

RELATIVISTIC AND ELECTRON CORRELATION EFFECTS ON THE SPECTROSCOPIC PROPERTIES OF CrF AND CrCl

JAMES F. HARRISON, *Department of Chemistry and Center for Fundamental Materials Research, Michigan State University, East Lansing MI 48824-1322.*

The electronic structure of CrF and CrCl in the low-lying sextets and quartets has been studied, using large atomic natural orbital basis sets and a variety of ab-initio methods, including multi-reference configuration interaction and coupled clusters with perturbative triples. We report the effects of perturbative scalar relativistic corrections and the correlation of the 3s and 3p electrons of the transition metal on T_e , R_e , and w_e . These corrections are necessary for quantitative agreement with experiment.