INL/EXP-23-74184-Revision-0

Intrinsic Bonding and Reactivity of Actinide Clusters Poster

October 2024

Christopher A Zarzana, Corey David Pilgrim, JungSoo Kim, Brittany Dawn Marie Hodges

Changing the World's Energy Future

INL is a U.S. Department of Energy National Laboratory operated by Battelle Energy Alliance, LLC

INL/EXP-23-74184-Revision-0

Intrinsic Bonding and Reactivity of Actinide Clusters Poster

Christopher A Zarzana, Corey David Pilgrim, JungSoo Kim, Brittany Dawn Marie Hodges

October 2024

Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

Prepared for the
U.S. Department of Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517, DE-AC07-05ID14517

Intrinsic Bonding and Reactivity of Actinide Clusters

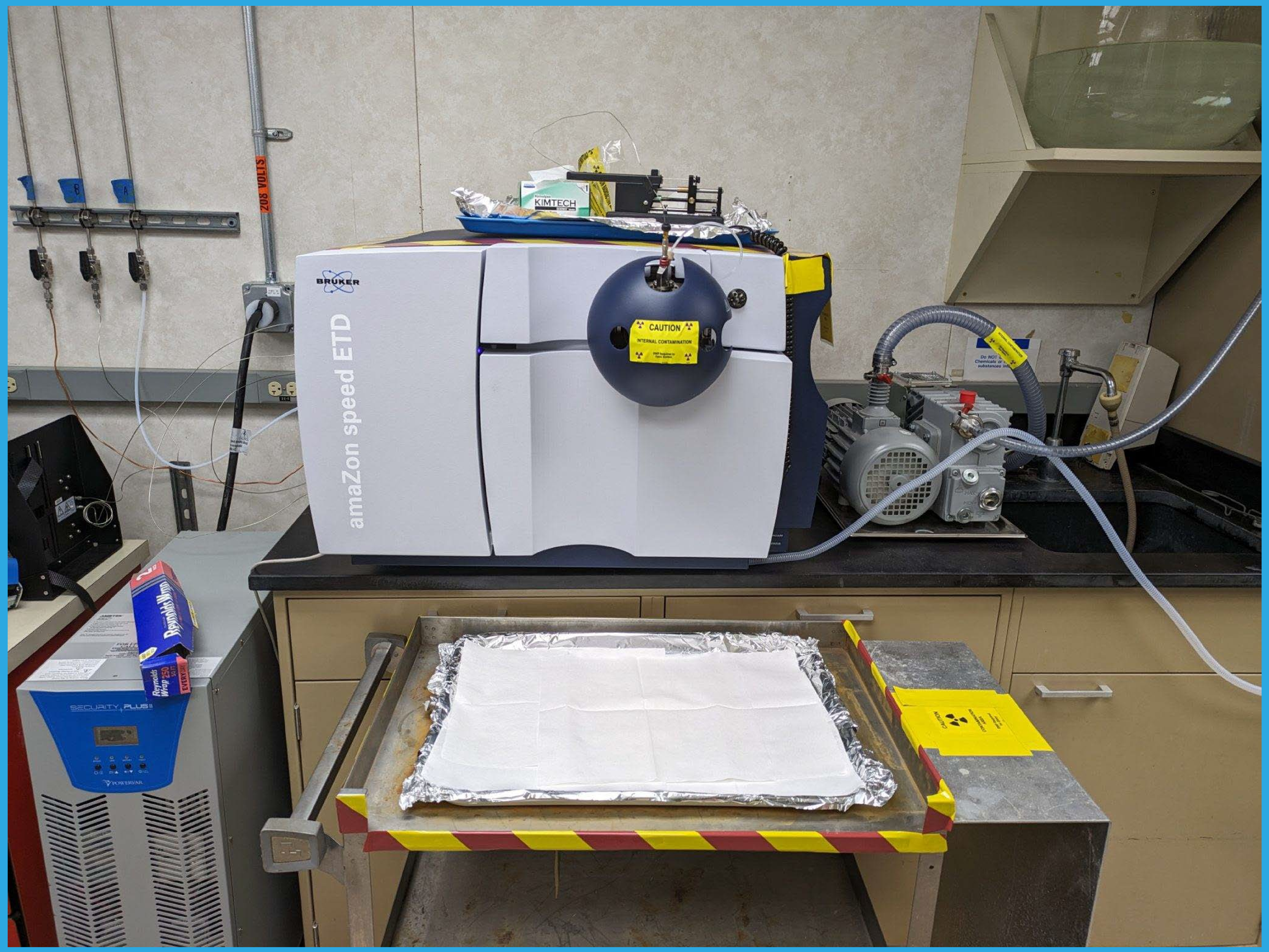
PRESENTER: **Christopher Zarzana**

New capability at Idaho National Laboratory for studying transuranic elements

