POTENTIAL ENERGY CURVE CONSTRUCTION OF THE $(4)^1\Sigma^+$ STATE OF KCs BASED ON $(4)^1\Sigma^+–X^1\Sigma^+$ TRANSITION STUDY

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The KCs molecule is a prospective object to produce the ultracold gas of polar diatomics with a large electric dipole moment. Detailed spectroscopic studies of KCs performed last years include the empirical potential energy curves (PEC) on KCs ground $X^1\Sigma^+$ and $a^3\Sigma^+$ states [1, 2], and the first excited $A^1\Sigma^+$ and $b^3\Pi$ states [3]. The excited $(4)^1\Sigma^+$ state attracts a particular interest for two reasons. First, as revealed in [1, 2], $(4)^1\Sigma^+$ state is connected with both $X^1\Sigma^+$ and $a^3\Sigma^+$ states by optical transitions. Thus, the information on the $(4)^1\Sigma^+$ state properties could facilitate, in particular, the selection of optical paths for efficient transformation of the ultracold molecules into the absolute rovibrational ground state (v = 0, J = 0) $X^1\Sigma^+$. Second, the specific "shelf" shape of its PEC at large internuclear distances caused by avoided crossing of ion-pair and valence adiabatic states yields favorable Frank-Condon factors to observe very high vibrational levels of the $X^1\Sigma^+$ state in $(4)^1\Sigma^+ \rightarrow X^1\Sigma^+$ transitions.

We present here a detailed study of the $(4)^1\Sigma^+$ state of KCs which has been performed by Fourier-transform spectroscopy of $(4)^1\Sigma^+ \rightarrow X^1\Sigma^+$ laser induced fluorescence using a high resolution Bruker IFS125HR spectrometer. The KCs molecules were produced at 290°C in a heat pipe. For excitation in the region [16000, 18000] cm^{-1} a ring dye laser Coherent 699-21 with Rhodamine 6G dye was used. Rotational assignment was made by accurate ground X-state PEC [1, 2]. The resulting 1800 rovibronic term values obtained with accuracy ca. 0.01 cm^{-1} are distributed in energy range from ca. 17000 cm^{-1} to 18300 cm^{-1} and J range from 1 to 180. These term values have been successfully fitted by a single diabatic PEC obtained in a point-wise form by the inverted perturbation approach, as well as by recently developed analytic form based on a combination of Chebychev polynomial and long range expansions. For both models the best fit was obtained assuming the lowest observed vibrational level being $v^{\prime}$ = 3. The striking fact that all experimental term values could be represented by a single diabatic potential while for most of them the spin-forbidden $(4)^1\Sigma^+ \rightarrow a^3\Sigma^+$ transition were observed means that the $(4)^1\Sigma^+$ state is only regularly perturbed, probably due to strong spin–orbit interaction with the remote triplet $^3\Pi$ states.

Support by Latvian Science Council grant No. 09.1036 is gratefully acknowledged.

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