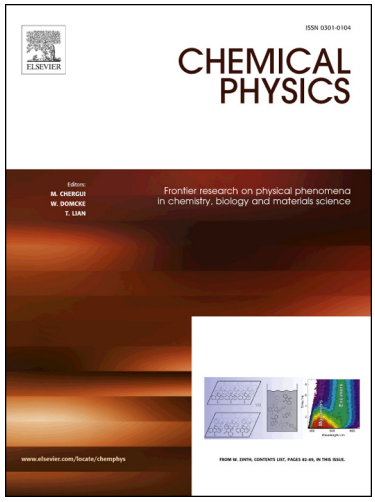

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Electronic Structure with the Calculation of the Rovibrational, and Dipole Moments of the Electronic States of the NaBr and KBr molecules

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Abstract

Due to the lack of the electronic structure of NaBr and KBr diatomic molecules, a systematic investigation of the electronic structure of these molecules was performed using *ab initio* CASSCF/(MRCI+Q) calculations. The adiabatic potential energy curves of the low-lying singlet and triplet electronic states in the representation $^{2s+1}\Lambda^{(+/-)}$ of NaBr and KBr molecules have been investigated. The spectroscopic constants T_e, R_e, ω_e, B_e, α_e, the dipole moment μ_e, and the dissociation energies D_e were calculated for the bound states in addition to the percentage ionic character f_{ionic} around the equilibrium position of two electronic states. Moreover, the static and the transition dipole moment curves have been calculated. The nuclear motion study has been performed using the canonical functions approach that allowed the determination of various rovibrational constants E_v, B_v, D_v and the abscissas of the turning points R_{min} and R_{max} for the investigated bound states. The investigated data are in a very good agreement with those given in literature. These results provide effective routes for many industrial applications and for the formation of cold alkali halide molecules in the low-lying vibrational states via experimental techniques.

1. Introduction

Recently, there was a noticeable growing interest in the production of cold and ultracold molecules in which the chemical reactions can be controlled by freezing most degrees of