THE ELECTRONIC STRUCTURE OF CrF AND CrCl

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We will discuss the electronic structures of CrF and CrCl in their ground and low-lying electronic states and will compare to recent experimental and theoretical results. We are particularly interested in the nature of the bonding in the sextet and quartet states and examine this as a function theoretical model (MCSCF, MRCI, CCSD, CCSD(T), etc.) using large single particle basis sets.