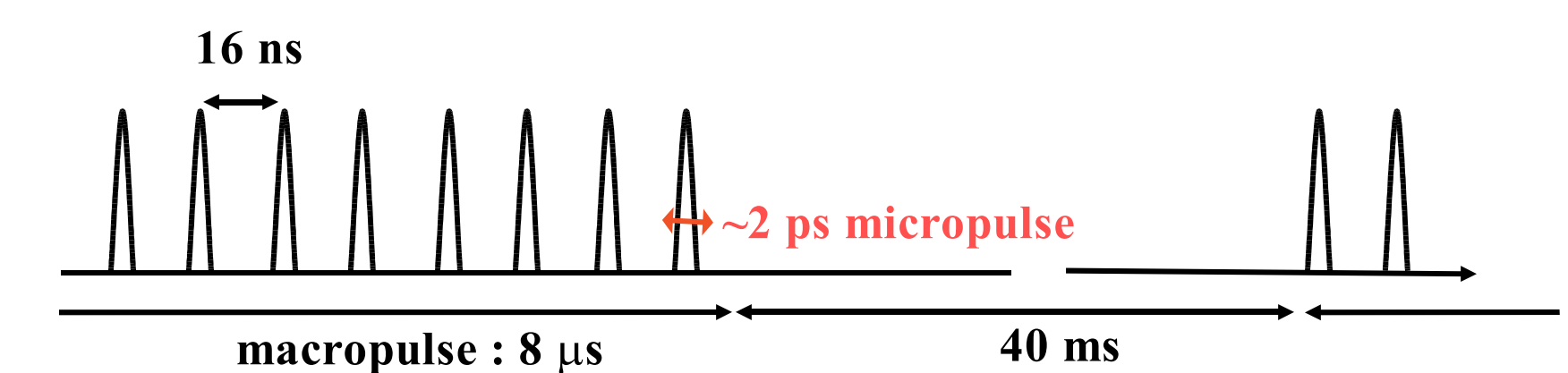
Continuously tunable over $\Delta\lambda/\lambda = 2.5$

Bandwidth 0.5% - 1%

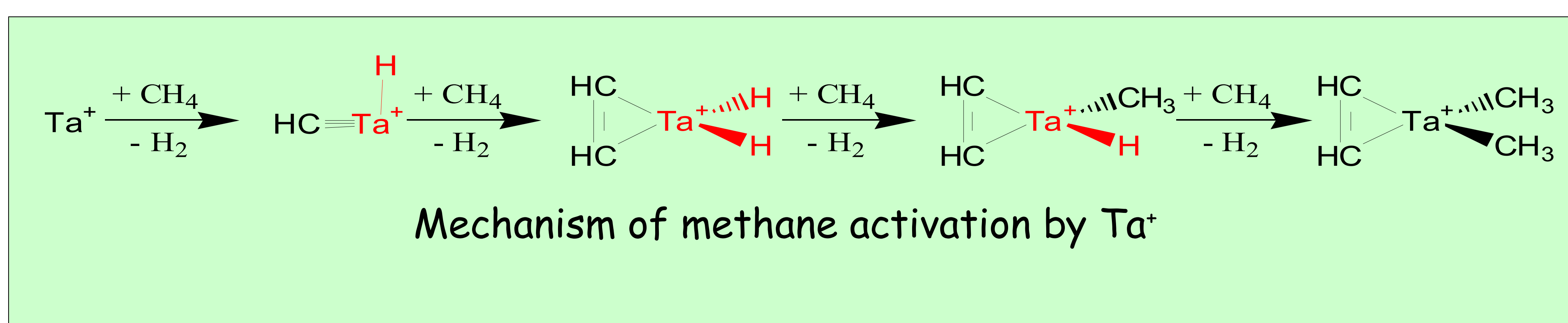
8 μs long macropulses, 25 Hz repetition rate

A macropulse contains 500 micropulses

The laser is focussed by a 1m focal length spherical mirror (waist diameter ~200 μm for $\lambda=5 \mu\text{m}$)



