THE ELECTRONIC STATES OF UF_6

QI WANG, RUSSELL M. PITZER, *Department of Chemistry, The Ohio State University, 100 W.18th Avenue, Columbus, OH, 43210*.

The ground and excited electronic states of UF_6 between 3 eV and 8 eV are investigated by *ab initio* configuration interaction (CI) calculations using relastivistic effective core potentials (RECPs) to replace the core electrons on both the uranium and fluorine atoms. Correlation-consistent polarized double-zeta (cc-pvdz) basis sets are used. The spin-orbit interaction and electron correlation are included using spin-orbit configuration interaction (SO-GUGA in the Columbus programs). Comparisions are made between this work and previous theoretical treatments as well as possible experimental results, particularly the extent of ligand-to-metal electronic transitions.