# Ion-Electron Coincidence Study of Thiophenone

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# Goal: Understand Electron Dynamics of Thiophenone

- Study fragmentation of thiophenone using XUV pulses and by recording photoions and photoelectrons in coincidence

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- Use coincidence spectroscopy to extract photoelectron energies corresponding to a specific photoion

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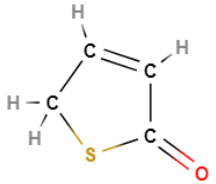
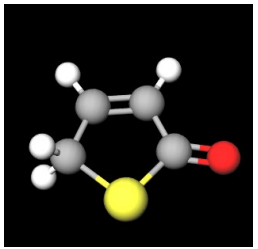
- Identify fragmentation pathways corresponding to the removal of an electron from a given molecular orbital of thiophenone

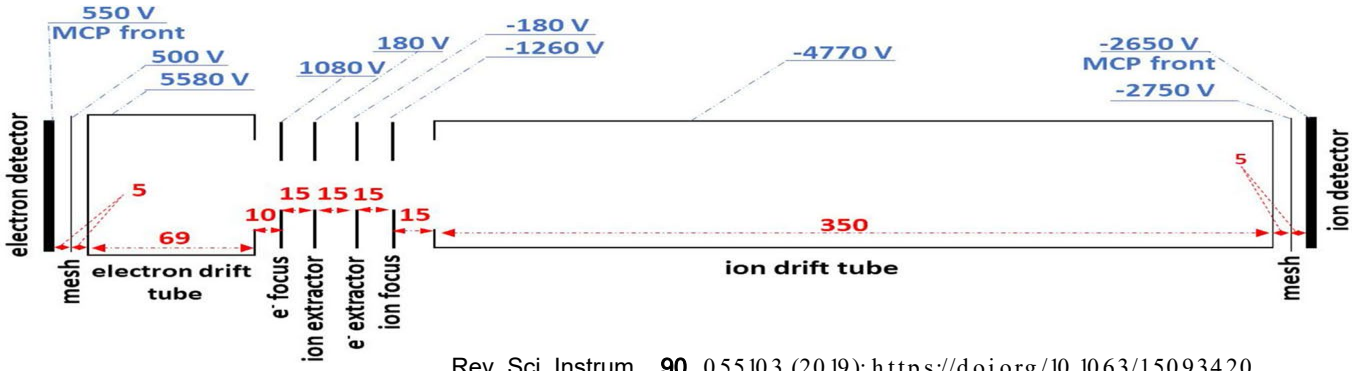
**Thiophenone - $C_4H_4OS$**



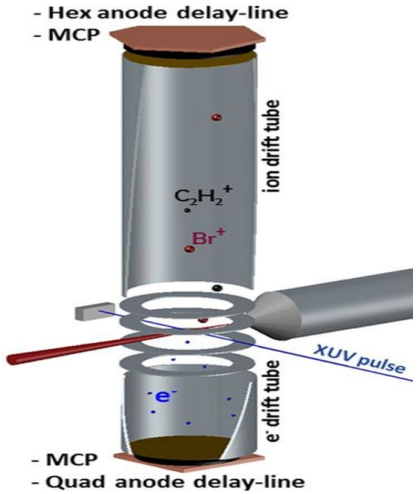



# Double-Sided VMI Spectrometer

- Molecule is ionized, bursts apart
- Records time of flight (TOF) and position data
- Measure ions and electrons in coincidence
- Electric field is not homogeneous, different from COLTRIMS

