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Vibrational spectroscopy of selectively prepared gas phase ions

by coupling a permanent magnet based FT-ICR-MS with a Free Electron Laser

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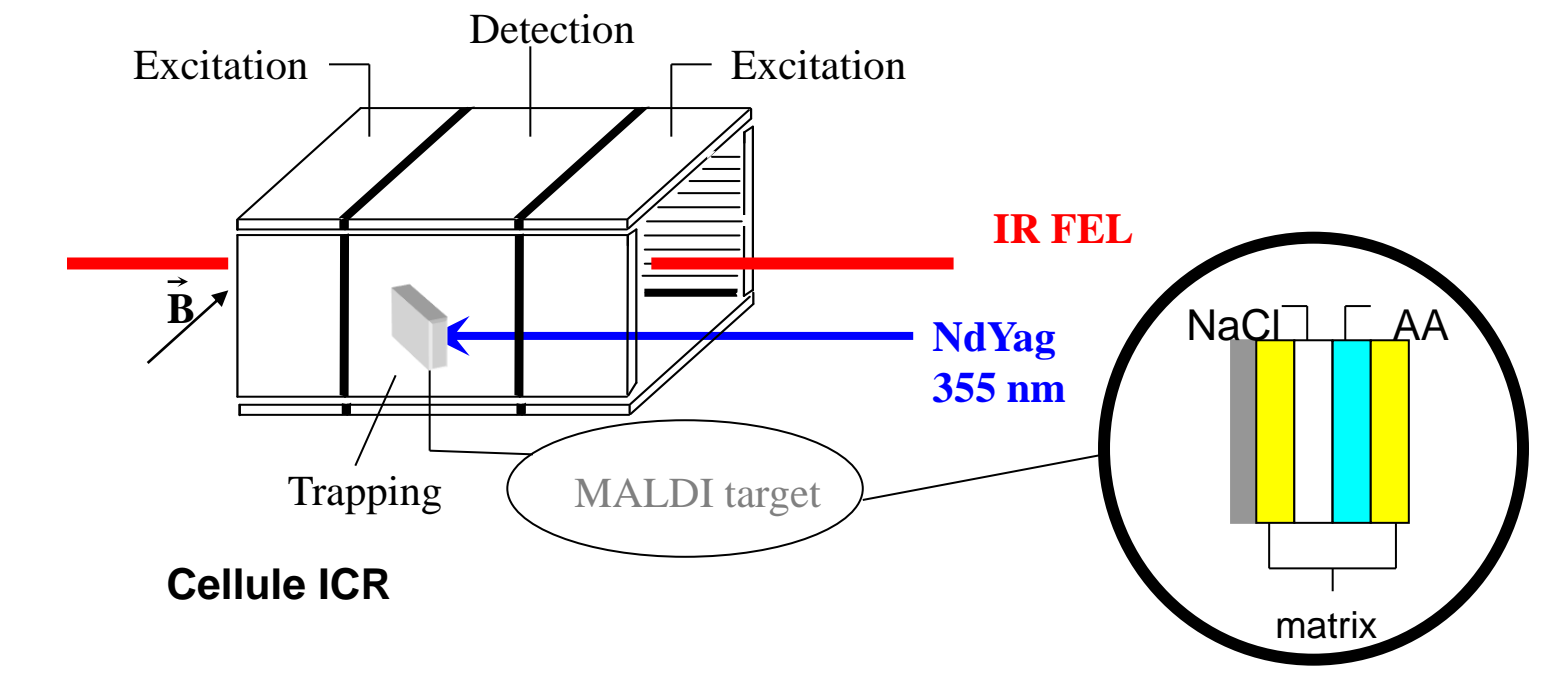
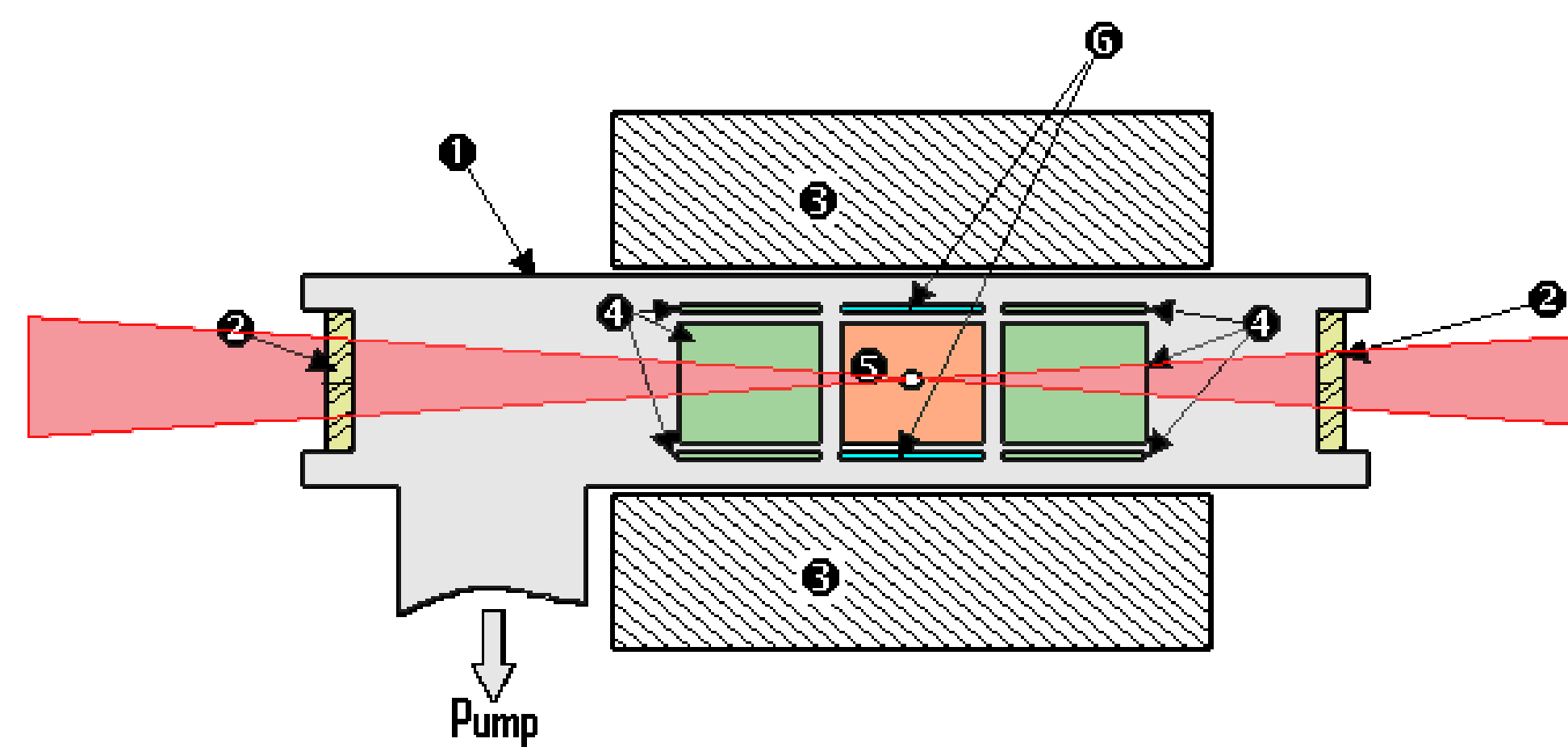
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The InfraRed Multiphoton Dissociation experiments are realised with a Mobile Ion Cyclotron Resonance Analyzer (MICRA), associated to the Orsay Free Electron Laser CLIO. The mass spectrometer is based on the use of a permanent magnet assembly (Halbach cylinder) producing a nominal magnetic field of 1.25T.