BACKGROUND: The purpose of this project is to develop new capability to study transuranic elements, increasing our understanding of chemical bond formation at the far edges of the periodic table. This is critical for solving technical challenges such as development of advanced nuclear fuel cycles and efficient rare earth separations, as well as a broader understanding of bonding across the entire periodic table.

RESULTS

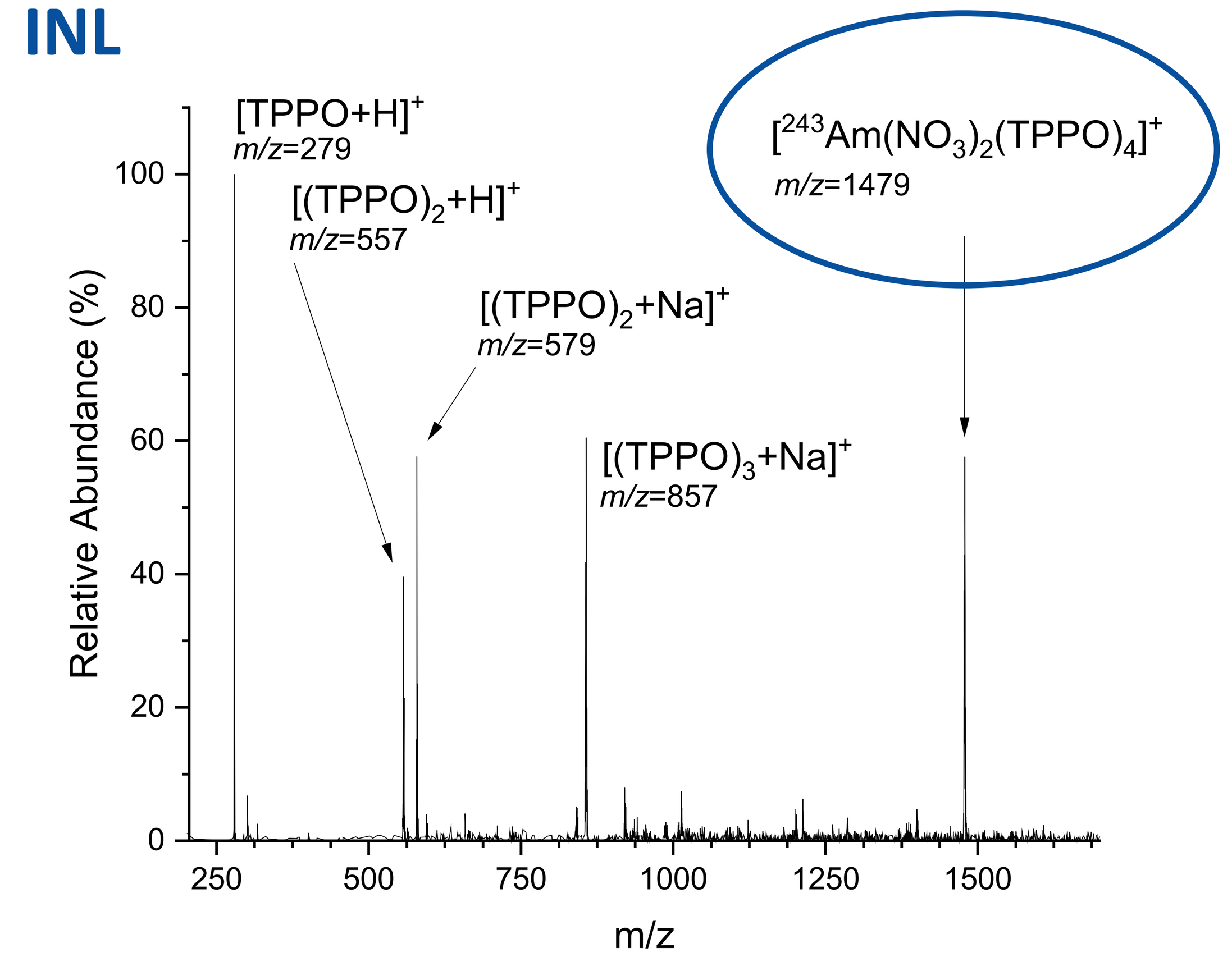
- Established the capability at INL to study gas-phase complexes containing transuranic atoms.
  - One of only three instruments in the world
- Spectra collected using approximately 500 ng (~0.2 µCi) of ^{243}Am. We believe we can cut that amount down by at least a factor of 10, decreasing the radiolytic hazards and expanding the envelope of transuranics that can be investigated.



