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Spin-orbit coupling effect on the $2^3\Pi$ state of $^{39}\text{K}^{85}\text{Rb}$ JIN-TAE KIM, Department of Photonic Engineering, Chosun University, Gwangju, 501-759, Korea, ANDREY V. STOLYAROV, Department of Chemistry, Moscow State University, Moscow, 119991, Russian Federation, WILLIAM C. STWALLEY, Department of Physics, University of Connecticut, Storrs, CT 06269-3046, USA — Recently we investigated the spin-orbit components ($\Omega = 0^+, 0^-, 1$, and 2) of the $2^3\Pi$ state of $^{39}\text{K}^{85}\text{Rb}$ by using experimental spectroscopy of ultracold molecules formed by photoassociation [1]. The separations ($\Delta(E_{\Omega=1} - E_{\Omega=0})$ and $\Delta(E_{\Omega=2} - E_{\Omega=1})$) between Ω components were unequal due to second-order perturbations by other electronic states. In the present work we investigate the spin-orbit coupling effect on the $2^3\Pi$ state of $^{39}\text{K}^{85}\text{Rb}$ in the framework of 1st and 2nd order non-degenerate perturbation theory based on an *ab initio* method. Required potential energy curves and electronic spin-orbit coupling matrix elements are evaluated over a wide range of internuclear distance in the basis of the spin-averaged wavefunctions corresponding to the pure Hund's case (a) coupling scheme. We compare the experimental spin-orbit splittings of the $2^3\Pi$ state with its *ab initio* counterparts, which agree well and elucidate the pronounced 2nd order perturbation effects caused by nearby electronic states.

[1] J. T. Kim *et al.*, New J. of Phys. **11**, 055020 (2009).

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