Abstract Submitted
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Spin-orbit coupling effect in the low-lying states of Rb_2, Cs_2 and RbCs molecules[1] ANDREY STOLYAROV, Department of Chemistry, Moscow State University, THOMAS BERGEMAN, Department of Physics and Astronomy, SUNY, Stony Brook — We present the results of *ab initio* calculations on the potential energy curves, transition dipole moments, spin-orbit and angular coupling matrix elements between the electronic states of Rb_2, Cs_2 and RbCs molecules converging to the lowest three dissociation limits. The quasi-relativistic matrix elements have been evaluated for a wide range of internuclear distance in the basis of the spin-averaged wavefunctions corresponding to pure Hund's coupling case (**a**) by using of small (9-electrons) effective core pseudopotentials of both atoms. The core-valence correlation has been accounted for a large scale multi-reference configuration interaction method combined with semi-empirical core polarization potentials. The calculated spin-orbit (SO) coupling matrix elements were involved in the deperturbation treatment of the of the fully mixed $A^1\Sigma^+$ and $b^3\Pi$ states as well as to estimate a second order SO effect in the ground singlet $X^1\Sigma^+$ and triplet $a^3\Sigma^+$ states. The resulting transition dipole moments and potentials were used to predict radiative lifetimes and emission branching ratios of excited vibronic states while the calculated angular coupling matrix elements were transformed to Λ-doubling constants of the $^1\Pi$ states. The accuracies of the present results are discussed by comparing with experimental data and preceding calculations.

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