MULTIREFERENCE CALCULATIONS ON THE GROUND AND EXCITED STATES AND DISSOCIATION ENERGIES OF LrF AND LrO

NUNO M. S. ALMEIDA, SASHA C. NORTH, TIMOTHÉ R. L. MELIN, ANGELA K. WILSON, *Department of Chemistry, Michigan State University, East Lansing, MI, USA*.

High-level ab initio approaches were performed on LrF and LrO detailing their numerous excited states, and spin multiplicities. Herein, multi reference methodologies such as the complete active space self-consistent field (CASSCF) and multireference configuration interaction (MRCI) were utilized to calculate ground and excited state properties of LrF and LrO. The potential energy curves for the ground, several excited states, and different dissociation channels are explored at CASSCF and MRCI+Q. Spin-orbit corrections were performed by diagonalizing the MRCI wavefunction on the basis of the Breit-Pauli Hamiltonian. For the second part of this work the bond dissocation energies (BDEs) of LrO and LrF were performed at different levels of theory using a range of basis sets. Core-valence, relativistic effects and spin-orbit contributions to the ground state are discussed. In addition, density functional theory (DFT) is also compared against wavefunction methods. Detailed spectra for intricate diatomic complexes such as actinide oxides and fluorides are essential for future experimental studies on heavy metal containing species.