Approach:

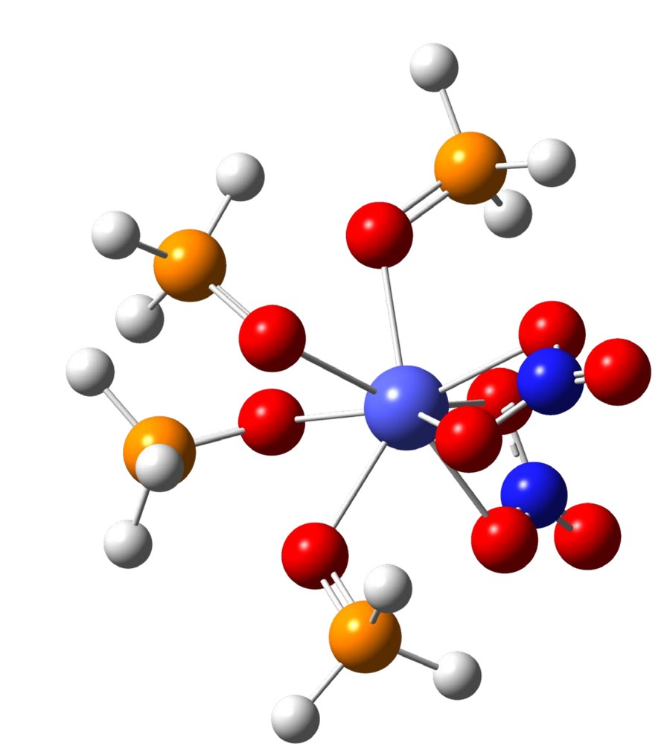
- Atmospheric pressure ionization mass spectrometry can form clusters containing actinide atoms from extremely small quantities of radioactive material
- Metal-ligand interaction is probed in the gas phase, revealing intrinsic behavior

First spectra of transuranic cluster ions at INL



TPPO=triphenyphosphine oxide

Quantum chemistry calculations are underway to understand electronic structure



Zarzana, Christopher; Pilgrim, Corey; Kim, JungSoo; Hodges, Brittany

Project Number: 21A1057-017FP

LRS Number: INL/EXP-23-74184

Work supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517."

www.inl.gov

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory