

Towards understanding of the spin-orbit interaction in the $A^1\Sigma^+ \sim b^3\Pi$ complex of KRb: spectroscopic observations and deperturbation analysis

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KRb is one of the most extensively studied molecules among the mixed alkali - metal dimers. A highly accurate ground state potential energy curve has been obtained in [1,2]. Several excited electronic states have been studied in detail. A variety of experiments with ultra-cold KRb molecules are on-going, see [3] for a review. Electronic structure calculations of KRb have been performed in [4,5]. At the same time, experimental data on the first excited states $A^1\Sigma^+$ and $b^3\Pi$ are very fragmentary and, to our best knowledge, a satisfactory description of these states is not achieved. The reason is the strong spin-orbit (SO) interaction between $A^1\Sigma^+$ and $b^3\Pi$ states leading to a great complexity of this mixed system forming an A–b complex.

Our previous experience in spectroscopic studies of the A–b complex of heavy alkali–metal dimers and in developing efficient deperturbation approach allowing to reproduce rovibronic term values with experimental accuracy, see e.g. [6] for KCs and [7] for NaCs, encouraged us to perform high resolution spectroscopy study of the A–b complex in KRb and to develop a multi-channel deperturbation model, which would allow us to describe the A–b complex in KRb with high accuracy. In this work, we will present the first experimental results and preliminary deperturbation analysis. In the experiment, the rovibronic levels of the KRb A–b complex were directly excited in $(A-b) \leftarrow X^1\Sigma^+$ transition by 980 nm and 1020 nm diode lasers. KRb molecules were produced in a heat pipe at a temperature about 570K. Laser induced fluorescence was dispersed by Bruker IFS–125HR Fourier transform spectrometer with an instrumental resolution 0.05 cm^{-1} . Spectra analysis allowed us to determine rovibronic term values of the A-b complex with accuracy of about 0.01 cm^{-1} . Overall we have obtained more than 1000 term values for $^{39}\text{K}^{85}\text{Rb}$, and more than 200 term values for $^{39}\text{K}^{87}\text{Rb}$, spanning over the energy range from 10900 to 13500 cm^{-1} .

The deperturbation model based on the rigorous coupled-channel approach considers the spin-orbit coupling effect between the singlet $A^1\Sigma^+$ and triplet $b^3\Pi$ states explicitly. The SO splitting of the b-state and spin-rotational interactions among its $\Omega=0,1,2$ -substates are taken into account as well. Both experimental and computational work is in progress.

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