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Ab Initio Spectroscopic Study of the Electronic Properties of the (Bana)+ Molecular Ion

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Abstract : In the present theoretical study, we investigated adiabatically the electronic structure of the (BaNa)+ by the use of the ab initio calculation. We optimized a large atomic GTO basis set for Na and Ba atoms. The (BaNa)+ molecular ion is considered a two-electron thank to a non-empirical pseudo-potentials approach applied to Ba and Na cores with the Core Polarization Potentials operator (CPP). Then, we performed the Full Configuration Interaction (FCI) method. Accordingly, we calculated the adiabatic Potential Energy Curves (PECs) and their spectroscopic constants (well depth De, transition energies Te, the equilibrium distances Re, vibrational constant e, and anharmonic constant exe) for 10 electronic states in Σ+ symmetry. Then we determined the vibrational level energies and their spacing, and the electric Permanent Dipole Moments (PDM).

Keywords : Ab initio, dipole moment, non-empirical pseudo-potential, potential energy curves, spectroscopic constants, vibrational energy
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