Energies and radiative properties of the $A^1\Sigma^+ - b^3\Pi$ complex in KRb: towards optimal ground-state transfer ultracold molecules

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Recently high resolution Fourier Transform (FT) spectroscopy and rigorous coupled-channel deperturbation analysis of the low-lying spin-orbit coupled $A^1\Sigma^+$ and $b^3\Pi$ states of KRb molecule have been performed [1]. The resulting mass-invariant deperturbed molecular parameters represent the termvalues of the $A-b$ complex of the different KRb isotopologues within accuracy of the measurements. A comparative study of the *ab initio* calculated $A^1\Sigma^+ - X^1\Sigma^+$ and $b^3\Pi - a^3\Sigma^+$ transition dipole moments demonstrate the remarkable agreement (with few percent) of the theoretical results obtained by the different quantum chemistry methods [2]. The highly accurate empirical adiabatic potential energy curves (PECs) for the ground singlet $X^1\Sigma^+$ and triplet $a^3\Sigma^+$ states of KRb up to their common dissociation limit became available as well [3]. This provides confidence that the energies and radiative properties of the KRb $A-b$ complex could be simulated at a high (close to experimental) level of accuracy in a wide range of the rovibronic excitation.

The goal of the present work is to perform a detailed theoretical analysis of the spectroscopic and radiative properties of KRb in order to identify the reasonable candidates for the stimulated Raman transitions between initial Feshbach resonance states (consist of the mutually mixed $X^1\Sigma^+$ and $a^3\Sigma^+$ levels due to hyperfine and magnetic external field perturbations), the spin-orbit coupled levels of the A$\sim$b complex and absolute ground $X^1\Sigma^+$ ($v=0$,$J=0$) state [4]. We have used the brand new deperturbed molecular PECs, spin-orbit coupling functions and transition dipole moments to predict the rovibronic energies and radiative lifetimes of the $A-b$ complex along with transition probabilities from the complex to weakly bound levels of the both $X^1\Sigma^+$ and $a^3\Sigma^+$ states near dissociation threshold as well as absolute ground X-state. The calculated $A-b \to X$ spontaneous emission coefficients are in a good agreement with the relative intensity distributions measured for long laser-induced fluorescence progression on the well-bound levels of the X-state. The theoretical lifetime predicted for the metastable b$^3\Pi(v=0)$ state 33.8 μs is remarkably close to its experimental counterpart [5]. The overall $A-b \leftrightarrow a$ transition probabilities are confirmed to be extremely weak due to the small $b-a$ transition moment [2,4]. At the same time the $A-b \leftrightarrow X$ transition probabilities from the highest vibrational levels of the X-state become comparable with the strength of the relevant transitions to the lowest $v_X = 0$ level of the ground X-state.

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