Adding an optical spectroscopy dimension to mass spectrometric analysis

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"These instruments alone are able to reveal the principles of the natural substances; hence chemists should be ordered to employ them rigorously in all their experiments."
Antoine-Laurent Lavoisier, 1786
Traditional structural analysis in mass spectrometry: “MS”

\[ M^+ \cdot Y + Ar \rightarrow M^+ + Y \]

Extend to obtain UV/Vis/IR spectra of each ion: MS-IR

Ultrasensitive metabolomics
Can't measure FTIR spectra of ions...not enough of them to see attenuation of light

\[ M^+ \cdot \text{He} + h\nu \rightarrow M^+ + \text{He} \]

Grow an H\_2 “ice cap” on a target ion

\[ \tau_{\text{vib}} \sim 50 \text{ fs} \]
\[ \tau_{\text{IVR}} \sim 10 \text{ ps} \]
\[ \tau_{\text{evap}} \sim \text{ns} \]

Parent Ion

Delay to extraction

10 ms

Sequential addition of H\_2 molecules

30 ms

40 ms

50 ms

Mass ->
Get structures of non-covalently bound complexes and folded biopolymers using local bond frequencies: “isotope-edited” spectroscopy

Site-specific isotopomers
Self Assigning spectral!

Garand et al., Science, 335, 694-698 (2012)
Infrastructure needs

• Machine shop (WL + student shop)
• Mass spec support (coordinate Keck, WC and CBIC (new position/Fabian Menges)
• Electronics support (missing!!): Digital and analogue/computer-driven IO interfaces
(Could have used this yesterday to mix two high voltage RF frequencies in an ion trap!!!