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A Correlation Potential Method for Electron Scattering Total Cross Section Calculations on Several Diatomic and Polyatomic Molecules over Energy Range 10～5000 eV

LIU Yu-Fang,[1] SHI De-Heng[1,2,3] SUN Jin-Feng,[1] ZHU Zun-Lue,[1] and YANG Xiang-Dong[2]

[1] Department of Physics, Henan Normal University, Xinxiang 453007, China

[2] Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China

[3] Department of Foundation, the First Aeronautical College of Air Force, Xinyang 464000, China

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Abstract: A complex optical model potential correlated by the concept of bonded atom, which considers the overlapping effect of electron clouds between two atoms in a molecule, is firstly employed to calculate the total cross sections for electron scattering on several molecules (NH_3, H_2O, CH_4, CO, N_2, O_2, and C_2H_4) over the energy range 10～5000 eV using the additivity rule model at Hartree-Fock level. The difference between the bonded atom and the free one in states is that the overlapping effect of electron clouds of bonded atoms in a molecule is considered. The quantitative total cross sections are compared with the experimental data and with the other calculations wherever available and good agreement is obtained over the energy range 10～5000 eV. It is shown that the correlated calculations are much closer to the available experimental data than the uncorrelated ones at lower energies, especially below 500 eV. Therefore, considering the overlapping effect of electron clouds in the complex optical model potential could be helpful for the better accuracy of the total cross section calculations of electron scattering from molecules.

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Key words: total cross section, additivity rule, atomic and molecular collision

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