IR spectroscopy of reactive intermediates

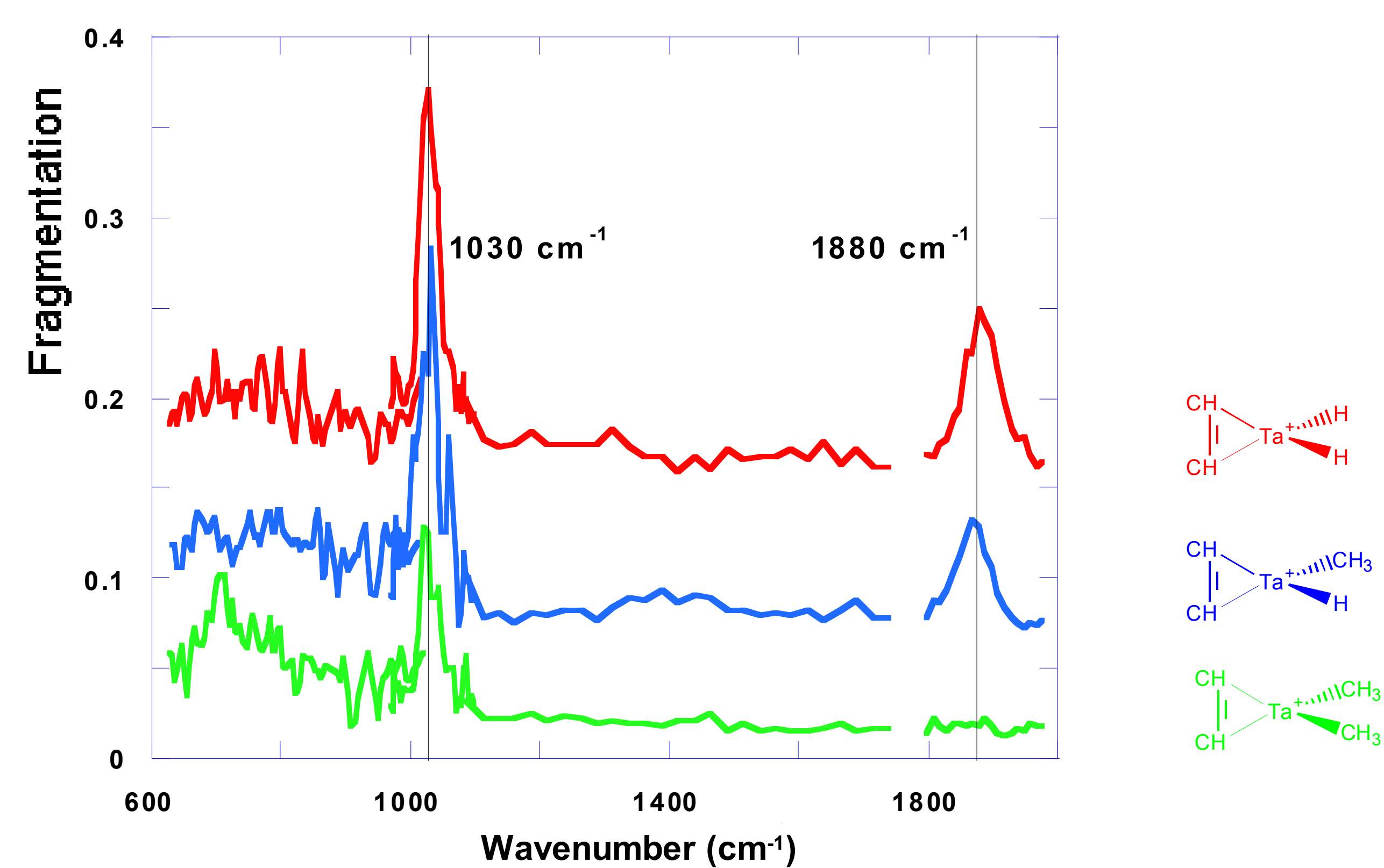


IRMPD has been used to characterize the mechanism of the sequential dehydrogenation of four methane molecules by third row transition metal cation Ta⁺.

Ta⁺ was produced by laser ablation on a tantalum foil. After reaction with methane the different reaction intermediates TaC_nH_{2n}⁺, n=2-4 have been isolated and characterized by their infrared spectra.

The band at 1880 cm⁻¹, characteristic of the Ta-H bond is observed for TaC₂H₄⁺ and TaC₃H₆⁺ but not for TaC₄H₈⁺ while the band at 1030 cm⁻¹ characteristic of the metallacycle is observed for the three intermediates.

These results provide evidence for methane activation through σ-bond metathesis..



Sodiated amino acids : salt bridge versus charge solvation structures

The sodium complexes of glycine and proline are formed by MALDI on a target located in front of the trapping plate.

They are transferred in the ICR cell, trapped and irradiated with the IR beam. The resulting experimental dissociation spectra are compared with the calculated spectra for the low energy isomeric forms.

In the case of Pro-Na⁺ the complex is found to have a salt bridge structure while in the case of Gly-Na⁺ the observed spectra corresponds to charge solvation by chelation of Na⁺ between nitrogen and the carbonyl oxygen.

