FOURIER-TRANSFORM SPECTROSCOPY AND POINT-WISE POTENTIALS OF THE $B(1)^1\Pi$ STATES IN KCs AND RbCs

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The lowest $B(1)^1\Pi$ states (*B*-states for short) of alkali diatomic molecules are involved in the processes exploited in numerous applications such as producing cold and ultra-cold diatomic species [1], measuring and imaging external electric and magnetic fields [2], and other. At the same time the data on their potential energy curves (PECs) based on high accuracy spectroscopic information is scarce for heavier diatomics due to numerous perturbations caused by strong spin-orbit (SO) interaction with closely lying triplet states. We report on the experimental studies and PEC construction of the *B*-states in KCs and RbCs.

We recorded back-scattered laser-induced fluorescence (LIF) $B \rightarrow X$ from a linear heat-pipe filled with K and Cs or Rb and Cs metals operating at about 290 ^{0}C. Tunable diode lasers with 685, 705 and 730 nm central frequencies were used for excitation. LIF spectra were dispersed with a resolution 0.03 cm^{-1} by Fourier-transform spectrometer Bruker IFS – 125HR. Term values of the *B*-state were obtained, with typical accuracy better than 0.01 cm^{-1}, by adding term value of the respective ground *X*-state $E(v'',J'')$ [3,4] to the frequency of the respective LIF line. Since it appeared not possible to accomplish a full multi-channel deperturbation routine due to the lack of representative data on the neighbouring triplet states, the moderate accuracy point-wise PECs were constructed by fitting less perturbed term values applying the Inverted Perturbation Approach (IPA). The constructed PECs are compared with *ab initio* calculations.

Regarding ^{39}K^{133}Cs, *B*-state energy range $E \in$ [14070, 15200] cm^{-1} was studied; v'-assignment up to v'=10 was based on the data analysis applying accurate PEC from [5]. The latter was obtained from fitting low-lying levels $v' \in [0, 3]$ and reproduced the fitted data with standard deviation (sd) of 0.02 cm^{-1}; the data for ^{41}K^{133}Cs not included in the fit were satisfactory reproduced as well. Applying step by step the fitting procedure we managed to identify higher v' levels and construct a PEC up to v'=35. In total, about 3000 term values were included in the fit non-uniformly covering $v' \in [0, 35]$ and $J' \in [7,233]$. These data were reproduced by the obtained point-wise PEC with sd about 1 cm^{-1} within *R*-range from 3.55 to 9.00 Å.

The results for the *B*-state of RbCs [6] were obtained in a similar way. In total, 2664 term values for ^{85}Rb^{133}Cs and ^{87}Rb^{133}Cs were obtained from LIF spectra in the energy range $E \in$ [13770, 15200] cm^{-1} covering $v' \in [0, 35]$ and $J' \in [6,228]$; the data were reproduced by the constructed point-wise PEC with sd 0.95 cm^{-1}. The IPA PEC includes 27 grid points within *R*-range from 3.55 to 9.00 Å. The low-lying term values were described with much better accuracy; the obtained PEC reproduced abundant vibrational level energies for $v' \in [0, 2]$ with sd 0.08 cm^{-1} which is closer to experimental uncertainty. The inflection in the empirical PEC was observed around *R*=4.4 Å caused by avoided crossing of two Ω = 1 terms of $B(1)^1\Pi$ and $c^3\Sigma^+$ states.

The support from ERAF grant No. 2010/0242/2DP/2.1.1.1.0/10/APIA/VIAA/036 is gratefully acknowledged.

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