ELECTRONIC TRANSITIONS AND SPIN-ORBIT SPLITTING OF LANTHANUM DIMER

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Lanthanum dimer (La_2) was studied by mass-analyzed threshold ionization (MATI) spectroscopy and a series of high-level multi-configuration ab initio calculations (CASSCF, CASPT2, and MRCI). The MATI spectrum exhibits three band systems originating at 39044, 40312, and 40862 cm^{-1}, respectively. Above the band origin, the first band system displays a vibrational progression of $\sim$232 cm^{-1}, and the other two show vibrational progression with the same interval of $\sim$240 cm^{-1}. Below the band origin, the three systems exhibit the same vibrational interval of $\sim$207 cm^{-1}. These band systems are assigned to three electronic transitions from the ground state of La_2 to the low-lying electronic states of $La_2{}^+$: $^2\Sigma_g^+ \leftarrow {}^1\Sigma_g^+$, $^2\Pi_{u,1/2} \leftarrow {}^1\Sigma_g^+$, and $^2\Pi_{u,3/2} \leftarrow {}^1\Sigma_g^+$. The spin-orbit splitting in the $^2\Pi_u$ ion state is 550 cm^{-1}. In addition, the electronic states and bonding of La_2 will be compared with those of Sc_2 and Y_2.