# Analytical Potential Energy Function for the Ground State X$^1\Sigma^+$ of Lanthanum Monofluoride

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(Received: 2002-7-23; Revised: )

Abstract: The equilibrium geometry, harmonic frequency and bond dissociation energy of lanthanum monofluoride have been calculated using Density-Functional Theory (DFT), post-HF methods MP2 and CCSD(T) with the energy-consistent relativistic effective core potentials. The possible electronic state and reasonable dissociation limit of the ground state of LaF are determined based on atomic and molecular reaction statics. Potential energy curve scans for the ground state X$^1\Sigma^+$ have been performed at B3LYP and CCSD(T) levels, due to their better results of harmonic frequency and bond dissociation energy. We find that the potential energy calculated with CCSD(T) is about 0.6 eV larger than the bond dissociation energy, when the internuclear distance is as large as 0.8 nm. The problem that single-reference ab initio methods do not meet dissociation limit during calculations of lanthanide heavy-metal elements is analyzed. We propose the calculation scheme to derive the analytical Murrell-Sorbie potential energy function. Vibrotational spectroscopic constants $B_e$, $\omega_e$, $\omega_e\chi_e$, $\alpha_e$, $\beta_e$, $D_e$ and $H_e$ obtained by the standard Dunham treatment coincide well with the results of rotational analyses on spectroscopic experiments.

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