Theoretical insights into the low-lying states of the RaF molecule promising for laser cooling

Y.V. Osika, M.B. Shundalau
Faculty of Physics, Belarusian State University, Minsk, Belarus,
e-mail: *shundalau@bsu.by*

Ultracold polar molecules offer prospects for the creation of the molecular Bose-Einstein condensate with possible applications for quantum information and precision measurements [1].

Recently [2, 3], it was shown that radium fluoride RaF is a promising candidate for the direct laser cooling in order to use it for measuring molecular parity violation. According to the *ab initio* FS-CCSD calculations [3], the equilibrium internuclear distances for the ground and first excited states of the RaF molecule almost coincide, which provides high values of the diagonal FCFs.

In this study, *ab initio* state-of-art calculations at the FS-CCSD level of theory of the low-lying potential energy curves (PECs) of the RaF molecule were performed for the first time (Fig. 1). The PECs and spectroscopic parameters were calculated for the following low-lying RaF terms: ground state $X^2\Sigma^+$, and excited states $A^2\Pi_{1/2}$ (T_e = 13298 cm^{-1}), $B^2\Delta_{3/2}$ (T_e = 14988 cm^{-1}), $A^2\Pi_{3/2}$ (T_e = 15332 cm^{-1}), $B^2\Delta_{5/2}$ (T_e = 15745 cm^{-1}), and $C^2\Sigma^+$ (T_e = 16628 cm^{-1}). The results of our calculations are in excellent agreement with experimental values [2].

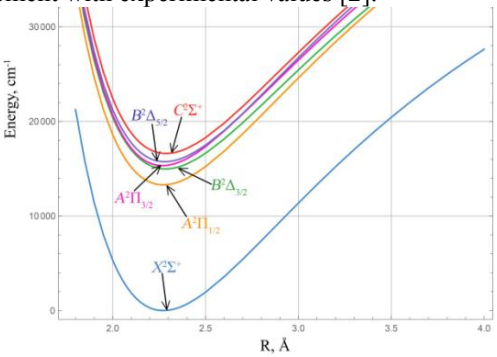

Fig. The PECs of the low-lying doublet states of the RaF molecule.

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References

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