



2023 American Society for Mass Spectrometry (ASMS) 71st Annual Conference on Mass Spectrometry and Allied Topics

June 2023

Changing the World's Energy Future

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Investigation of Transient Species through Metal Clusters of Triphenylphosphine Chalcogenides with Group I Metals

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***71st Conference on Mass Spectrometry and Allied Topics
American Society For Mass Spectrometry, Houston, TX***

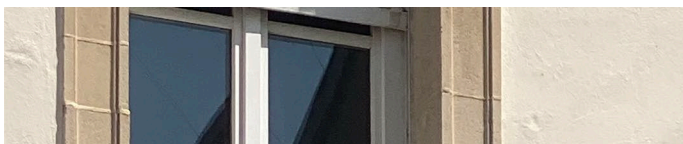
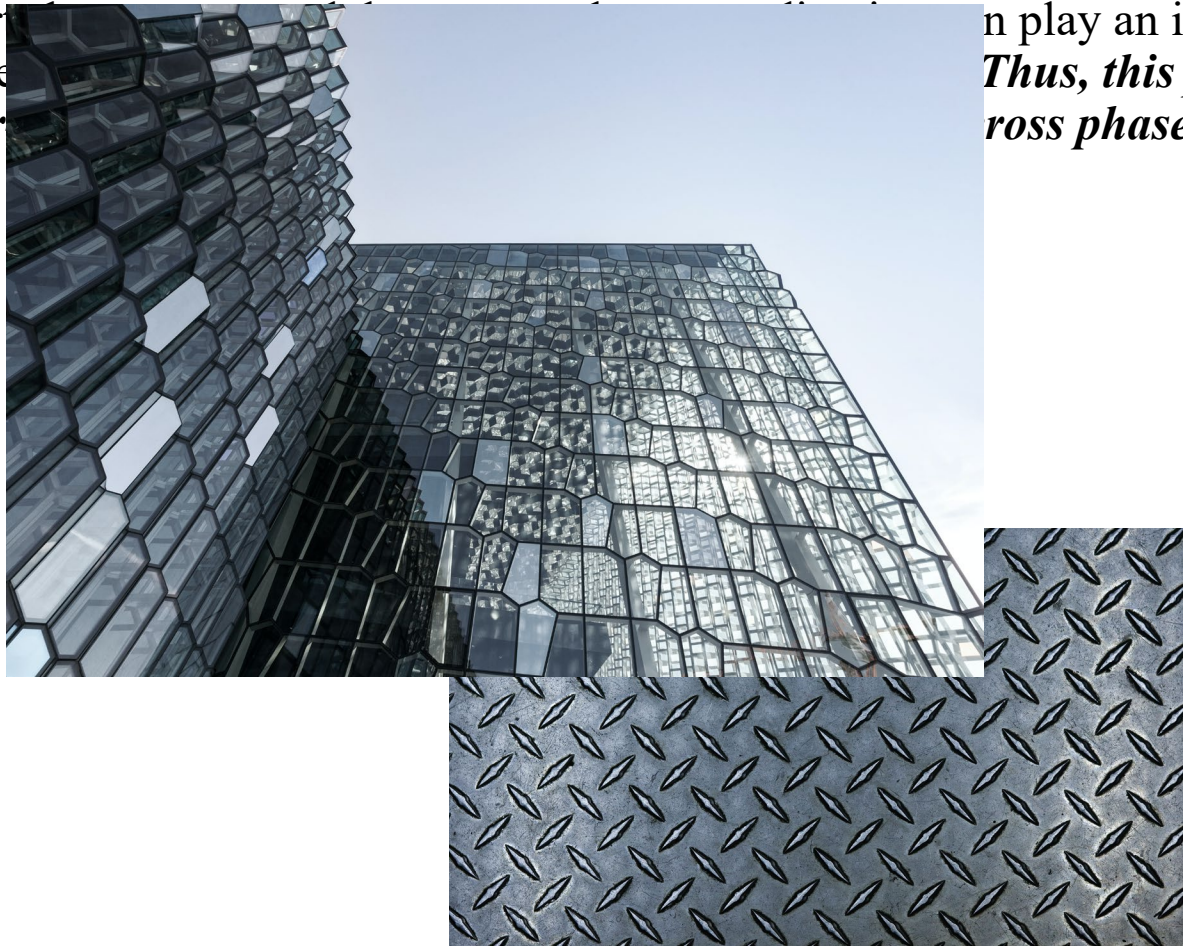
June 8, 2023 ThOD PM



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Transport of metal ions across a boundary from an aqueous to an organic phase is a critical step in nuclear fuel reprocessing and critical material recovery. As the initial metal coordination environment is significantly different from the final, the metal must transition through a series of transient species as it passes from one phase to another. The chemistry of these transition species is critical to the overall chemistry of transport. Recent reports suggest that certain species may play an important role in transport, but this is less well understood. *Thus, this proposal seeks to understand the role of these species in the cross phase boundary transport.*



