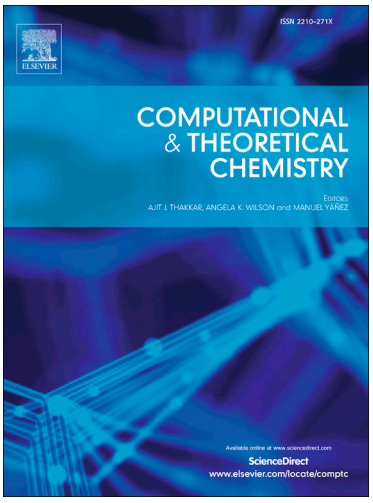

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Theoretical study of LuH molecule: Potential energy curves, spectroscopic constants and spin-orbit couplings

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Abstract

SA-CASSCF and ic-MRCI methods have been performed to calculate 26 low-lying $^{(2s+1)}\Lambda^{(\pm)}$ electronic states located below 40250cm^{-1} for ^{175}Lu^{1}H molecule. The potential energy curves (PECs) for these states are displayed in the range of 1.00 to 3.50Å. The spectroscopic constants such as R_e, T_e, ω_e and $\omega_e\chi_e$ are reported for the first time. Moreover, the permanent and transition electric dipole moments are plotted versus internuclear distance (R). Subsequently, for the first 13 $^{(2S+1)}\Lambda^{(\pm)}$ states located below 30000cm^{-1}, the spin-orbit coupling (SOC) of 30 $\Omega^{(\pm)}$ states is calculated with their spectroscopic constants.

***Keywords**: SA-CASSCF, ic-MRCI, $^{(2s+1)}\Lambda^{(\pm)}$ and $\Omega^{(\pm)}$ states, LuH , SO coupling, PEC, spectroscopic constants, electric dipole moments.*

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