APPROXIMATE THEORETICAL MODEL FOR THE FIVE ELECTRONIC STATES (Ω = 5/2, 3/2, 3/2, 1/2, 1/2) ARISING FROM THE GROUND $3d^9$ CONFIGURATION IN NICKEL HALIDE MOLECULES AND FOR ROTATIONAL LEVELS OF THE TWO Ω = 1/2 STATES IN THAT MANIFOLD

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An effective Hamiltonian for a non-rotating diatomic molecule containing only crystal-field and spin-orbit operators has been set up to describe the energies of the five spin-orbit components that arise in the ground electronic configuration of the nickel monohalides. The model assumes that bonding in the nickel halides has the approximate form Ni^+X^-, with an electronic $3d^9$ configuration plus closed shells on the Ni^+ moiety and a closed shell configuration on the X^- moiety. Least-squares fits of the observed five spin-orbit components of the three lowest electronic states in NiF and NiCl are then carried out in terms of the three crystal field parameters C_0, C_2, C_4 and the spin-orbit coupling constant A. Following this, the usual effective Hamiltonian $B(\mathbf{J}\text{-}\mathbf{L}\text{-}\mathbf{S})^2$ for a rotating diatomic molecule is used to derive expressions for the unusually large Ω-type doubling parameter p in the two Ω = 1/2 states in the $3d^9$ manifold. These expressions show (for certain sign conventions) that the sum of the two p values should be $-2B$, but that their difference can vary between $-10B$ and $+10B$. The theoretical magnitudes for p are in good agreement with the two observed p values for both NiF and NiCl, but the signs are not. The experimental signs can be brought into agreement with the theoretical signs by a fairly massive change in +/- parity assignments in the NiF and NiCl literature. The last part of the talk will focus on the theoretical and experimental implications of these parity changes.