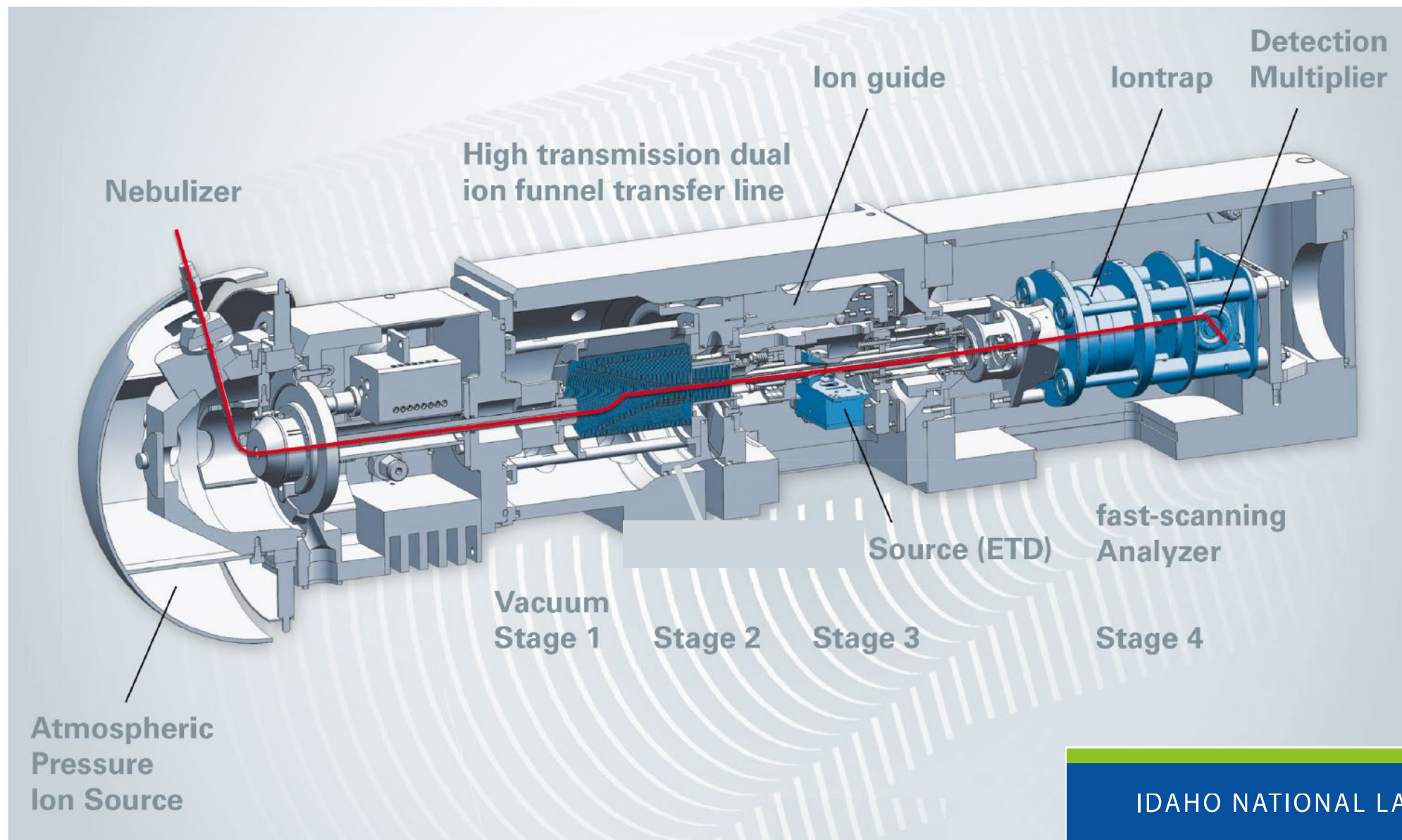
Methods

- Metal cluster ions of sodiated ligands were formed via direct electrospray using the commercial Bruker ion source
- Homodimers or Heterodimers of the ligands were formed.
 - Recipe
- Sodium containing dimers isolated in the gas phase, and fragmented with collisionally induced dissociation to investigate fragmentation patterns
- Experiments were performed on either a Bruker microTOF-QII or a Bruker amaZon ETD instrument.



