The $(2)^1\Pi$ state in KCs: Fourier-transform spectroscopy and potential construction

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Spectroscopic information on the mixed excited states of heteronuclear alkali diatomics is of particular interest because of their application as an intermediate state for producing molecules in cold and ultracold conditions, preferably in the lowest $X^1\Sigma^+$ rovibronic state. The ultracold KCs molecules have not been produced yet, but optical schemes for its production are proposed in [1,2]. A different scheme which involves photoassociation via the mixed $(2)^1\Pi$ and $(2)^3\Pi$ states was used in [3] for RbCs. In present study we report on the first spectroscopic data and construction of the pointwise potential energy curve (PEC) for the $(2)^1\Pi$ state of KCs [4].

Similar to our previous KCs experiments [5,6], we recorded the back-scattered laser induced fluorescence (LIF) by Fourier-transform spectrometer Bruker IFS-125HR at a resolution of 0.03 cm^{-1}. KCs molecules were produced in a linear heat-pipe, filled with 10g of K and 7g of Cs, at about 300 ^{o}C temperature. For excitation we used the laser diodes (658 nm and 685 nm) and a Coherent CR 699 ring dye laser (Rh6G and DCM dyes). A Hamamatsu R928 photomultiplier was employed as a detector. The uncertainty of the line positions was estimated as 0.003 cm^{-1}.

From 180 recorded LIF spectra we obtained 2121 term values of e and f parity rovibronic levels. The assingment of quantum numbers v'', J'' and J' for each LIF progression was based on the accurate ground state PEC [7]. The data set included vibrational $v' \in [0, 28]$ and rotational $J' \in [7, 274]$ levels. The experimental uncertainty of the term energy was estimated as 0.01 cm^{-1}. For systematically over J' data within $v' \in [0, 10]$ it was possible to determine the Λ-doubling constant, or q-factor. For $v' \in [0, 6]$ and $J' > 50$ the obtained q-factor values have not revealed significant perturbations. Therefore we averaged these values to $\bar{q} = (1.8 \pm 0.1) \times 10^{-6}$ cm^{-1}, being in excellent agreement with the $q = 1.84 \times 10^{-6}$ cm^{-1} value calculated in [8].

The $(2)^1\Pi$ state PEC of KCs was constructed using the Inverted Perturbation Approach. The empirical PEC consists of 29 grid points in the internuclear distance range from 3.6 to 8.6 and describes the 67% of its well depth. The standard deviation (std) of the fit is 0.5 cm^{-1}, while for $v' \in [0, 7]$ the std is 0.008 cm^{-1}. The presented PEC obtained in one-state model can be used as the first step in further analysis of this state, which would require a more detailed spectroscopic information also on perturbing $(3)^3\Sigma^+$ and $(2)^3\Pi$ states.

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