



# Modeling the Fundamental Radiation Chemistry of the Organic Diluent, and the Effect of Metal Ion Complexation on the Radiochemical Behavior of Active Compounds

*Changing the World's Energy Future*

Gregory P Horne



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Center for Radiation  
Chemistry Research

# **(i) Modeling the Fundamental Radiation Chemistry of the Organic Diluent, and (ii) the Effect of Metal Ion Complexation on the Radiochemical Behavior of Active Compounds**

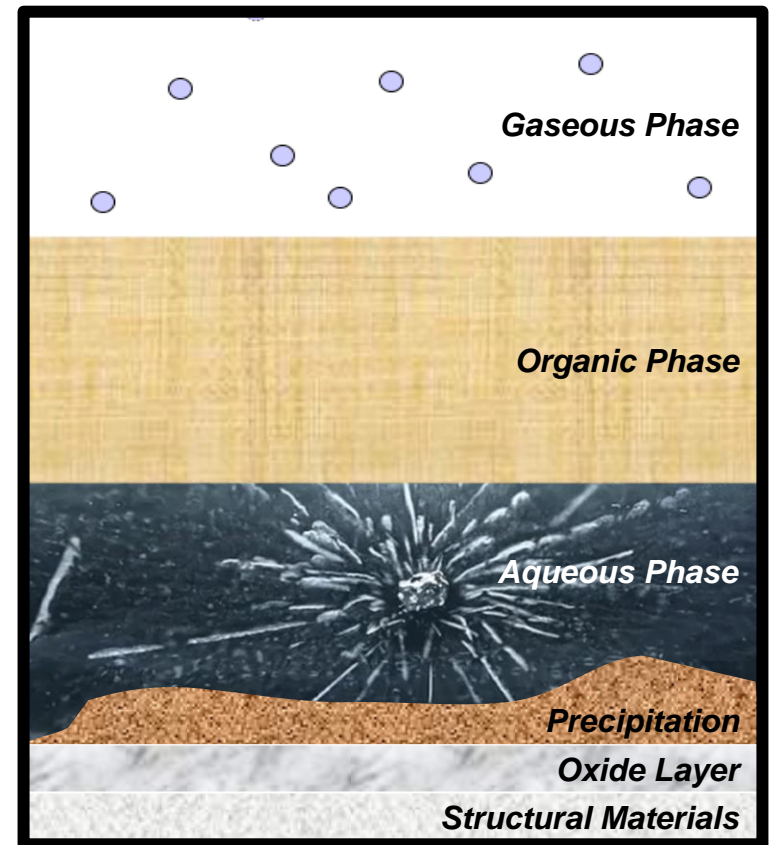
**Innovative Separations R&D Needs For Advanced Fuel  
Cycles Workshop 2021, 30<sup>th</sup> August – 1<sup>st</sup> September**