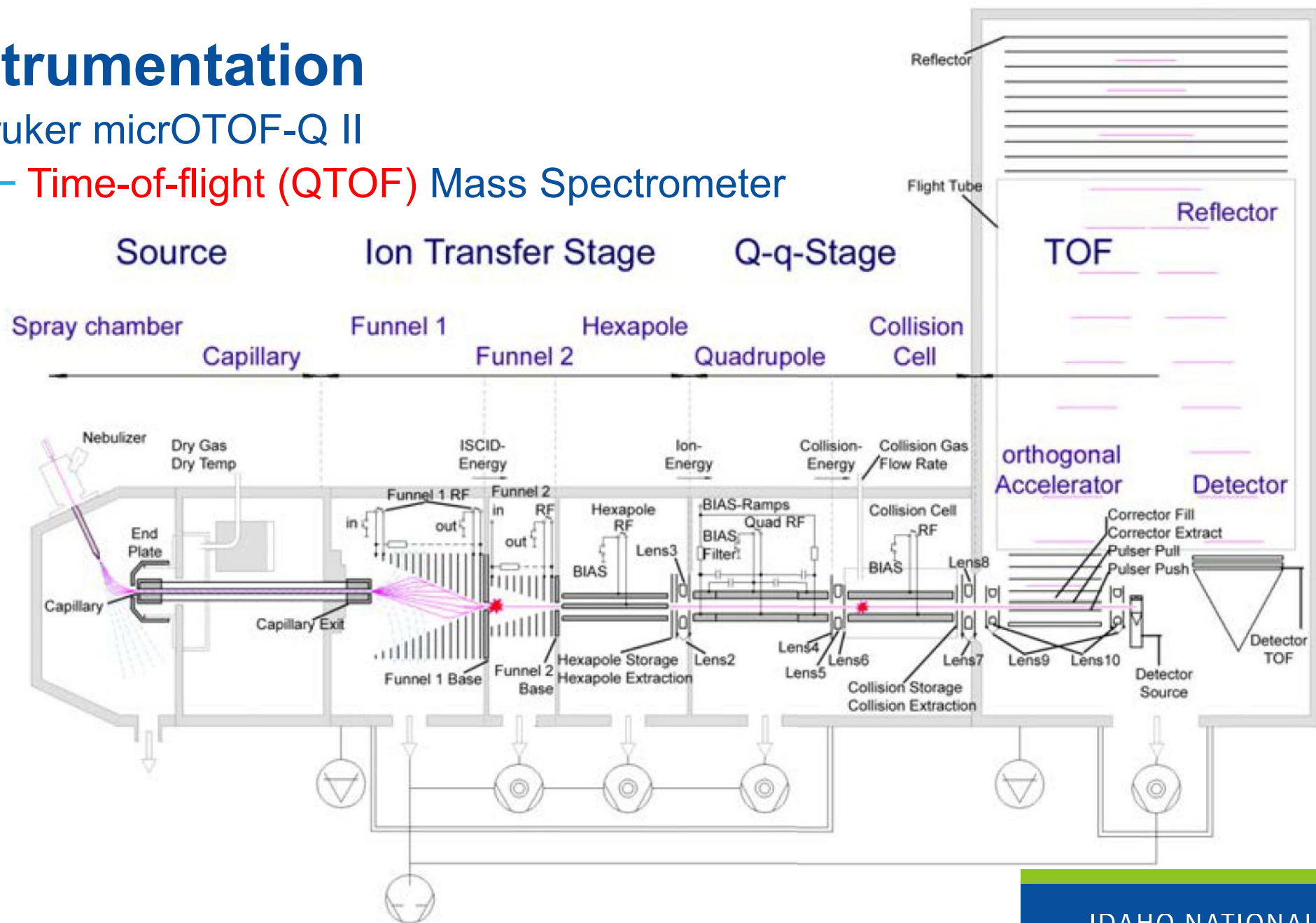
Instrumentation

- Bruker amaZon speed ETD
 - Quadrupole **Ion Trap** Mass Spectrometer

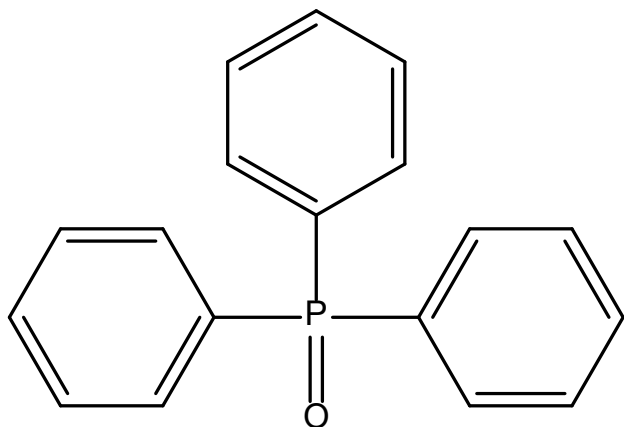


Instrumentation

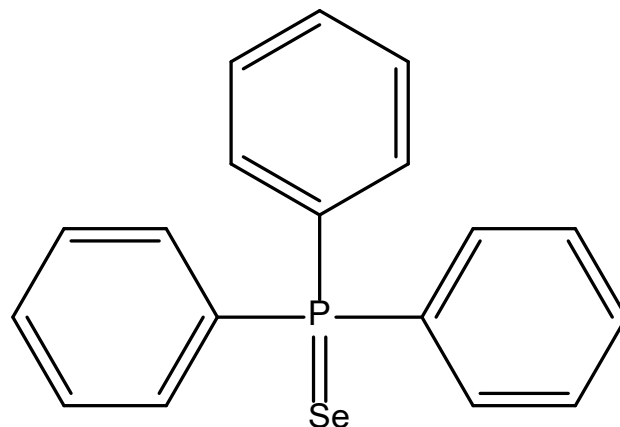
- Bruker micrOTOF-Q II
 - Time-of-flight (QTOF) Mass Spectrometer



