New spectroscopic data and deperturbation analysis of the $A^1\Sigma^+$ - $b^3\Pi$ states in KCs

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In heteronuclear alkali diatomic molecules containing heavy atoms the lowest excited $A^1\Sigma^+$ and $b^3\Pi$ states are coupled due to the strong spin-orbit interaction forming $A^1\Sigma^+$~ $b^3\Pi$ complex with complicated and irregular energy levels structure. These states are of great importance due to the possibility of their usage as intermediate states for transferring the vibrationally excited ultra-cold molecules into the absolute [rovibronic] ground state $X^1\Sigma^+$ (v_X =0; J_X = 0).

In our recent studies [1,2] direct $(A^1\Sigma^+\sim b^3\Pi)\leftarrow X^1\Sigma^+$ excitation by various diode lasers (830-1060 nm) was applied followed by laser-induced fluorescence (LIF) A~b→X. LIF was dispersed by Fourier transform spectrometer Bruker IFS 125HR and recorded with the resolution of 0.03 - 0.05 cm^{-1}. More than 3600 A~b term values within energy range $E\in$[10040, 13272] cm^{-1} were obtained with average accuracy of 0.01 cm^{-1} and included in a global multichannel deperturbation analysis.

The goal of the present study was to expand the experimental energy range of A~b state term values of KCs to upper levels as well as to reach “dark” levels of the $b^3\Pi$ state well below the bottom of the $A^1\Sigma^+$ state. This was accomplished by the analysis of $(4)^1\Sigma^+\rightarrow$A~b LIF spectra. KCs molecules were produced in a stainless steel heat pipe at a temperature about 310 ^oC. The $(4)^1\Sigma^+$ state was excited using a single mode CR-699-21 ring dye laser with Rhodamine 6G dye. The Fourier-transform spectra $(4)^1\Sigma^+\rightarrow(A^1\Sigma^+\sim b^3\Pi)$ and $(4)^1\Sigma^+\rightarrow X^1\Sigma^+$ were recorded. We used the InGaAs room temperature diode to detect transitions (around 7700 cm^{-1}) to the lowest levels of the $b^3\Pi_0$ state and the thermoelectrically cooled InGaAs diode for transitions in 4500 – 7000 cm^{-1} spectral range to detect levels of higher energy. The most complicated task of identifying the complicated $(4)^1\Sigma^+\rightarrow$ A~b spectra became feasible by comparison with their predicted counterparts calculated by previous set of deperturbation parameters of the A~b state complex [2]. As a result, more than 3000 new rovibronic term values in expanded energy range $E\in$[9190,13813] cm^{-1} were added to the data field of [1,2]. In particular $b^3\Pi_{0^-}$ sub-state term values for v_b = 3 were obtained. By including all data into the multichannel deperturbation processing, refined structure parameters were derived which reproduce about 96% of all experimental $^{39}K^{133}Cs$ term values of the $A^1\Sigma^+\sim b^3\Pi$ states within experimental uncertainty.

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References:

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