THEORETICAL STUDIES OF THE NaK $3\,^3\Pi$ DOUBLE MINIMUM STATE

R. D. MILES, A. WILKINS, L. MORGUS, J. HUENNEKENS, A. P. HICKMAN, *DEPARTMENT OF PHYSICS, LEHIGH UNIVERSITY, BETHLEHEM, PA 18015*.

The hyperfine structure of various ro-vibrational levels of several excited electronic states of the NaK molecule has been analyzed using a model based on diabatic electronic states. The patterns of the experimentally observed hyperfine levels exhibit considerable variation, which can be interpreted by associating different hyperfine coupling constants with each diabatic state contributing to a given adiabatic potential curve. The theoretical work is based on performing *ab initio* electronic structure calculations for several adiabatic states (using the GAMESS code) and then determining diabatic curves using the block diagonalization method.
The *ab initio* calculations for the $3\,^3\Pi$ state clearly show that the double minimum arises from the crossing of diabatic states. Using the *ab initio* results as a guide to the correct form, we parametrized the diabatic potential curves and fitted the experimental data using parameterized, diabatic potential curves and coupling terms. Further calculations yield the hyperfine and spin-orbit coupling constants (b_F and A_v, respectively) for each region of the potential.