An Analysis of the Complex Electronic State Manifold and Disssociatiom Channels LuF

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Understanding the spectroscopic and thermochemical properties of lanthanide compounds require the use of *ab initio* correlated methods combined with multireference wavefunction approaches. Complete active space self-consistent field (CASSCF) calculations were performed for LuF describing a total of 132 states, including four dissociation channels. Multiconfiguration interaction (MRCI) calculationss were utilized to describe the bond lengths, excited states, and spectroscopic constants at a quadruple-ζ basis set level quality. In addition, the Breit-Pauli Hamiltonian was employed to account for the spin-orbit effects on the ground and the first few excited states, aiding in revealing the state ordering. In addition, both scalar and spin-orbit relativistic effects were incorporated in the calculations in the prediction of bond dissociation energies (BDEs) of LuF. Since the 1960s, experimental BDE measurements on many of the lanthanide diatomics, including lanthanide fluoride molecules such as LuF have varied significantly, mainly due to the use of empirical models and the lack of direct measurements. This work provides new insight about LuF.