

ELECTRONIC STRUCTURE CALCULATION OF $U(BH_4)_4$ WITH A CORRELATION CONSISTENT BASIS SET

ZHIYONG ZHANG and RUSSELL M. PITZER, *Department of Chemical Physics, The Ohio State University, Columbus, OH43210.*

A correlation consistent basis set, through g functions, is developed for uranium. Calculations are carried out for $U(BH_4)_4$ using a relativistic effective core potential and the spin-orbit effect included at the configuration interaction level. The calculated electronic energy levels are compared with experimental data and previous assignments and calculations. The effect of basis set size on f→f excitation energies is discussed.