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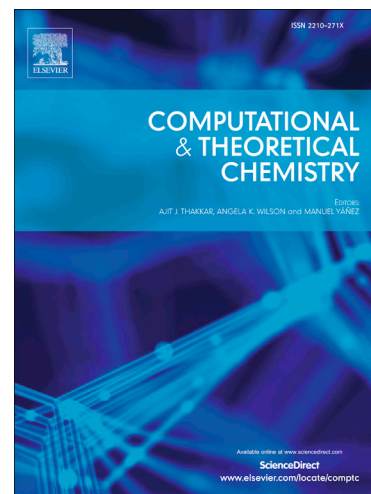
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Theoretical study of LuH molecule: Potential energy curves, spectroscopic constants and spin-orbit couplings

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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 $^{175}\text{Lu}^1\text{H}$ molecule. The potential energy curves (PECs) for these states are displayed in the range of 1.00 to 3.50\AA . The spectroscopic constants such as R_e , T_e , ω_e and $\omega_e x_e$ 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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