

THE *AB INITIO* STUDY OF UO AND UO₂ MOLECULES IN THE GAS PHASE

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

Ab initio calculations are performed on UO and UO₂ molecules. Ionization potential and electronic structure for the high and low lying states are calculated using the spin-orbit configuration interaction technique. Finally, these calculated results are compared with experimental results and with results that have been obtained by utilizing other theoretical methods.