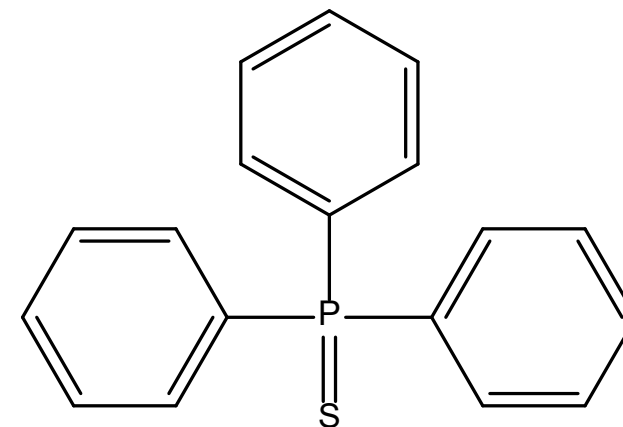
Triphenylphosphine Ligands with Oxygen, Selenide, and Sulfur



Triphenylphosphine Oxide
(TPPO)

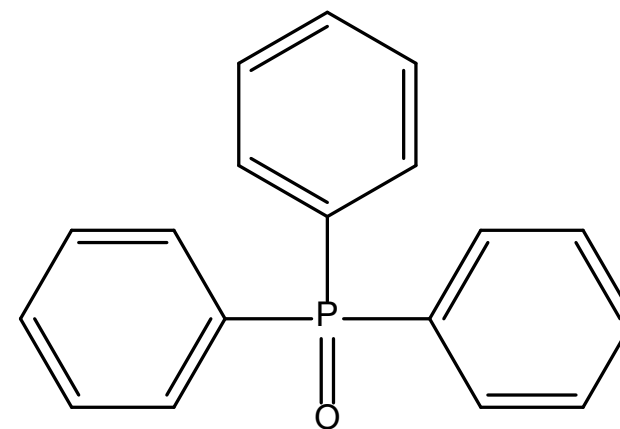
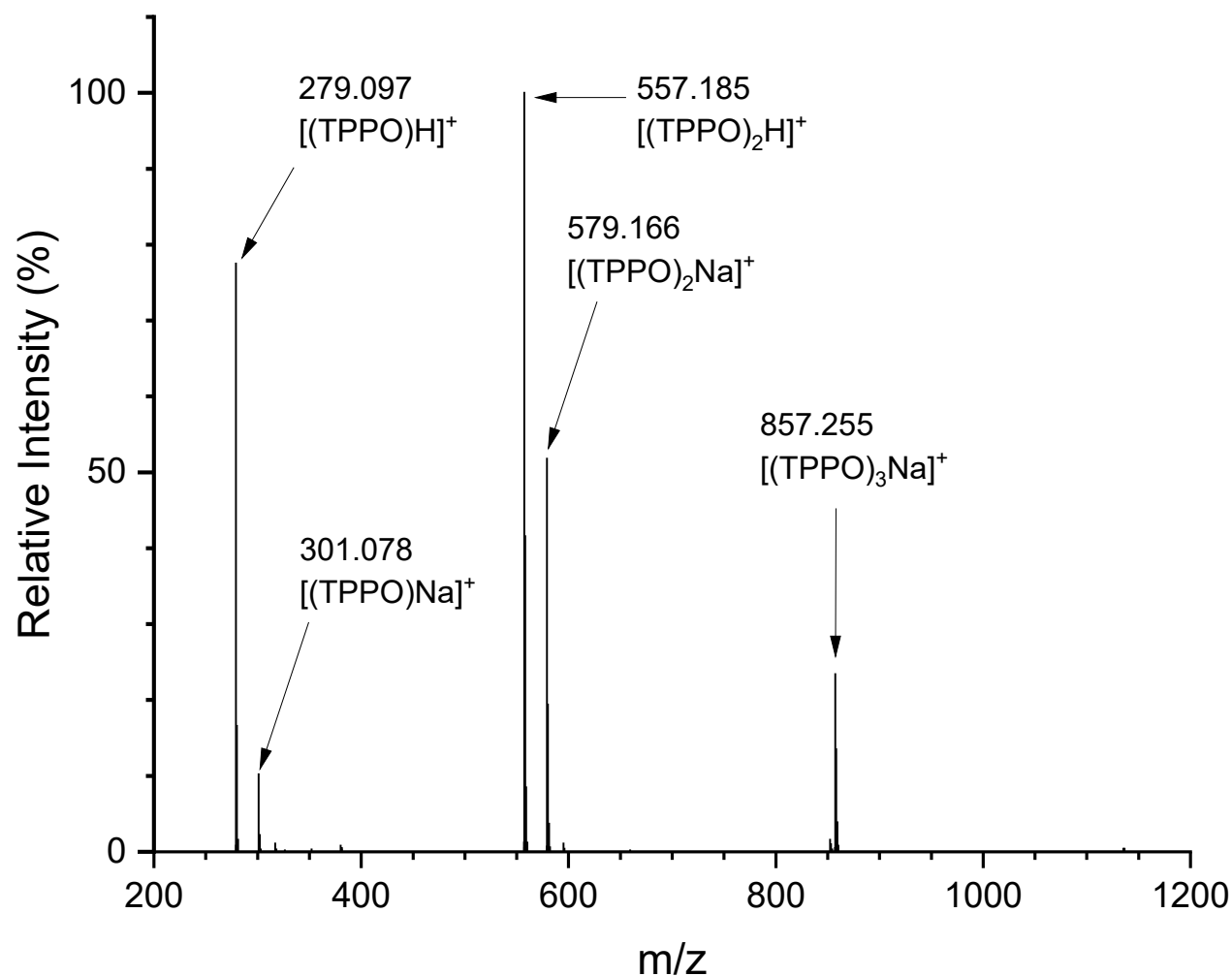


