THEORETICAL STUDY OF THE ELECTRONIC STATES WITH SPIN-ORBIT EFFECTS AND ROVIBRATIONAL CALCULATIONS OF THE MOLECULE LiCs

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Due to the advancement in the ultracold alkali atom trapping developments, which are at the root of photoassociation spectroscopy, the potential energy curves have been calculated for the 82 lowest electronic states of the molecule LiCs including the spin orbit effect within the range 3.0a_o to 28.0a_o of the internuclear distance R for the symmetries $^{1,3}\Sigma$, $^{1,3}\Pi$, $^{1,3}\Delta$, and Ω=0^-, 0^+, 1, 2, 3 along with the spectroscopic constants for 66 electronic states. To investigate the electronic structure of these electronic states, the atoms Li and Cs have been treated through non-empirical relativistic effective one-electron core potential of the Durand and Barthelat type. Gaussian basis sets have been used in this calculation for the Li and Cs atoms. Core valence effects including core-polarization and core valence correlation are taken into account by using an l-dependent core-polarization potential. In order to reproduce the experimental splitting with a very good agreement for Li and Cs, semi-empirical spin orbit pseudo-potential has been designed for these atoms. The molecular orbitals of the molecule LiCs have been derived from self consistent field (SCF) calculation and full valence configuration interaction (CI) calculations were performed. The core-core interaction calculations are performed as the Hartree-Fock energy of the ion $(LiCs)^{2+}$. The calculations were performed in a pseudo-potential scheme. To investigate the electronic structure including the spin-orbit effects (SO) we used the package CIPSO which allows a full CI calculation as well as perturbative CI calculations with SO effects. Using the canonical functions approach, the values of the eigenvalue E_v, the abscissas of the turning points (R_{min}, R_{max}), the rotational constants B_v, and the centrifugal distortion constants D_v have been calculated up to 76 vibrational levels for 20 states. Through the same approach, the dipole moment functions have been calculated for most of the states in the Λ-representation along with the vibrational matrix elements for the states $(1)^1\Sigma^+$, $(1)^3\Sigma^+$, $(1)^1\Pi$, and $(1)^3\Pi$. The comparison of the present results with those available in the literature shows a very good agreement.