**Research Product:** Control, Knowledge, and Model

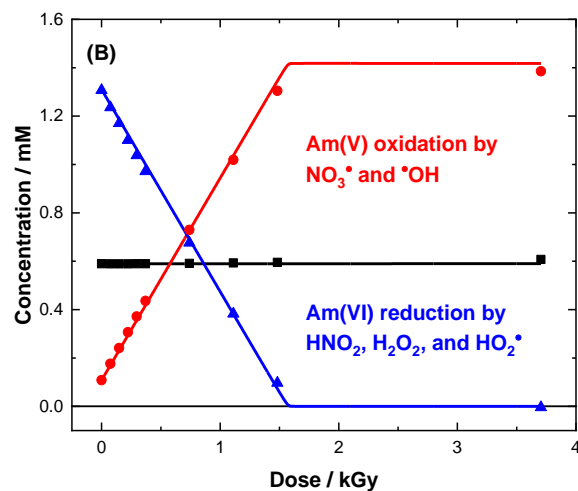
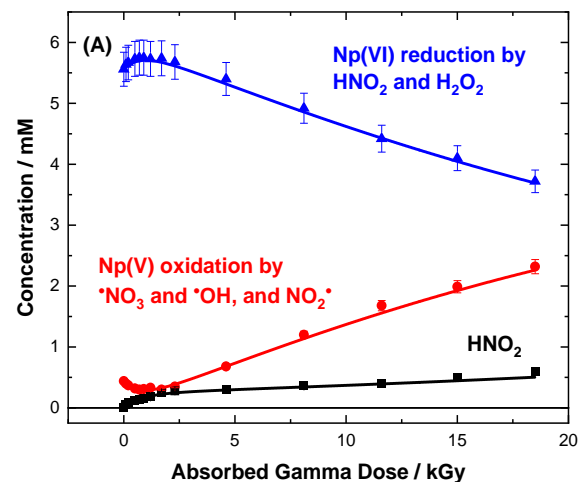
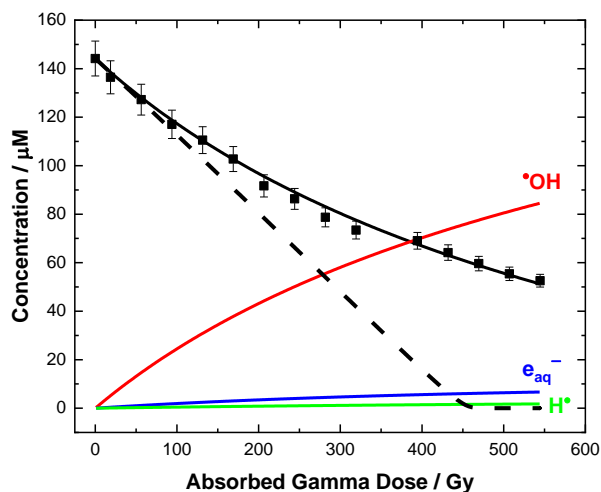
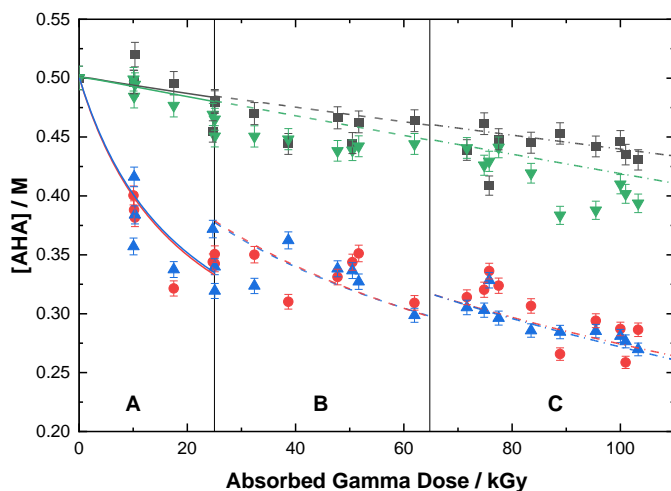


# Innovative Separations R&D Needs For Advanced Fuel Cycles – Radiation Chemistry

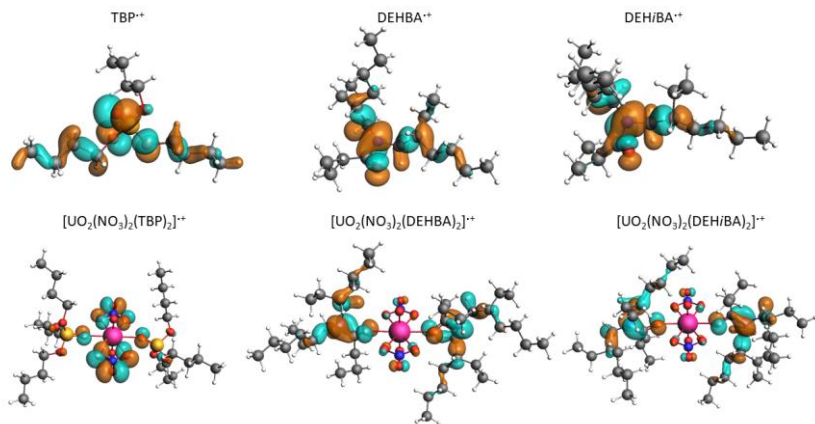
- Actinides and radiation studies need to be core to future work
- Design radiation models to support direction of R&D and process scale tests
- Move away from simulants
- Study realistic systems