Triphenylphosphine Selenide
(TPPSe)



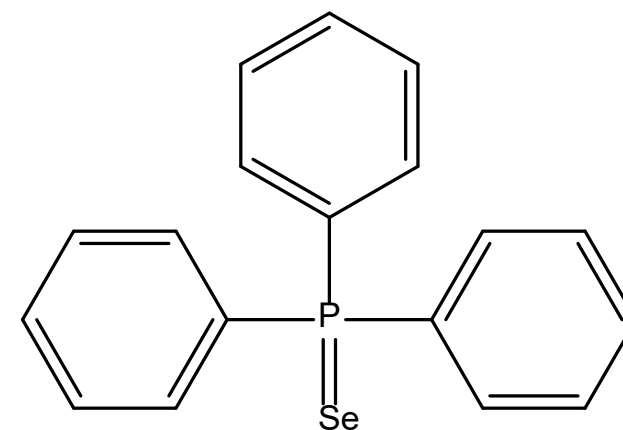
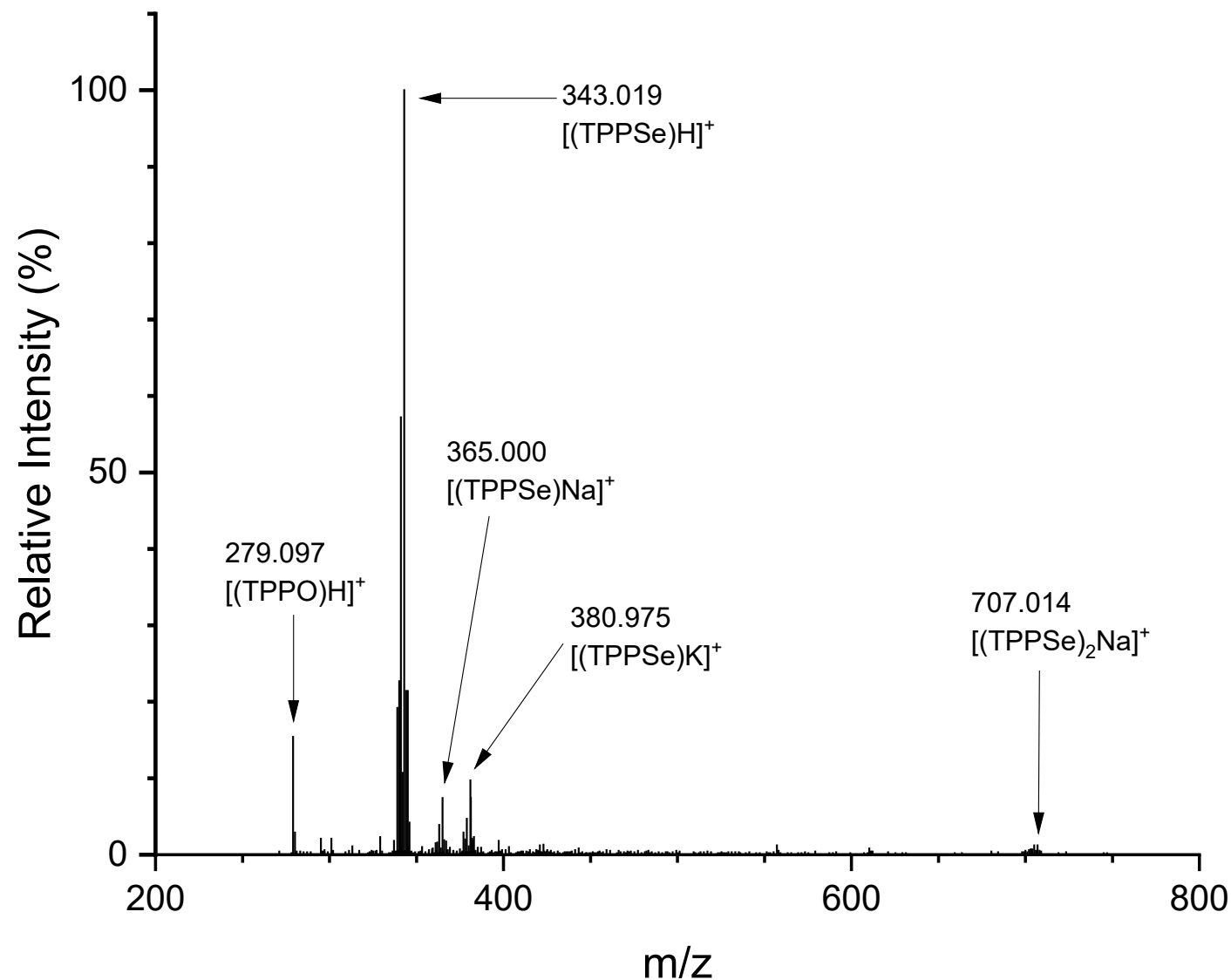
Triphenylphosphine Sulfide
(TPPS)