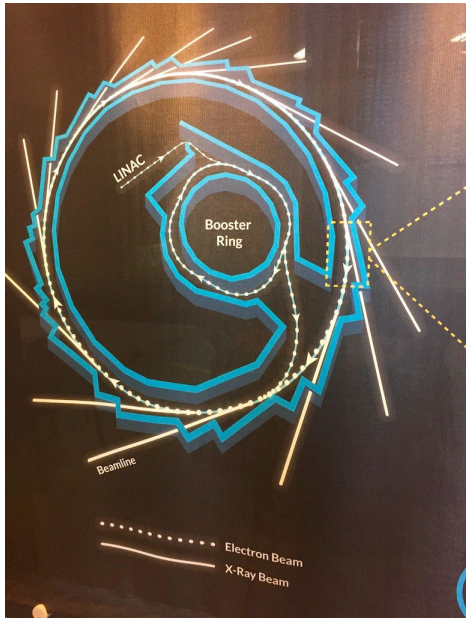


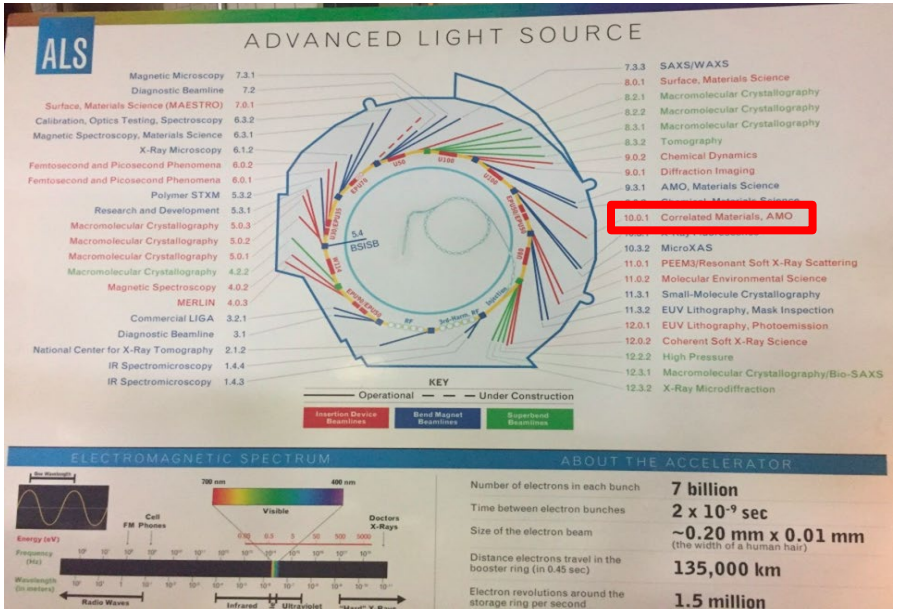

Rev. Sci. Instrum. **90**, 055103 (2019); https://doi.org/10.1063/1.5093420



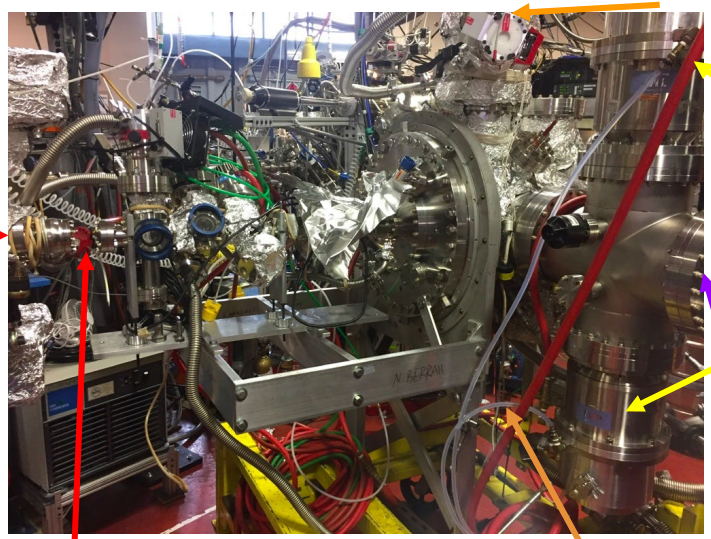

Ablikim, U. *et al.* Identification of absolute geometries of *cis* and *trans* molecular isomers by Coulomb Explosion Imaging. *Sci. Rep.* **6**, 38202; doi: 10.1038/srep38202 (2016).

# Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory



# Experimental End-Station (Double-sided VMI)



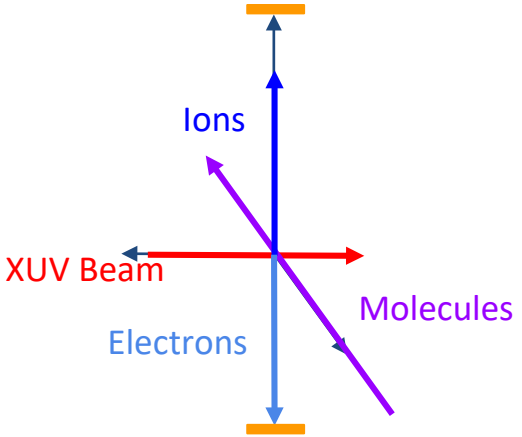
Spectrometer

Turbo Pumps

Molecular Beam

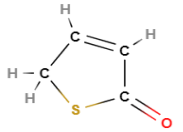
XUV Beam
Enters Here

Spectrometer

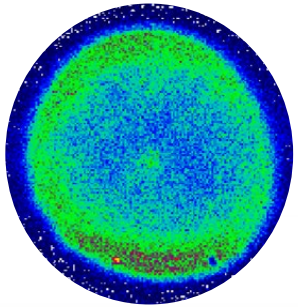


# Data Analysis

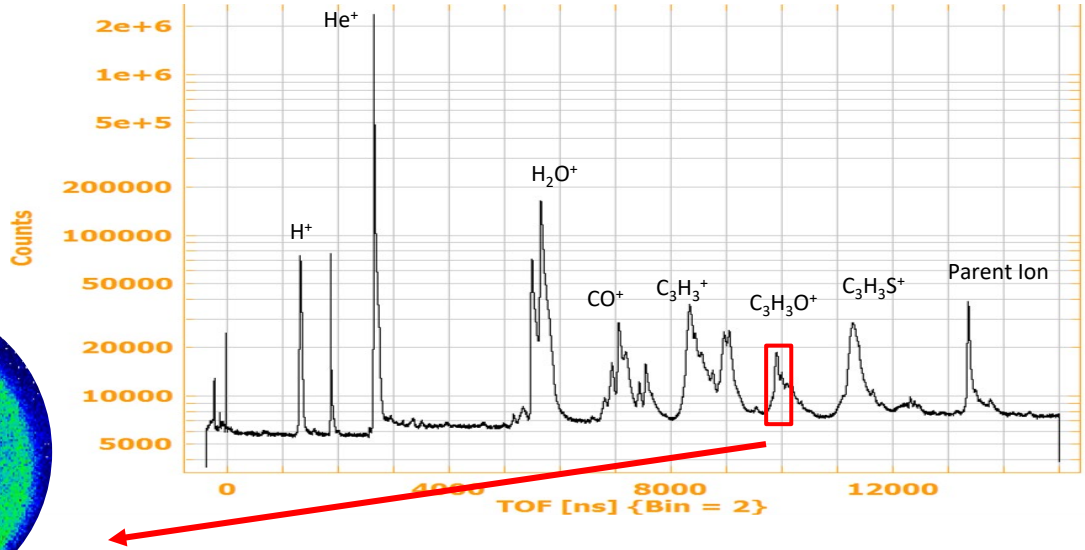
$C_4H_4OS$



- Analyze TOF data and use mass-to-charge ratio in order to identify ions
- Gate on specific ions to focus on just their electrons
- Analysis focused on electrons rather than ions, unlike previous experiments