The geometry of the ICR cell allows an easy optical access to the cell center : the cell is derived from a cubic cell where the two excitation plates are replaced by two tunnels made of four interconnected electrodes.



Available ionisation modes :

-Electron impact

-Formation of metal cations by laser ablation ionisation on a metallic target

-MALDI

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

Characteristics of the Free Electron Laser CLIO

Tuning range : 3 – 120 μm

Average power : 1W peak power 40 MW

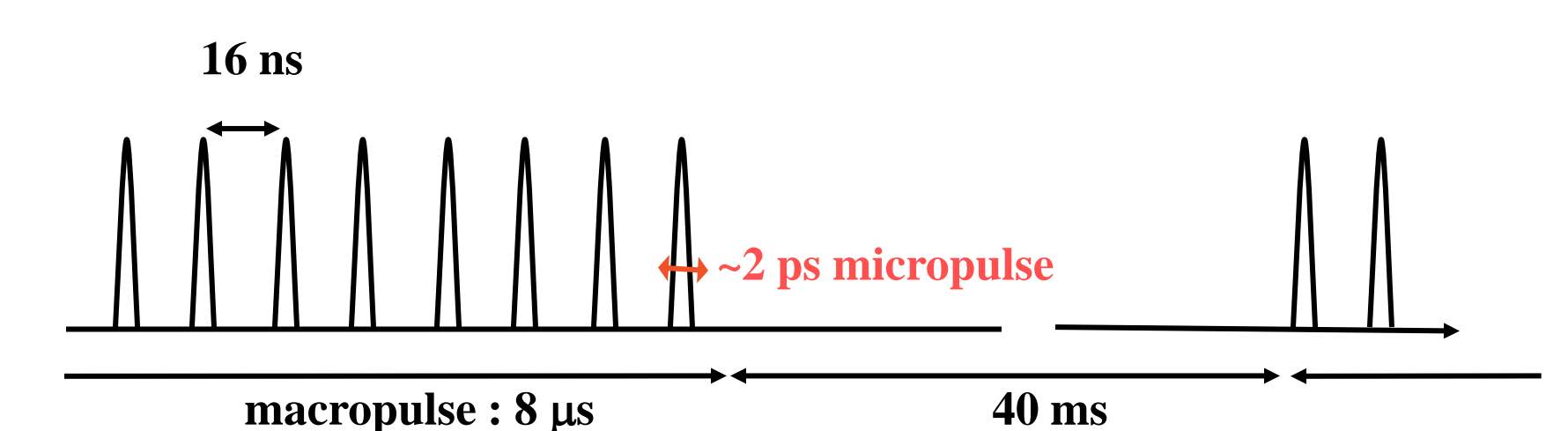
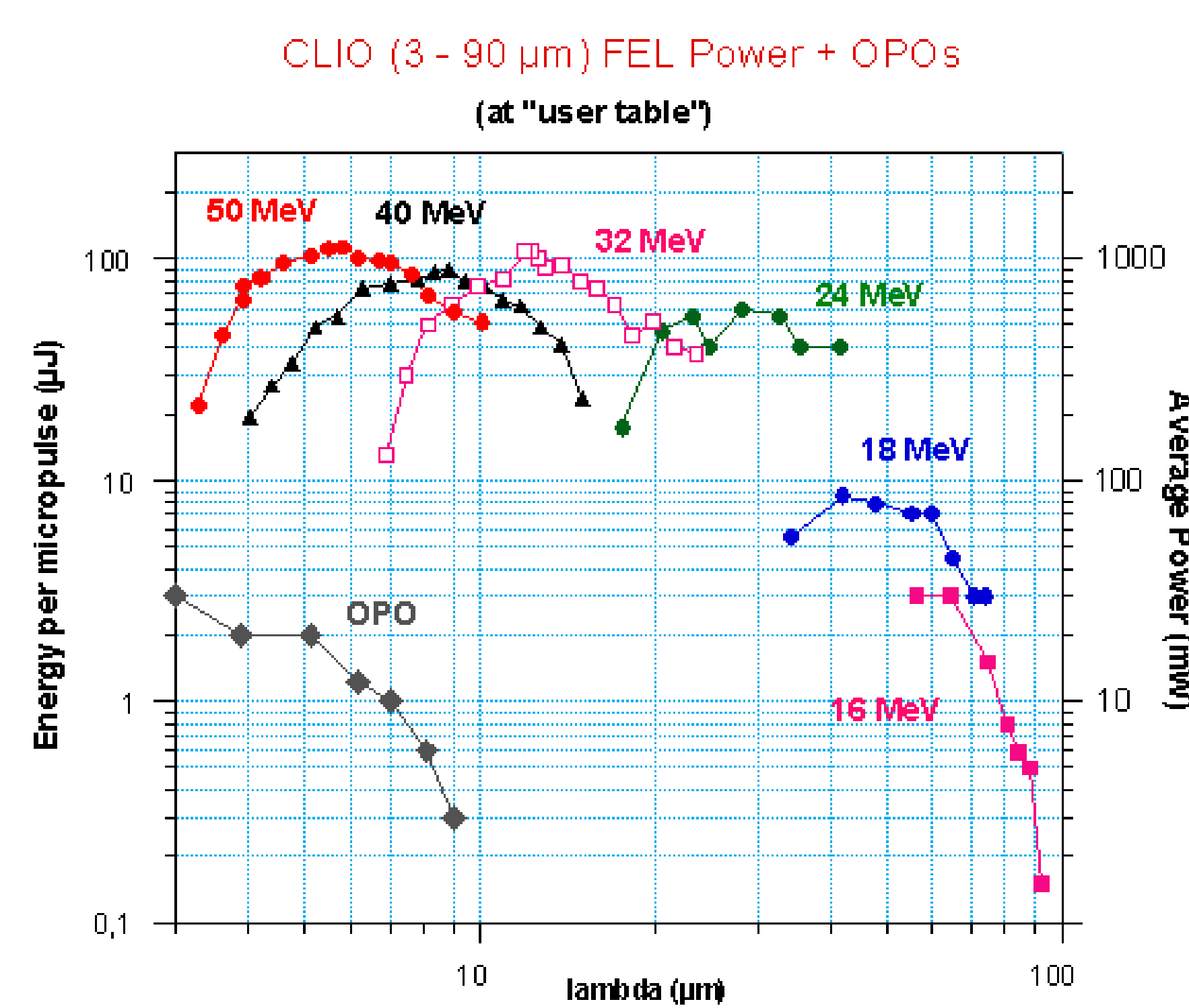
Continuously tunable over $\Delta\lambda/\lambda = 2.5$

