Experimental description of the $6^1\Sigma^+$ - $4^3\Pi$ states in KCs

J. Szczepkowski¹, A. Grochola¹, W. Jastrzebski¹, P. Kowalczyk², E. Pazyuk³ A. Stolyarov³, A. Pashov⁴

¹Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland

²Institute of Experimental Physics, Faculty of Physics, University of Warsaw, *ul. Pasteura 5, 02-093 Warsaw, Poland*

³Department of Chemistry, Moscow State University, Leninskie gory 1/3, Moscow 119991, Russia

⁴Faculty of Physics, Sofia University St. Kliment Ohridski, 5 J. Bourchier blvd., 1164 Sofia, Bulgaria

E-mail: pashov@phys.uni-sofia.bg

Since the first experimental description of the KCs excited state $6^1\Sigma^+$ [1] with a single channel model, no attempt has been undertaken to resolve the reported perturbations by the neighbouring $4^3\Pi$ triplet electronic state. The problem is challenging since the "perturber" was observed only through local perturbations with the singlet state, thus the shape of its potential energy curve can be determined experimentally with great ambiguity. Additional complications arise from the vibrational numbering of the singlet state, established only from distribution of the experimental line intensities, based on the single channel Frank-Condon factors.

The present contribution reports on theoretical calculations of the R-dependent matrix element of the electric dipole operator between the ground $X^1\Sigma^+$ and the excited $6^1\Sigma^+$ electronic states and the spin-orbit operator. These radial functions are then used to model the experimental observations in a coupled channels model, which accounts for the spin-orbit interaction between the coupled stated.

AP acknowledges partial support from National Science Fund of Bulgaria Grants DTNS/Russia/01/10 and DN18/12/11.12.2017.

References:

1. J. Szczepkowski, A. Grochola, W. Jastrzebski, P. Kowalczyk, Chem. Phys. Lett. 614, 36–40 (2014).