Ab initio investigation of the electronic and vibrational properties for the (CaLi)(+) ionic molecule

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Abstract

A wide adiabatic study has been performed for numerous electronic states of CaLi+ molecular ion. The adiabatic potential energy curves and their spectroscopic constants (R-e, D-e, omega(e) and T-e) have been calculated using an ab initio approach including a nonempirical pseudo-potential for the Ca and Li cores with the core polarisation potentials operator through full configuration interaction (FCI). Thereafter, the energies of vibrational levels and their spacing for all these states have been reported. In addition, the electric dipole moment curves have been investigated for the (1-19) Sigma, (1-12) Pi and (1-8) Delta electric states. Moreover it lets us check the extreme transition dipole moments (TDM). These behaviours of TDM are more accustomed to estimate the radiative lifetimes for all vibrational levels in 2(1)Sigma(+) and 3(1)Sigma(+) states. Also, the bound-bound and the bound-free contribution have been calculated precisely and by employing a Franck-Condon (FC) approximation.

[GRAPHICS]

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