Bandwidth 0.5% - 1% of the central wavelength

8 μs long macropulses, 25 Hz repetition rate

A macropulse contains 500 micropulses

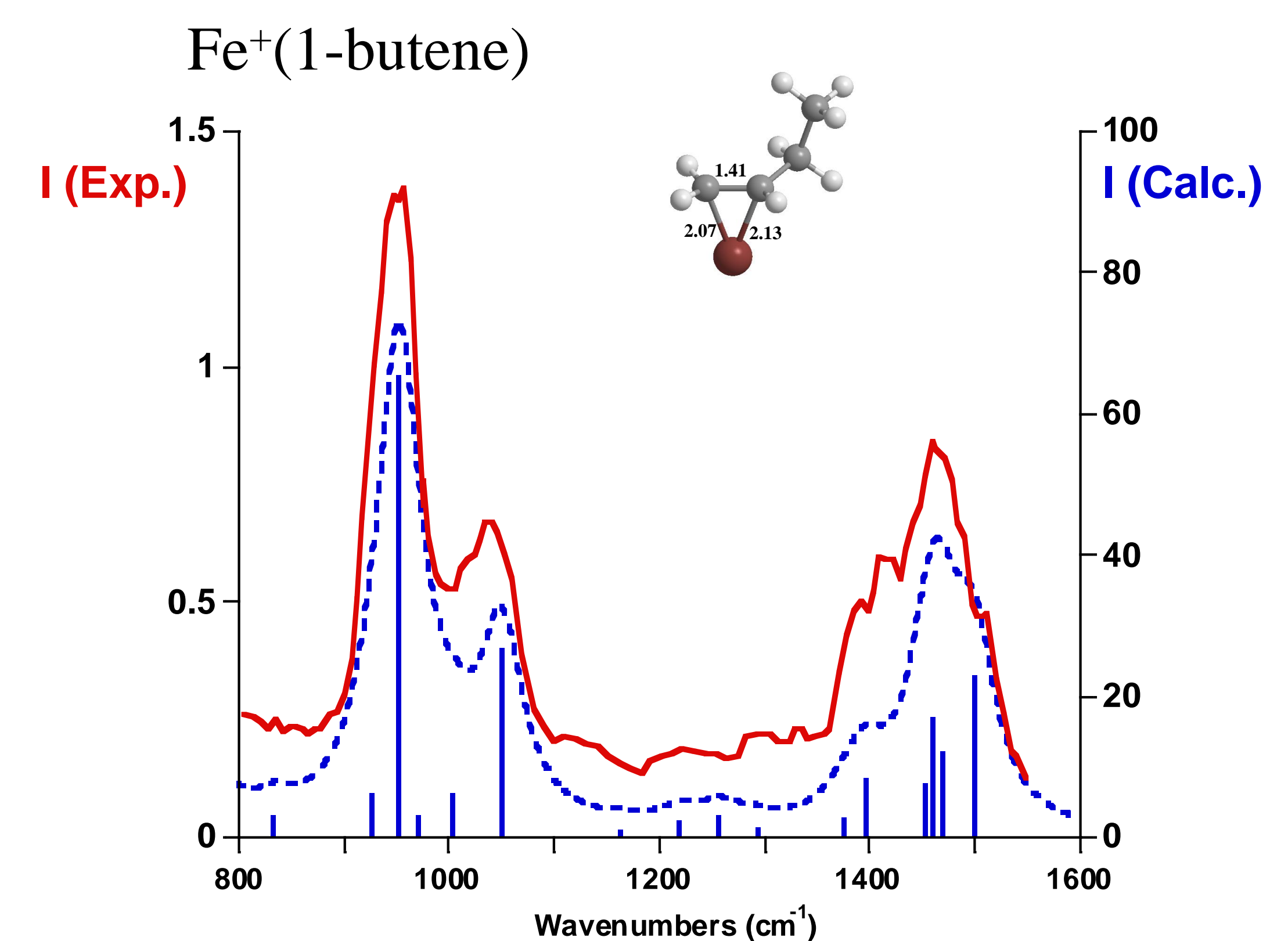
