MASS ANALYZED THRESHOLD IONIZATION OF LUTETIUM DIMER

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Lu_2 is produced in a pulsed laser-vaporization metal-cluster source and studied by mass-analyzed threshold ionization (MATI) spectroscopy. The MATI spectrum displays several long progressions from the transitions between various vibrational levels of the neutral and ion electronic states. From the spectrum, the upper limit of the ionization energy of the dimer is determined to be 43996 cm^{-1}, and the vibrational frequencies are measured to be 121 cm^{-1} in the neutral state and 90 cm^{-1} in the ion state. By combining with ab initio calculations at CASPT2 level, the ground state of Lu_2 is identified as $^3\Sigma_g^-$. The $^3\Sigma_g^-$ state has an electron configuration of $6s\sigma_g^2 5d\pi_u^1 5d\pi_u^1 6s\sigma_u^2$, which is formed by the interactions of two Lu atoms in the $^2D(5d6s^2)$ ground state. Ionization of the neutral state removes a $5d\pi_u$ bonding electron and yields a ion state with a considerably longer bond distance. Lu_2 has a very different bonding feature from La_2, for which a $^1\Sigma_g^+$ ground state was previously identified with an electron configuration of $5d\pi_u^4 6s\sigma_g^2$ formed by the interactions of two La atoms in the $^4F(5d^2 6s)$ excited state.[a]

[a] Yang Liu, Lu Wu, Chang-Hua Zhang, Serge A. Krasnokutski, and Dong-Sheng Yang, *J. Chem. Phys.* **135**, 034309 (2011).