Collision Induced Dissociation of of Sodiated tris-Triphenylphosphine Oxide $[(\text{TPPO})_3\text{Na}]^+$



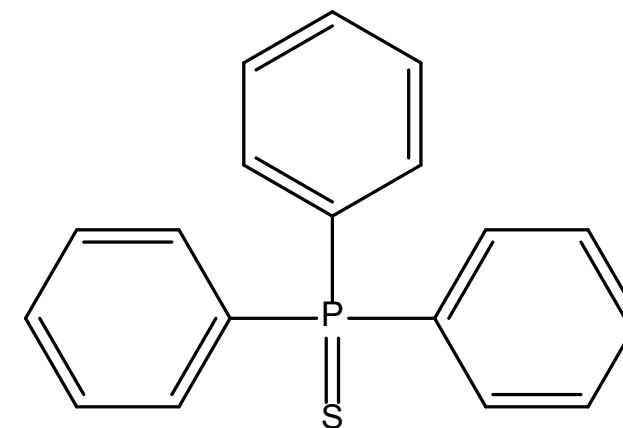
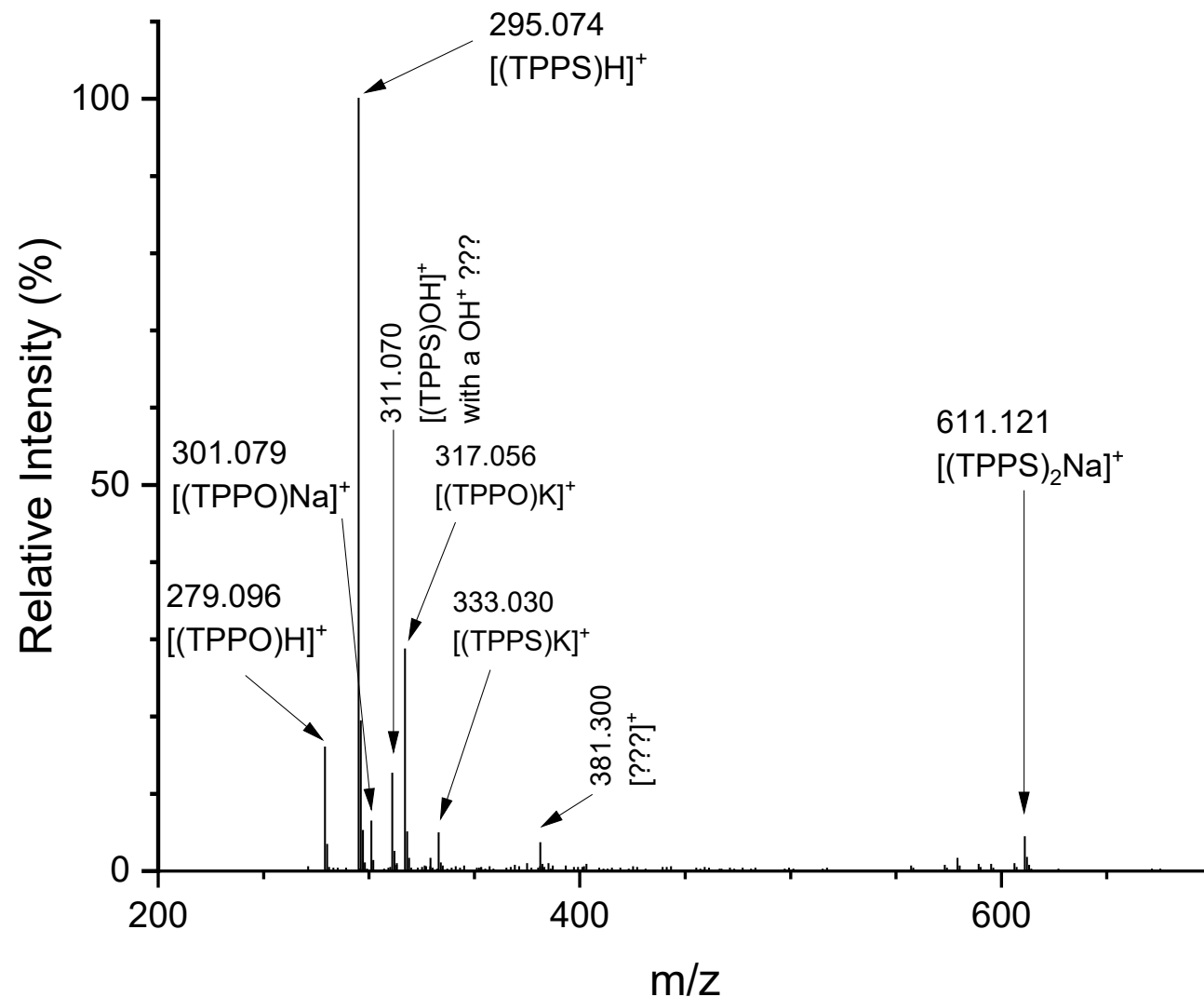
Triphenylphosphine Oxide
(TPPO)