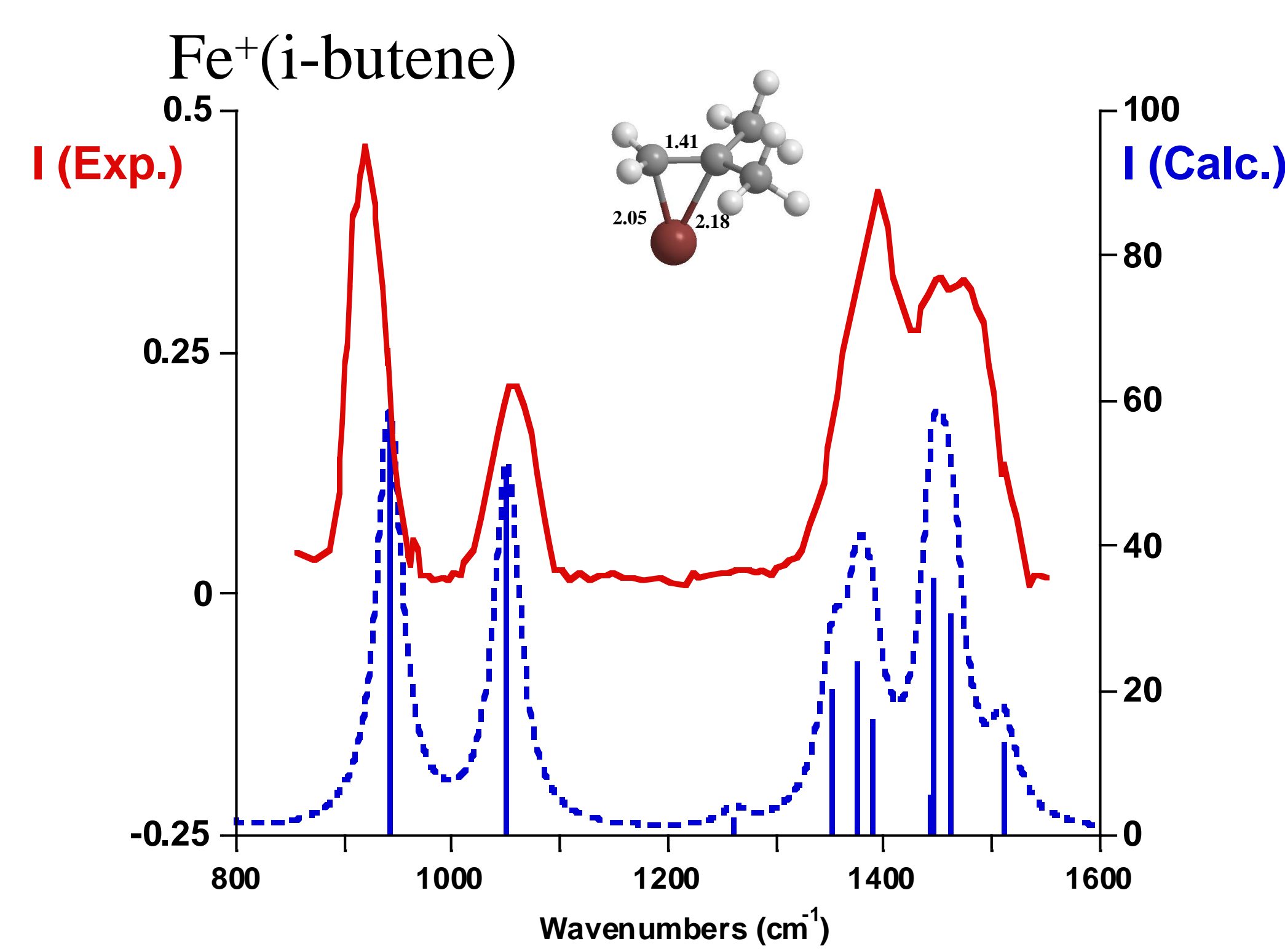
The laser is focussed by a 1m focal length spherical mirror (waist diameter $\sim 200 \mu\text{m}$ for $\lambda = 5 \mu\text{m}$)



