

## Radiation-Induced Interhalogen Chemistry in Molten Salts

June 2023

Gregory Peter Holmbeck, Jacy Kathleen Conrad





#### DISCLAIMER

This information was prepared as an account of work sponsored by an agency of the U.S. Government. Neither the U.S. Government nor any agency thereof, nor any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness, of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. References herein to any specific commercial product, process, or service by trade name, trade mark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the U.S. Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the U.S. Government or any agency thereof.

# Radiation-Induced Interhalogen Chemistry in Molten Salts

Gregory Peter Holmbeck, Jacy Kathleen Conrad

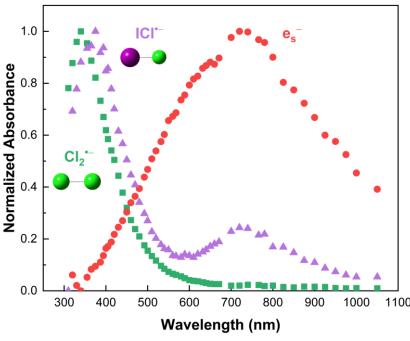
June 2023

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

### Radiation-Induced Interhalogen Chemistry in Molten Salts



Normalized, deconvoluted transient spectra from the electron pulse irradiation of molten KI (10 wt.%) in LiCI-KCI eutectic at  $400^{\circ}$ C (ICI<sup>--</sup> = iodine-chlorine radical anion,  $\text{Cl}_2^{\text{--}}$  = dichlorine radical anion, and  $\text{e}_{\text{S}}^{\text{--}}$  = solvated electron).

J.K. Conrad, K. Iwamatsu, M.E. Woods, R. Gakhar, B. Layne, A.R. Cook, and G.P. Horne, *PCCP* **2023**, DOI: 10.1039/d3cp01477k.

This work was performed at Idaho and Brookhaven National Laboratories (INL and BNL) and used resources of the BNL Accelerator Center for Energy Research.

### **Scientific Achievement**

The transient interhalogen species (**ICI** has been identified and observed for the first time in irradiated iodide-containing molten chloride salt mixtures, exhibiting a lifetime on the order of microseconds.

### **Significance and Impact**

The radiation chemistry of interhalogen species in molten salt reactors is unknown. The formation of **ICI** has significant implications for the transport and accumulation of fission-product iodine in these extreme environments.

#### **Research Details**

- Transient spectra and chemical kinetics were measured to determine the impact of iodide ions on the fundamental radiation chemistry of molten chloride salt mixtures as a function of temperature (400–700°C).
- Spectro-kinetic analysis (SK-Ana) software, and gas-phase density functional theory calculations were employed for spectral deconvolution and transient identification, respectively.