Collision Induced Dissociation of of Sodiated di-Triphenylphosphine Selenide ($\text{Na}(\text{TPPSe})_2$)



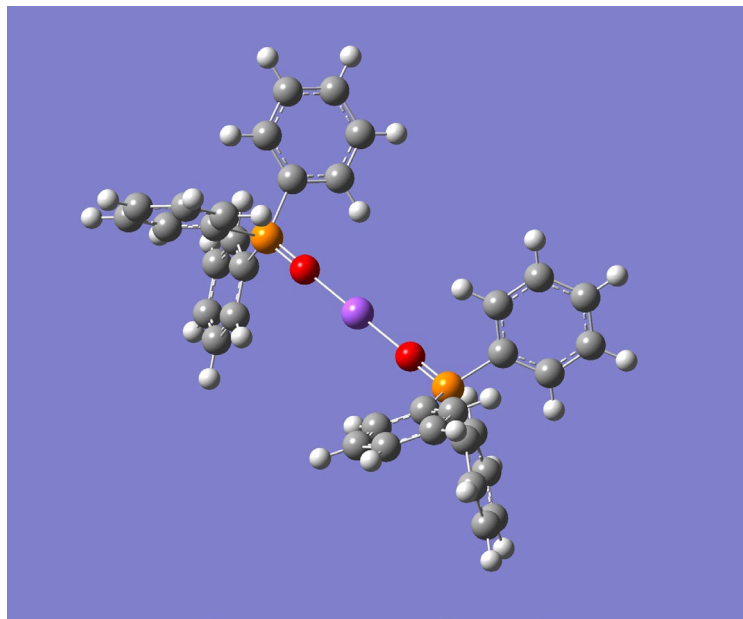
Triphenylphosphine Selenide
(TPPSe)

Collision Induced Dissociation of of Sodiated di-Triphenylphosphine Sulfide ($\text{Na}(\text{TPPS})_2$)

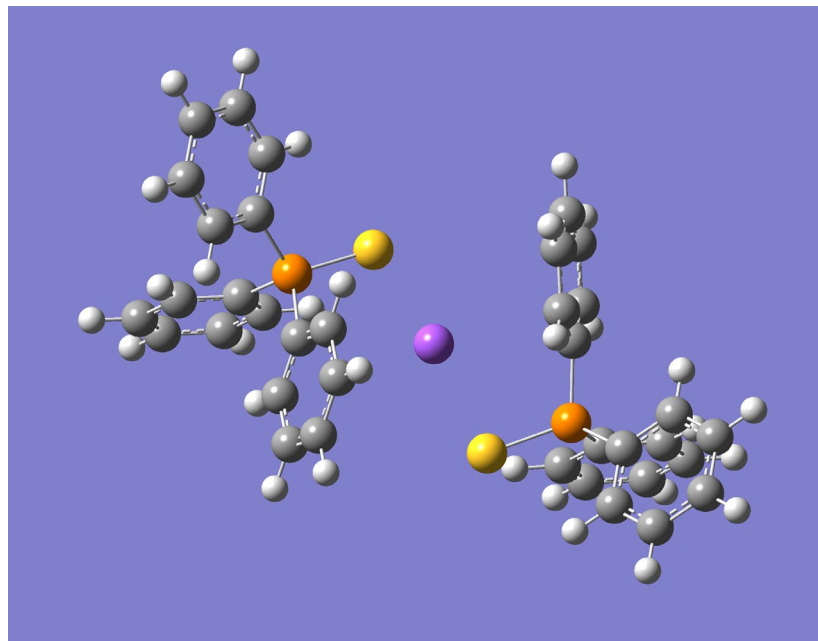


Triphenylphosphine Sulfide
(TPPS)

