ANALYSIS OF PERTURBATIONS OBSERVED IN THE FT SPECTRA OF CuCl₂

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Abnormally large e-f separations have been observed in the (ν₁, 0, ν₃) levels of the ground X²Π₉/₂₊ state of CuCl₂ about 2500 cm⁻¹ above the lowest vibrational level (0,0,0). The largest splittings are accompanied by extra lines in the dispersed fluorescence spectra. Some of the extra lines have resolvable Cu hyperfine structure; they are assigned as transitions to levels which result from mixing essentially between X²Π₉/₂ and a nearby ²Σ₊ state.

We have used an effective Hamiltonian to model the ²Π ~ ²Σ interaction and derived molecular constants for the unknown ²Σ state using a non-linear least-squares fitting routine. Taking an arbitrary value of the spin-orbit parameter Aᵢ of -300 cm⁻¹, we estimate the ²Σ state to lie around 3000 cm⁻¹ above the (0,0,0) level of the X²Π₉/₂₊ ground state.