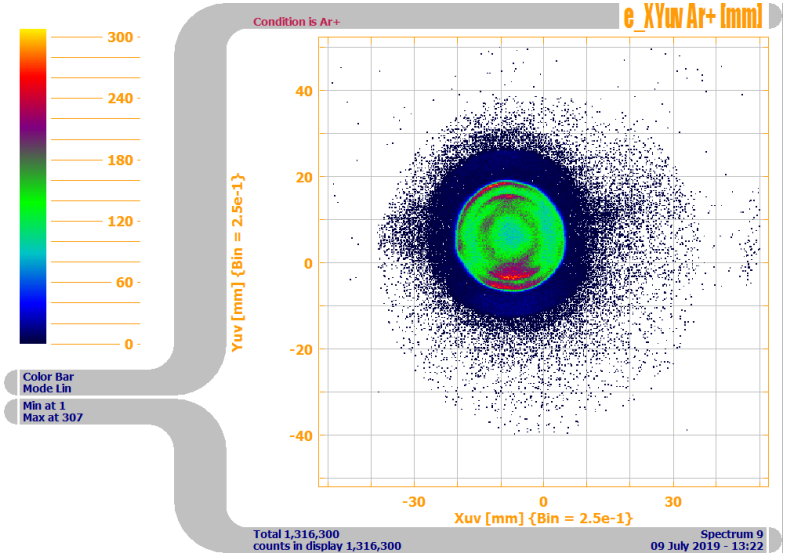


Thiophenone Time of Flight Spectrum -- photon energy = 23 eV



# Velocity Map Imaging

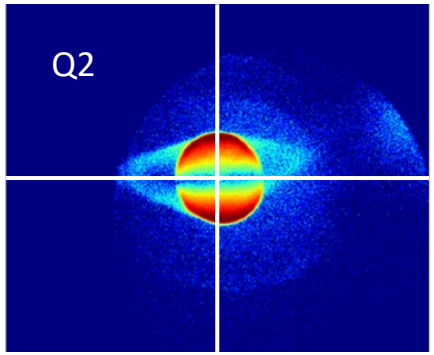
- Find kinetic energies of electrons at the moment of emission
- Set electric field such that all electrons of the same energy hit the detector at the same radius
- Each distinct ring should correspond to a different energy
- Should reflect the photoelectron spectrum of the molecule (i.e., the different energy shells and binding energies)



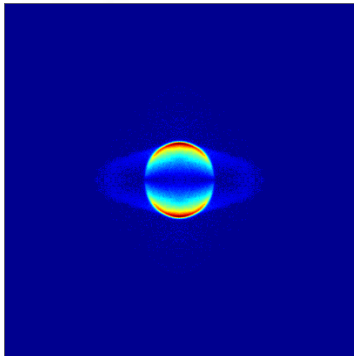

Photon energy of 50 eV -- calibration molecule is Ar

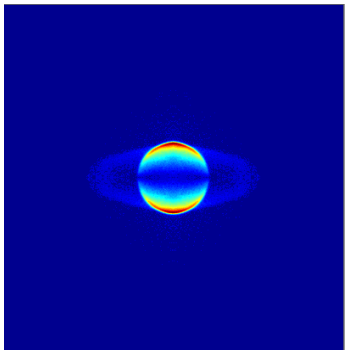
# Circularization

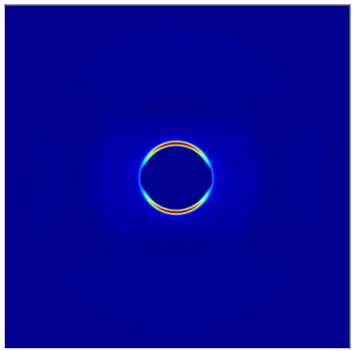
- Reflect quadrant 2 onto other three quadrants
- Circularize symmetrized image
- Invert image to get calibration between radius and energy
- Apply the same technique for molecule fragments that we wish to study



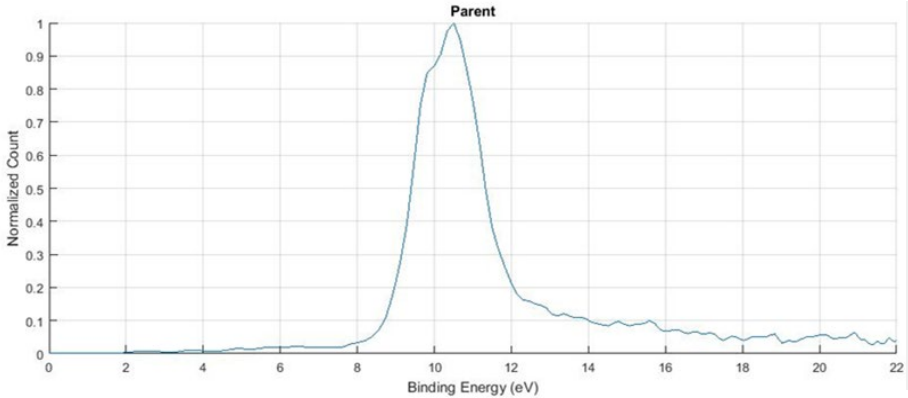
He 28eV -- raw

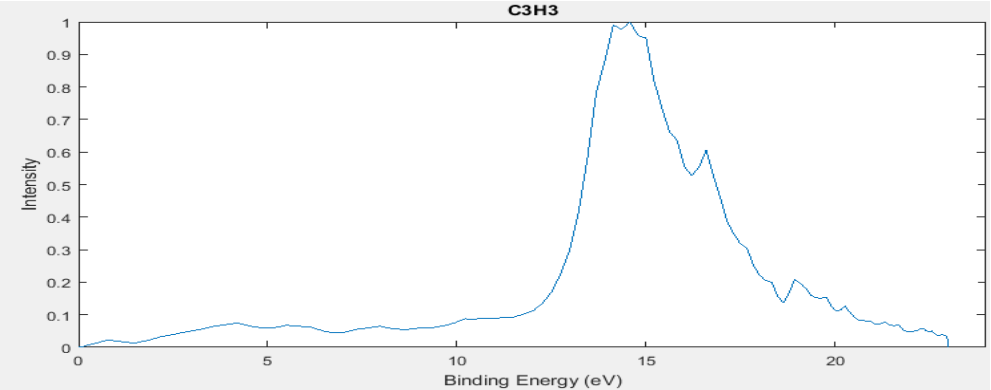

Q2 reflected


Circularized

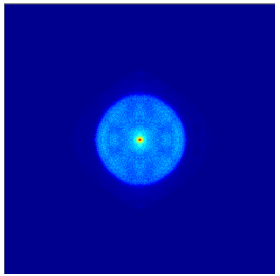

Inverted

# Extracting Photoelectron Spectrums

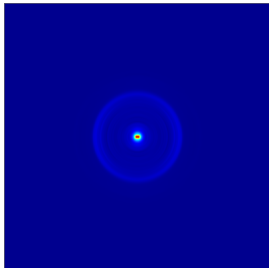



- Applied to the main fragments we identify
- All together, they should sum up to the total electron spectrum of the molecule