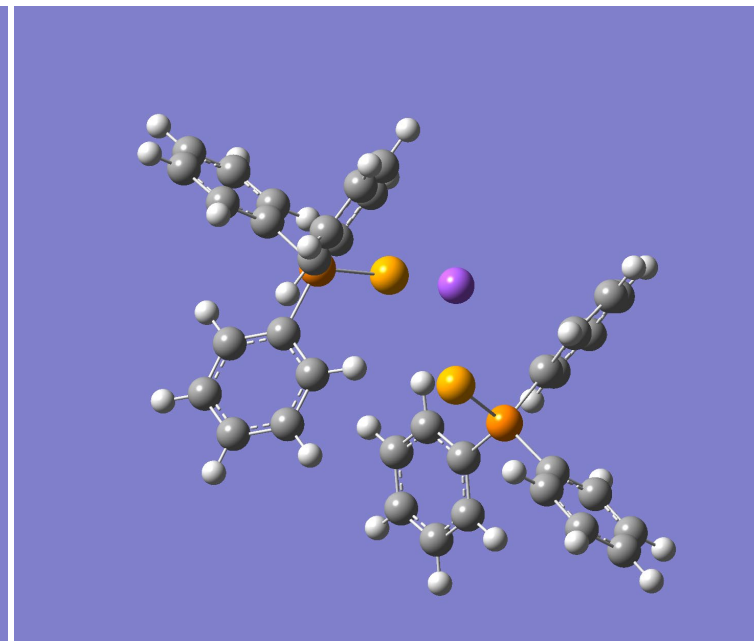
Density Functional Theory Calculations



TPPO+Na Homodimer



TPPS+Na Homodimer



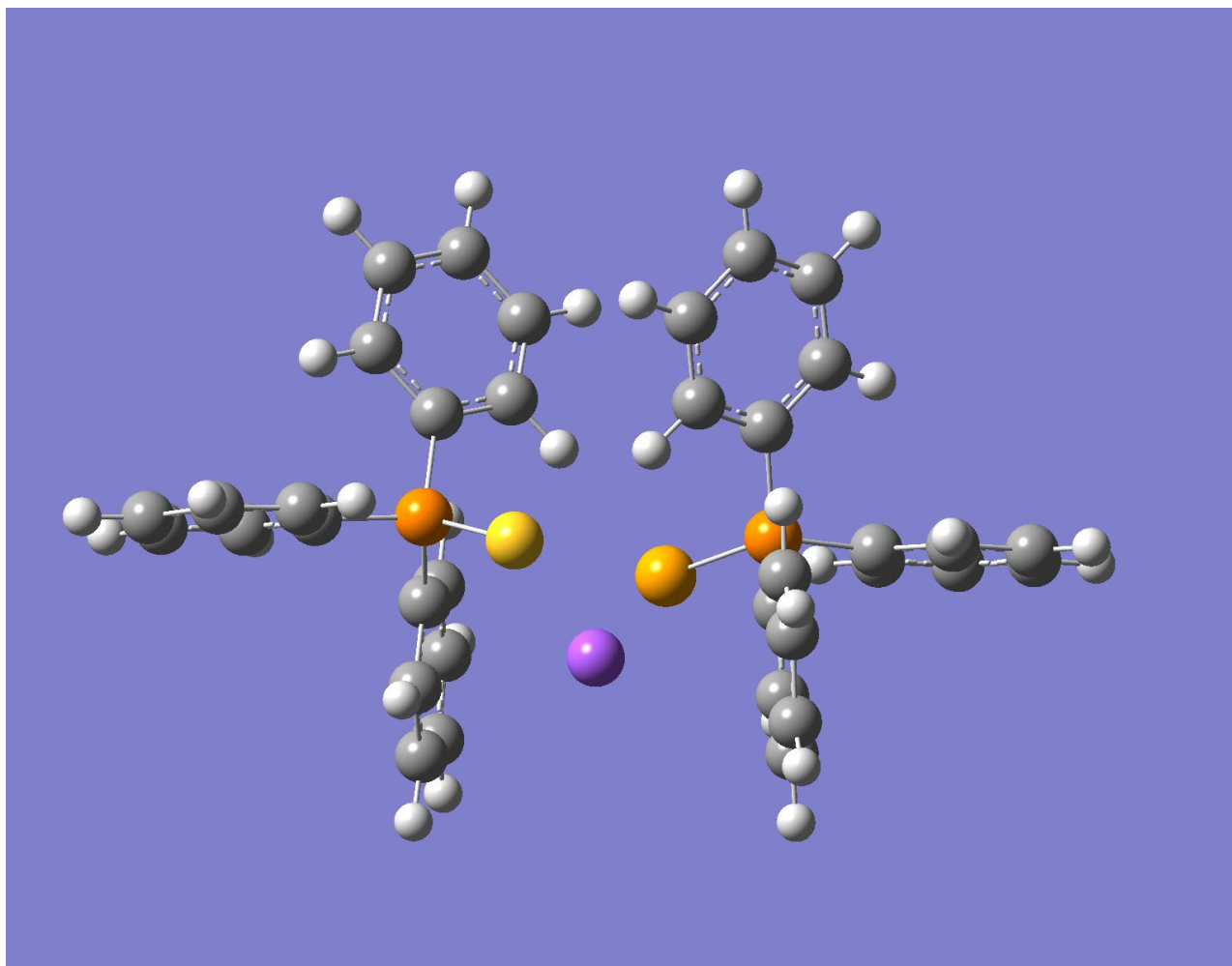
[(TPPSe₂Na] Homodimer

- Calculations were performed using Gaussian and viewed in GaussView 6.0.16 (<https://gaussian.com/>)
- Density Functional Theory Calculations were optimized with B3LYP

GaussView, Version 6, Roy Dennington, Todd A. Keith, and John M. Millam, Semichem Inc., Shawnee Mission, KS, 2016.

Gaussian 16, Revision C.01, M. J. Frisch, et al, Gaussian, Inc., Wallingford CT, 2016.

Density Functional Theory Calculations- Heterodimers of Triphenylphosphine Sulfur and Selenium with Sodium





Conclusions

- Dimers of triphenylphosphine chalcogenides (TPPX) and sodium were generated via electrospray and investigated via collisionally induced dissociation on a Bruker MicroTOF II.
- The collision induced dissociation of the ligands demonstrated that

Acknowledgements



Christopher A. Zarzana



Brittany D.M. Hodges



JungSoo Kim



Collaborative Computing Center
Idaho National Laboratory

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<https://hpc.inl.gov/SitePages/Home.aspx>



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