ANALYSIS OF PERTURBATIONS OBSERVED IN THE FT SPECTRA OF $CuCl_2$

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Abnormally large e-f separations have been observed in the (v_1, 0, v_3) levels of the ground $X^2\Pi_{g(3/2)}$ state of $CuCl_2$ 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 $^2\Pi_{g(1/2)}$ and a nearby $^2\Sigma_g$ state.

We have used an effective Hamiltonian to model the $^2\Pi \sim {}^2\Sigma$ interaction and derived molecular constants for the unknown $^2\Sigma$ state using a non-linear least-squares fitting routine. Taking an arbitrary value of the spin-orbit parameter A_Π of -300 cm^{-1}, we estimate the $^2\Sigma$ state to lie around 3000 cm^{-1} above the (0,0,0) level of the $X^2\Pi_{g(3/2)}$ ground state.