COUPLED-CHANNEL ANALYSIS OF THE $D~^1\Pi~-d~^3\Pi$ COMPLEX IN NaK; POTENTIAL ENERGY CURVES AND SPIN-ORBIT FUNCTIONS

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Two-colour polarization labeling experiments measuring the $D \leftarrow X$ system of NaK have characterised more than 99 % of the potential well of the $D^{-1}\Pi$ state of NaK^a, the last observed level being located 7 cm⁻¹ below the Na(3p⁻²P_{3/2}) + K(4s) atomic asymptote. The vibrational progressions all exhibit irregular intervals, because of strong interactions with the nearby $d^{-3}\Pi$ state. A comprehensive analysis has now been made of all available data concerning the $D^{-1}\Pi$ and $d^{-3}\Pi^b$ states. The potential curves are represented by Morse/Lennard Jones analytical functions, with *ab initio* constraints on the long-range part of V(R). Morse functions are also used to represent the *R*-dependent diagonal and off-diagonal spin-orbit terms. Initial values for the spin-orbit coupling matrix elements were extracted from quasi-relativistic *ab initio* calculations. In total, 29 parameters were required to recalculate 95 % of the 1400 observed term energies to within experimental uncertainty, giving an unweighted standard deviation 0.03 cm⁻¹.

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^bP. Kowalczyk J. Mol. Spectrosc. <u>136</u> 1 (1989)