Ab Initio Spectroscopic Study for the NaRb Molecule in Ground and Excited States

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Abstract

A wide adiabatic study is performed for NaRb molecule, involving 15(1)sigma(+) electronic states including the ionic state Na-Rb+, as well as 14(3)sigma(+), 1-9(1,3), and 1-5(1,3) states. This investigation is performed using an ab initio approach which involves the effective core potential, the core polarization potential with l-dependent cut-off functions. The NaRb system has been treated as a two-electron system and the full valence configuration interaction is easily achieved. The spectroscopic constants R-e, D-e, T-e, (e), (e)x(e), B-e, and D-0 for all these states are derived. We have also computed the vibrational levels as well their spacing for different values of J. In addition, permanent and transition dipole moments are determined and analyzed. The Dunham coefficients have been used to perform experimental spacing to compare directly with our results. The present calculations on NaRb extend previous theoretical works to numerous electronic excited states in the various symmetries. (c) 2014 Wiley Periodicals, Inc.

Keywords

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