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Towards the experimental accuracy deperturbation analysis of the fully mixed $A^1\Sigma^+$ and $b^3\Pi$ states of Rb_2, Cs_2 and RbCs molecules ANDREY STOLYAROV, Department of Chemistry, Moscow State University, THOMAS BERGEMAN, Department of Physics and Astronomy, SUNY, Stony Brook — The laser production and manipulation of the ultracold molecular assembles would be greatly facilitated by accurate knowledge of the structure and dynamic properties of the electronic states involved. In spite of the recent progress in the systematic spectroscopic investigation of the promising diatomic species such as Rb_2, Cs_2 and RbCs, the reduction of the raw experimental data available for fully mixed $A^1\Sigma^+$ and $b^3\Pi$ states to the precise structure parameters (potential and interaction matrix elements) is very challenging and still unambiguous procedure. We present here a review of physical models and numerical recipes currently developed for the comprehensive deperturbation treatment of the strongly coupled diatomic states in a wide range of excitation energy and internuclear distance. The crucial role of ab initio calculations on the spin-orbit coupling matrix elements in the deperturbation analysis is demonstrated. The interpolation and extrapolation properties of the resulting non-adiabatic models are discussed with respect to accuracy required for the adequate reproduction of experimental data sets.

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