Ab initio calculation of ground and low excited state spectroscopic data and transition properties of SBr+

guosen Wang[1], XinGuan Tan[1], Chuanyu Zhang[1], and Yulin Wang[2]

[1]Chengdu University of Technology
[2]Sichuan University of Science and Engineering

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Abstract

In this paper, the potential energy curves of the Λ-S and Ω states of SBr^+ are reported for the first time, and the spectrum data of some low excited bound states are obtained. The differences in the spectrum properties of main group molecules and SBr^+ were compared and analyzed, providing a sufficient theoretical basis for the subsequent study of main group molecules. The phenomenon of avoided crossing that occurs in the Ω state is analyzed, and finally it is concluded that this phenomenon mainly occurs in the energy region between 20000 cm^{-1} and 40000 cm^{-1}. Potential transitions in the Ω state capable of achieving laser cooling of SBr^+ are explored. The Franck-Condon factor, radiation lifetime and Einstein coefficient between $X^3\Sigma^-_{0^+}$ and $21\Sigma^+_{0^+}$ are calculated. From the calculation results, we concluded that direct laser cooling of SBr^+ is not feasible. What we have studied in this paper provides a theoretical basis for subsequent computational exploration of the spectrum properties of SBr^+.

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