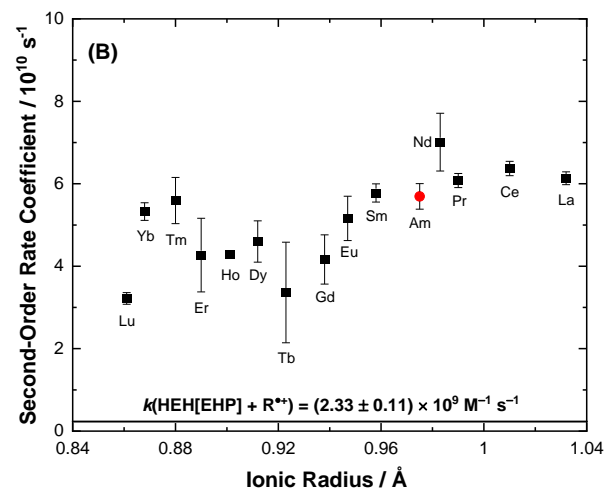
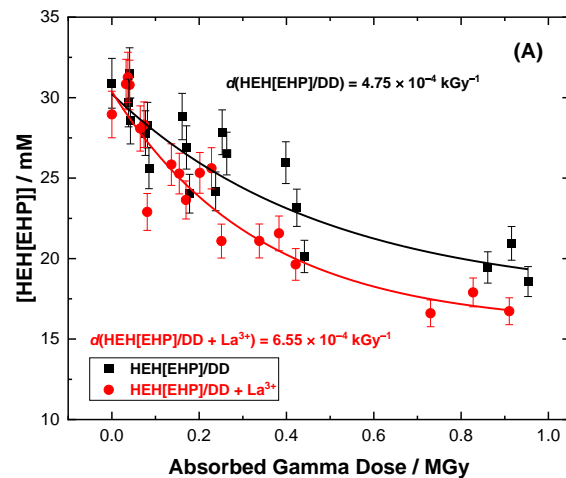
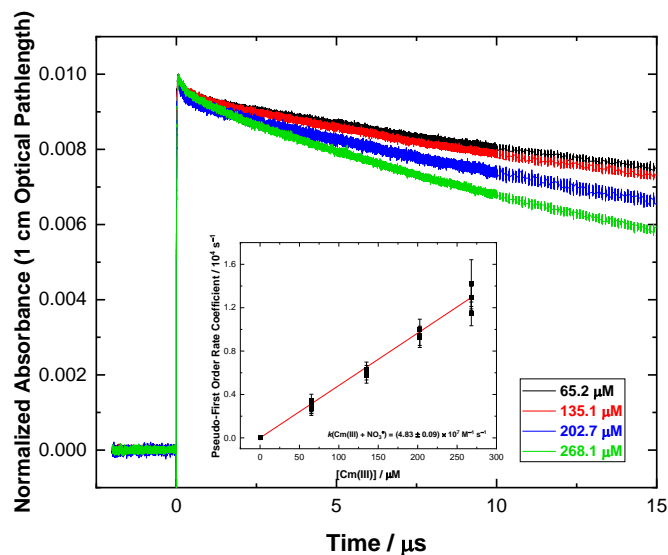
# Modeling the Fundamental Radiation Chemistry of the Organic Diluent



# Effect of Metal Ion Complexation on the Radiochemical Behavior of Active Compounds



Canonical Kohn-Sham molecular orbitals of the electron holes in the geometry-optimized radical cation species for TBP, DEHBA, and DEH/BA.



# Breakout Session Questions

- **What aspect of separations is improved through this ‘*technology*’?**
  - Radiation-induced processes are pervasive throughout separations, and yet their understanding is an after thought.
- **What are the primary benefits this ‘*technology*’ could offer?**
  - Predictive radiation models and studying metal loaded systems will accelerate the innovation of separation technology and reduce research costs.
- **How wide-ranging are these impacts?**
  - Impacts all proposed separation technologies, including pyrochemical processes under a different guise.
- **What are the primary technological risks associated with this ‘*technology*’?**
  - All computational and experimental techniques are available. The key risk is time, expertise are running out.