Abstract

The positronic bound state for the non-polar carbon disulfide (CS_2) was experimentally identified, while previous theoretical investigations, which dedicated to studying the positronic CS_2 monomer, cannot reasonably reproduce the experimentally measured positron affinity. In the present study, we performed analysis of the vibrational averaged positron affinity for the positronic CS_2 dimer, $[C_2S_4;e^+]$, using the Hartree-Fock and configuration interaction level of multi-component molecular orbital method combined with the self-consistent field level of vibrational variational Monte Carlo method. We obtained that the equilibrium structure of the non-polar C_2S_4 can have the positronic bound state with the positron affinity of about 46.18 meV in configuration interaction level while 0 meV in Hartree-Fock level. Furthermore, by taking into account the vibrational effect, we succeeded in reproducing the resonant positron kinetic energies lying close to the experimental value, where the vibrational averaged positron affinity becomes greater with increased dipole moment and dipole polarizability. We also showed possible mechanisms effectively to enhance the resonant positron capture for $[C_2S_4; e^+]$, associated with both infrared active and infrared inactive vibrational modes.