InfraRed spectroscopy of metal-ligand complexes : differentiation of isomers

$\text{Fe}^+(\text{i-butene})$ is prepared by deshydrogenation of i-butane by mass selected Fe^+

$\text{Fe}^+(\text{1-butene})$ is formed by ligand displacement from mass selected FeCO^+ by 1-butene

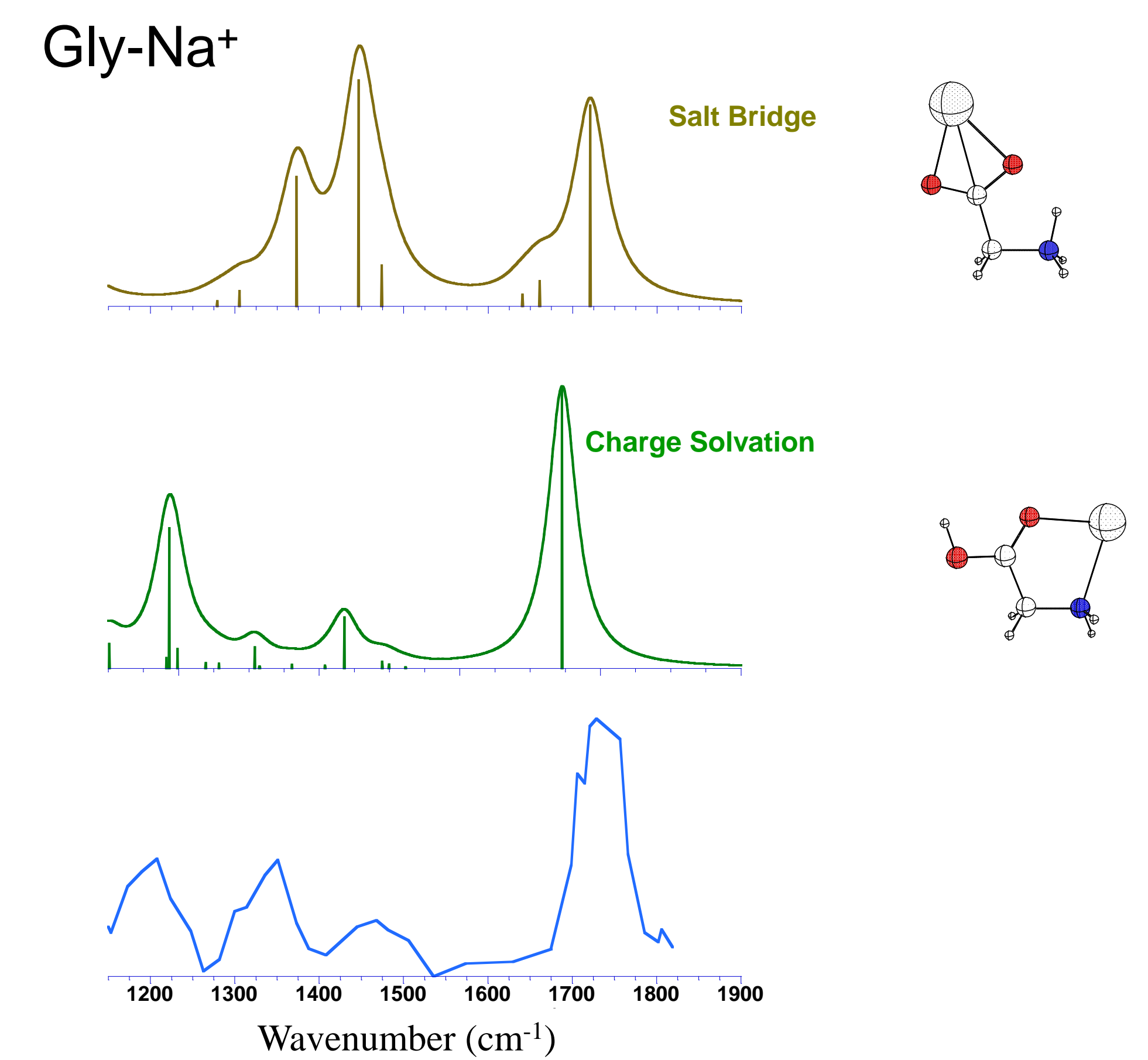
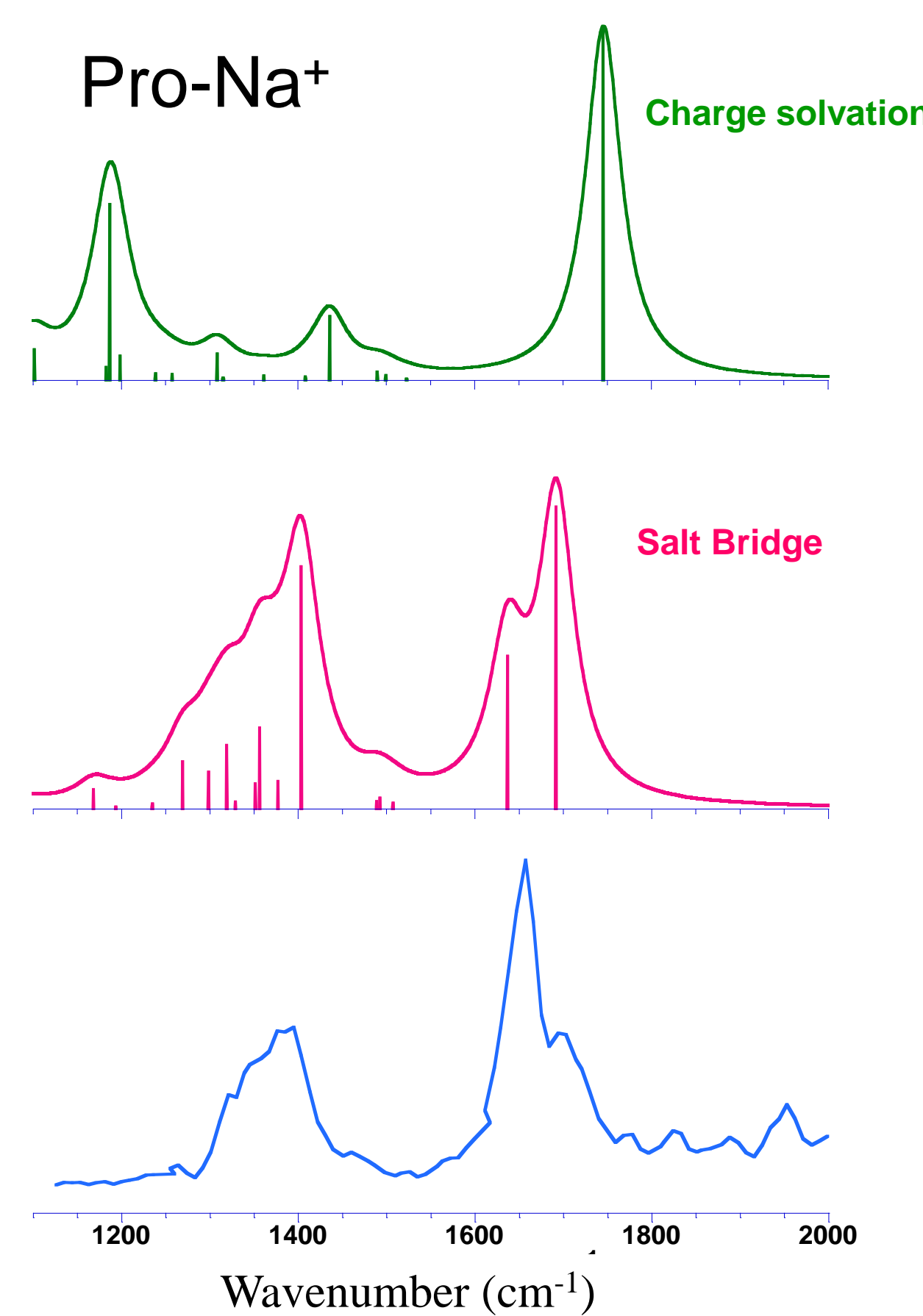


Sodiated amino acids

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.



IRMPD rate efficiency as a function of laser intensity

The dependance of the multiphoton dissociation rate with laser intensity has the form of an S shape curve exhibiting a threshold behavior at low intensity and a saturation behavior at high intensity.

The threshold intensity under which no dissociation is observed can be very different from one system to another.

The spectra are generally realised in the region where the behavior is close to linearity.