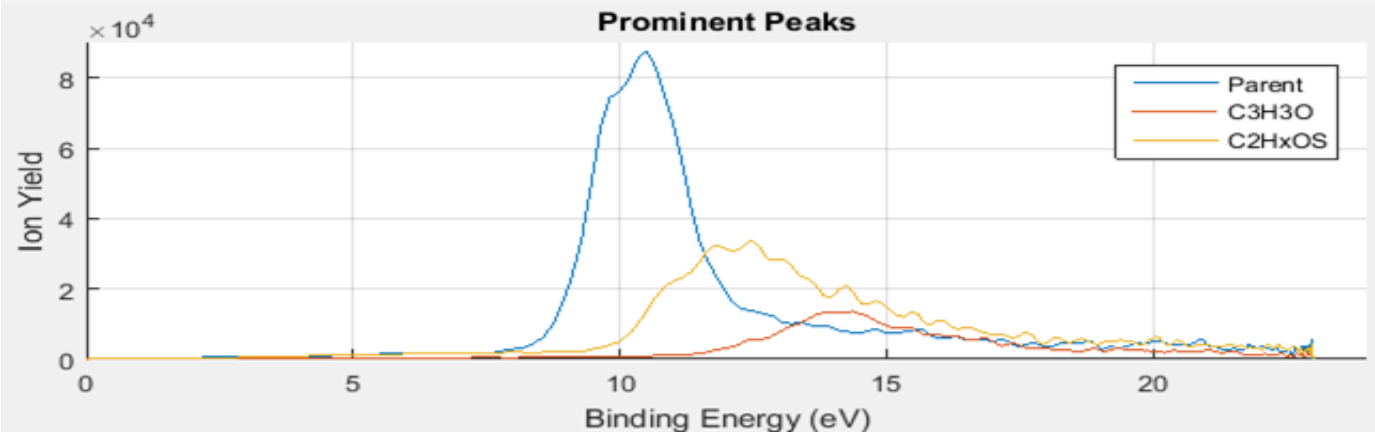


Circularized

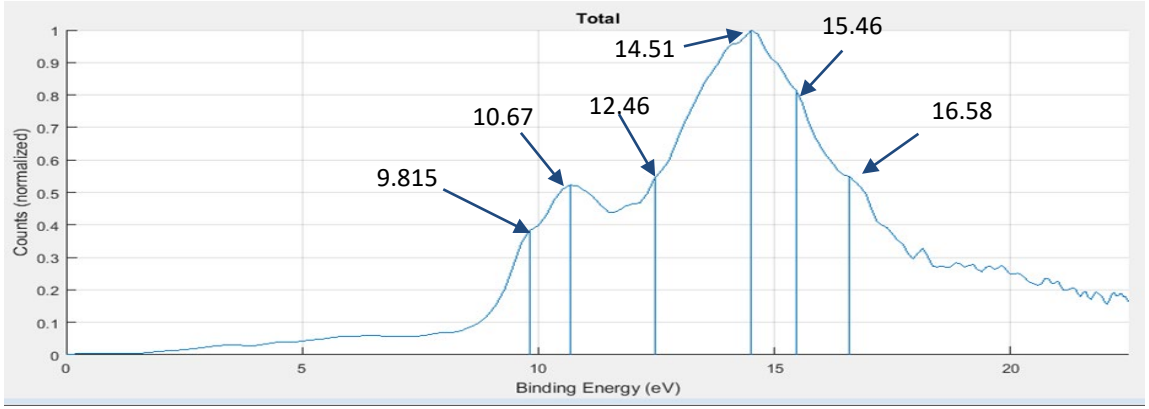


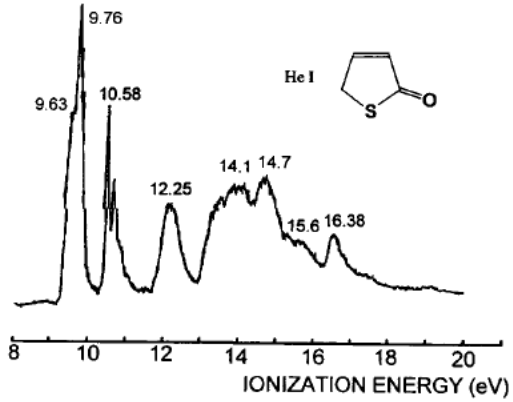
Inverted

# Prominent Spectra



# Total Spectrum

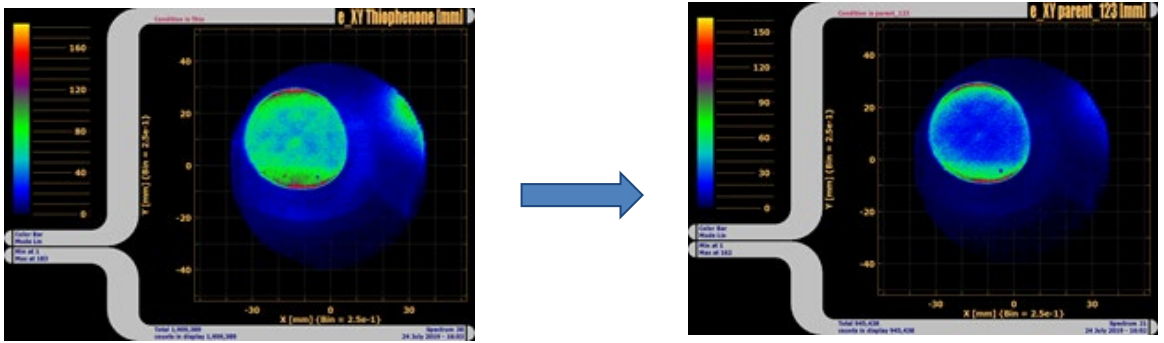



Chin, W. *et al.* He I and He II photoelectron spectra of thiophenones. *J. Electron Spectrosc. Relat. Phenom*88-91 (1998) pp 97-101; doi: 10.1016/S0368-2048(97)00253-3

# Future Outlook

- Use narrower gates, and gate on position as well as time
- Look for theoretical support to understand fragment dependent photoionization spectrum
- Use the information of the electron dynamics in future pump-probe experiments that lead to molecular movies



# Thanks To...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- Dr. Loren Greenman
- Kansas State University
- National Science Foundation
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