POTENTIAL ENERGY SURFACES OF M+NG, M = K, RB, CS AND NG = HE, NE, AR

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Pressure broadening (PB) plays an important role in the operation of optically pumped alkali lasers (OPAL) by broadening the absorption features of the alkali metal via a perturbing noble gas. While sophisticated PB models exist, they require a knowledge of the interaction potentials involved to become predictive. As a first step toward studying the PB at work in OPAL systems, ab initio potential energy surfaces have been generated for a series of combinations of alkali metals (K, Rb, and Cs) and noble gas atoms (He, Ne, and Ar) which potentially may comprise such systems. These surfaces include the ground state $X^2\Sigma^+_{1/2}$, as well as the excited states $A^2\Pi_{1/2}$, $A^2\Pi_{3/2}$, and $B^2\Sigma^+_{1/2}$. They are calculated using the multi-configurational singles and doubles configuration interaction method, including the spin-orbit interaction through the use of two-component pseudopotentials, implemented in the COLUMBUS suite of molecular structure programs. Where possible, results are compared to both experimentally measured and previous theoretical predictions of spectroscopic constants as well as experimentally determined vibrational energy levels.